Correlations and Topology in Quantum Materials

Spanish-German WE-Heraeus-Seminar

21 – 24 January 2024

at the Physikzentrum Bad Honnef/Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the Spanish-German WE-Heraeus-Seminar "Correlations and Topology in Quantum Materials":

Recent insight thanks to improved methods for calculating the band structure of solids has shown that many compounds might host topological excitations at the surface, potentially presenting dissipationless transport and novel fermionic excitations, such as Dirac, Weyl or multiple fold fermions. This includes many bulk systems but also in particular graphene and layered quasi two-dimensional compounds. On the other hand, some of these systems present novel phases emerging from the electronic interactions, which have been traditionally difficult to address using band structure calculations. These novel phases include topologically non trivial phases, providing for example unconventional superconductivity, anomalous magnetism, nematicity or anomalous charge density waves.

The purpose of this seminar is to bring together groups addressing the problem of quantum phases of bulk layered quasi two-dimensional materials and single layer systems from different perspectives. We aim to create a fertile ground for new collaborations, particularly among researchers of Spanish and German institutions.

There are ongoing collaborations in the subject, often centered around traditional approaches. Many new experiments show that electronic correlations are important. Taking electronic correlations into account and understanding the full breadth of their consequences requires a collaborative effort which provides a fertile ground to reinforce established collaborations and initiate new ones.

Scientific Organizers:

Dr. Leni Bascones, ICMM-CSI, Madrid, Spain
E-mail: leni.bascones@csic.es

Prof. Dr. Hermann Suderow, Universidad Autónoma de Madrid, Spain
E-mail: hermann.suderow@uam.es

Prof. Dr. Roser Valentí, University of Frankfurt, Germany
E-mail: valenti@itp.uni-frankfurt.de

Introduction

Administrative Organization:

Dr. Stefan Jorda
Mojca Peklaj

Wilhelm und Else Heraeus-Stiftung
Kurt-Blaum-Platz 1
63450 Hanau, Germany

Phone +49 6181 92325-11
Fax +49 6181 92325-15
E-mail peklaj@we-heraeus-stiftung.de
Internet: www.we-heraeus-stiftung.de

Venue:

Physikzentrum
Hauptstraße 5
53604 Bad Honnef, Germany

Conference Phone +49 2224 9010-120

Phone +49 2224 9010-113 or -114 or -117
Fax +49 2224 9010-130
E-mail gomer@pbh.de
Internet: www.pbh.de

Taxi Phone +49 2224 2222

Registration:

Mojca Peklaj (WE Heraeus Foundation)
at the Physikzentrum, Reception Office
Sunday (17:00 h - 21:00 h) and Monday morning

Program

Program *(CET)*

Sunday, 21 January 2024

17:00 – 21:00	ARRIVAL and REGISTRATION	
18:30	*BUFFET SUPPER*	

Monday, 22 January 2024

08:00	*BREAKFAST*	
08:50 – 09:00	Organizers	**Welcome**
Session chair: Roser Valentí		
09:00 – 09:45	Maia Vergniory	**Topological Quantum Chemistry and Single Particle Greens' Function for Correlated Topological Materials**
09:45 – 10:15	Jörg Schmalian	**Topologically Enabled Superconductivity**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:30	Claudia Felser	**Magnetic Topological Materials with Electronic Instabilities**
11:30 – 12:00	Victor Pardo	**Interplay Between Charge density Waves, Magnetism and Super-conductivity in Transition Metal Dichalcogenides**
12:00 – 12:30	Anna Boehmer	**Tuning Quantum Materials**
12:30 – 12:45	**Conference Photo (outside at the main entrance)**	
12:45 – 14:00	*LUNCH BREAK*	

Program *(CET)*

Session chair: Leni Bascones		
14:00 – 14:30	Kristin Willa	**Interplay of Stripe and Double-Q Magnetism with Superconductivity in $Ba_{1-x}K_xFe_2As_2$ Under the Influence of Magnetic Fields**
14:30 – 15:00	Jochen Wosnitza	**Unconventional High-Field Phases in Organic Superconductors**
15:00 – 15:30	Maria Navarro Gastiasoro	**Superconductivity in $KTaO_3$ Interfaces**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 16:30	Gertrud Zwicknagl	**Heavy Fermion Systems: Recent Surprises and New Frontiers**
16:30 – 17:00	Miguel M. Ugeda	**Collective Electronic States in a Two-dimensional Heavy-fermion System**
17:00 – 17:30	Gabriel Sánchez Santolino	**Polar Vortex Patterns in Twisted Freestanding Oxides**
17:30 – 17:45	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
17:45 – 18:30	**Poster Flash I**	
18:30 – 19:30	*DINNER*	
19:30 – 20:30	**Poster Session I**	
20:30	**Social Event: Ham Tasting** *(Lichtenberg Cellar)*	

Program *(CET)*

Tuesday, 23 January 2024

08:00	*BREAKFAST*	

Session chair: Hermann Suderow

09:00 – 09:45	Angel Rubio	**Cavity Materials Engineering: Novel Non-equilibrium Phenomena in Two Dimensional Heterostructures**
09:45 – 10:15	María José Calderon	**The Unconventional Normal State of Twisted Bilayer Graphene**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:30	Tim O. Wehling	**Electron Correlations in Moiré Superlattices**
11:30 – 12:00	Tobias Stauber	**Phase Diagram of Magic Angle Bilayer Graphene**
12:00 – 12:30	Laura Classen	**Field Control of Many-body Phases in Frustrated Moiré Bilayers**
12:30 – 14:00	*LUNCH BREAK*	

Session chair: Jörg Schmalian

14:00 – 14:30	Katharina Franke	**Yu-Shiba-Rusinov States in Artificially Constructed Adatom Structures: Quantum Spins, Band Formation and Chirality**
14:30 – 15:00	Dieter Koelle	**NanoSQUIDs for Sensing Magnetic Fields on the Nanoscale**
15:00 – 15:30	José María De Teresa	**Superconducting Devices Based on Bi_2Se_3 Junctions**
15:30 – 16:15	*COFFEE BREAK*	
16:15 – 17:00	**Poster Flash II**	
17:00 – 18:30	**Round Table: Promoting Collaborations**	
18:30 – 20:00	*HERAEUS DINNER at the Physikzentrum (with complimentary drinks)*	
20:00 – 21:00	**Poster Session II**	

Program *(CET)*

Wednesday, 24 January 2024

08:00	*BREAKFAST*	
Session chair: Anna Böhmer		
09:00 – 09:45	Eugenio Coronado	**2D Magnetic Heterostructures: From Artificial Magnets to Smart Molecular/2D Heterostructures**
09:45 – 10:15	Jairo Sinova	**The Emergent Research Landscape of Altermagnetism: Unconventional Magnetism and its New Connections**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:30	José J. Baldovi	**Magnon Straintronics and Chemical Tuning in 2D Magnetic Materials**
11:30 – 12:00	Sebastian Bergeret	**Nonreciprocal Superconducting Transport and the Spin Hall Effect in Gyrotropic Structures**
12:00 – 12:30	Johannes Hofmann	**Nonlinear Topological Thermoelectric Currents as Probes of Interaction Effects in Fermi Liquids**
12:30 – 12:40	**Poster Prizes and Concluding Remarks**	
12:40	*LUNCH*	

End of Seminar / Departure

Posters

Poster Session I, Monday, 22 Jan, 19:30 h (CET)

Miguel Águeda	**Tunneling Spectroscopy through the Magnetic Phases of Ce(Ru0.92Rh0.08)2Si2**
Olga Arroyo Gascón	**Universality of Moiré Physics in Collapsed Chiral Carbon Nanotubes**
Martin Braß	**Weyl-nodes and Electronic Correlations in Ce3Bi4Pd3**
Atasi Chakraborty	**Strain Induced Antiferromagnetic to Altermagnetic Transition in ReO2**
Lorenzo Crippa	**Heterogeneous Ta-dichalcogenide Bilayer: Heavy Fermions or Doped Mott Physics?**
Marli dos Reis Cantarino	**RIXS Investigation of Cr-substituted BaFe2As2**
Axel Fünfhaus	**Topological Phase Transitions of Interacting Phases in Commensurate Magnetic Flux**
Marta García Olmos	**Topology and Disorder in a 2D Semidirac Material**
Pablo García Talavera	**2D Lock-in Analysis of Ordered Phases in Superconductors**
Ana García-Page	**Chiral Quantum Phase Transition in Moiré Dirac Materials**
Celia González Sánchez	**Towards Hybrid van der Waals Josephson Junctions Based on NbSe2**
Thomas Günkel	**Complex Oxide Memristors for Cryogenic Neuromorphic Computing**

Poster Session I, Monday, 22 Jan, 19:30 h (CET)

Haojie Guo	Characterizing the Chemical Structure of Topological Defects of Graphene Surfaces by ncAFM
Florian Hirsch	Cold Atomic Excitons
Moritz Hirschmann	Fundamental Laws of Chiral Band Crossings
Sofie Castro Holbæk	The Interplay Between a Charge Density Wave Order and Superconductivity in the Kagome Materials
Mikel Iraola	Topology of SmB6 Revisited by Means of Topological Quantum Chemistry
Dilan Pérez	Microscopic Model for the Charge Transfer in Graphene/WS2 Heterostructure

Poster Session II, Tuesday, 23 Jan, 20:00 h (CET)

Simon Koch	**YBCO Heterostructures for SQUID-on-Si-lever**
Tim Kokkeler	**Spectroscopic Signature of Spin Triplet Odd-valley Superconductivity in Two-dimensional Materials**
Felix Lüpke	**Engineered Topological and Correlated States in van der Waals Heterostructures**
Elizabeth Martín Jefremovas	**Skyrmion Lattices in Magnetic Multilayers and Lateral Confinements**
Renjith Mathew Roy	**Magneto Optical Response of Bulk WTe2**
Jose Antonio Moreno	**Crossover from Isolated YSR States to Gapless Superconductivity in 2H-NbSe2-xSx at the Atomic Scale**
Kitinan Pongsangangan	**Transport Properties of Charged Two-dimensional Dirac Systems in Hydrodynamic Regime: The Role of Dynamical Screening and Plasmons**
Gautam Rai	**Dynamical Correlations and Order in Magic-angle Twisted Bilayer Graphene**
Amaia Sáenz-Hernández	**Fabrication Method for Hybrid Quantum Devices Involving Topological Insulators and Superconductors Using Focused Ion Beam Induced Deposition**
Sandra Sajan	**Evidence for Ground State Coherence in a Two-dimensional Kondo Lattice**
Miguel Sánchez	**Correlated Insulators in Magic-angle Graphene at one Magnetic Flux Quantum**

Poster Session II, Tuesday, 23 Jan, 20:00 h (CET)

Marco Schönleber	Spin-orbit Coupled States Arising in the Half-filled t_{2g} Shell
Mireia Tolosa Simeón	Analog Gravity in Moiré Dirac Materials
Jan Ullmann	Nb Constriction-Josephson Junction NanoSQUIDs on Cantilevers Patterned by He and Ne Focused Ion Beams
Igor Vasilevskiy	Plasmonic Response of a Nanorod in the Vicinity of a Planae Surface
Manish Verma	Tuning of the carrier localization, magnetic and thermoelectric properties in ultrathin (LaNiO3−δ)1 /(LaAlO3)1(001) superlattices by oxygen vacancies
Maxim Wenzel	Broadband Optical Investigations of the Antiferromagnetic Kagome Metal FeGe
Setareh Zahedi Azad	Two-step Growth of Wafer-sized NbSe2 Film

Abstracts of Lectures

(in alphabetical order)

Magnon straintronics and chemical tuning in 2D magnetic materials

D.L. Esteras,[a] A. Rybakov,[a] A.M. Ruiz,[a] G. Rivero-Carracedo[a] and José J. Baldoví[a]
[1]*Instituto de Ciencia Molecular (ICMol), University of Valencia, Paterna, Spain.*

The recent isolation of two-dimensional (2D) magnets offers tantalizing opportunities for spintronics and magnonics at the limit of miniaturization.[1] Among the key advantages of atomically-thin materials are their flexibility, which provides an exciting avenue to control their properties by strain engineering, and the more efficient tuning of their properties with respect to their bulk counterparts. In this presentation we will provide an overview of our recent results on this fascinating topic. First, we will focus on the magnetic properties, magnon dispersion and spin dynamics of the air-stable 2D magnetic semiconductor CrSBr (T_C = 146 K)[2] and will investigate their evolution under mechanical strain and Coulomb screening using first-principles.[3] Our results provide a deep microscopic analysis of the competing interactions that stabilize the long-range ferromagnetic order and the orientation of the spin in the monolayer.[4]

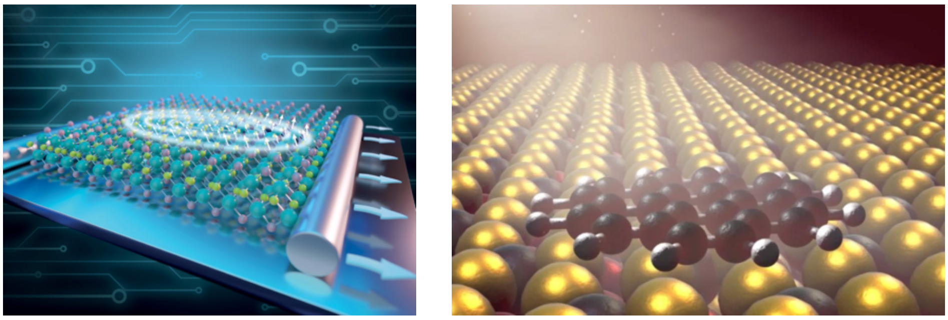


Figure 1. Artistic representation of (left) strain-engineering of spin waves in single-layer CrSBr and (right) a coronene molecule on the surface of a 2D magnetic material.

References:

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, X. Xu, Nature **546**, 270 (2017).
[2] K. Lee, A. H. Dismukes, E. J. Telford, R. A. Wiscons, J. Wang, X. Xu, C. Nuckolls, C. R. Dean, X. Roy, X. Zhu, Nano Lett. **21**, 3511 (2021).
[3] D. L. Esteras, A. Rybakov, A. M. Ruiz, J. J. Baldoví, Nano Lett. **22**, 8771 (2022).
[4] C. Boix-Constant, S. Mañas-Valero, A. M. Ruiz, A. Rybakov, K. A. Konieczny, S. Pillet, J. J. Baldoví, E. Coronado, Adv. Mater. **34**, 2204940 (2022).

Nonreciprocal superconducting transport and the spin Hall effect in gyrotropic structures

T. Kokkeler[1], I. Tokatly[1], and F.S. Bergeret[2]

[1], Donostia International Physics Center (DIPC), San Sebastian
[2] Materials Phyaics Center(MPC-CFM), CSIC, San Sebastian

The search for superconducting systems exhibiting nonreciprocal transport and, specifically, the diode effect, has proliferated in recent years. This trend encompasses a wide variety of systems, including planar hybrid structures, asymmetric SQUIDs, and certain noncentrosymmetric superconductors. A common feature of such systems is a gyrotropic symmetry, realized on different scales and characterized by a polar vector. Alongside time-reversal symmetry breaking, the presence of a polar axis allows for magnetoelectric effects, which, when combined with proximity-induced superconductivity, results in spontaneous non-dissipative currents that underpin the superconducting diode effect. This symmetry established, we present a comprehensive theoretical study of transport in a lateral Josephson junctions composed of a normal metal supporting the spin Hall effect, and attached to a ferromagnetic insulator. Due to the presence of the latter, magnetoelectric effects arise without requiring external magnetic fields. We determine the dependence of the anomalous current on the spin relaxation length and the transport parameters commonly used in spintronics to characterize the interface between the metal and the ferromagnetic insulator. Therefore, our theory naturally unifies nonreciprocal transport in superconducting systems with classical spintronic effects, such as the spin Hall effect, spin galvanic effect, and spin Hall magnetoresistance. We propose an experiment involving measurements of magnetoresistance in the normal state and nonreciprocal transport in the superconducting state. Such experiment, on the one hand, allows for determining the parameters of the model and thus verifying with a greater precision the theories of magnetoelectric effects in normal systems. On the other hand, it contributes to a deeper understanding of the underlying microscopic origins that determine these parameters.

References

T. Kokkeler, I. Tokatly, F. S. Bergeret, arXiv:2309.00495 (2023)

Tuning Quantum Materials

Anna E. Böhmer

Experimentalphysik IV, Ruhr University Bochum, Bochum, Germany

Quantum materials, which often exhibit collective orders such as magnetism or superconductivity, tend to react sensitively to small changes of composition or lattice parameters. This sensitivity allows to tune and control their properties. An exemplary class of quantum materials, that reacts sensitively to such deformations, are the iron-based superconductors. As this material class has by now reached “teen-age”, 15 years after its discovery, the large variety of possible chemical structures, the richness of realized phases and phase diagrams, as well as the diverse methods available to tune them, are even more appreciated. Related cobalt- and nickel-based materials show similarly complex phase diagrams featuring magnetism, charge density waves and/or superconductivity. Here, I will discuss how lattice deformations and chemical substitutions can be used as selective tuning parameters for the different phases of several iron- and cobalt-based 122-type materials. I will further show how we may approach the design and discovery of new materials.

The unconventional normal state of twisted bilayer graphene

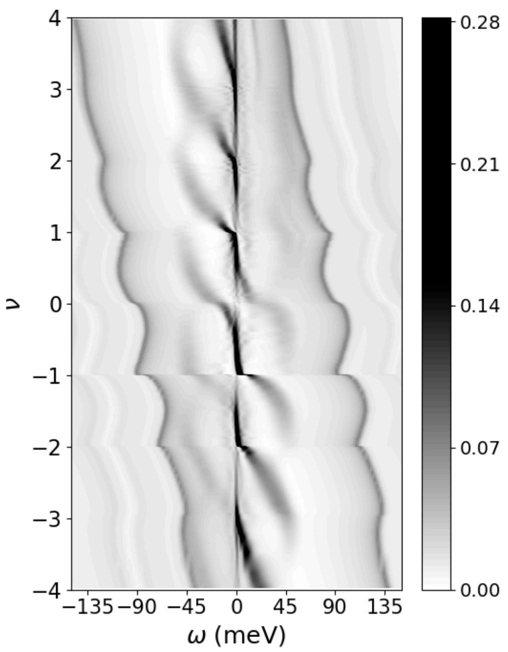
María José Calderón

Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC (Spain)

Twisted bilayer Graphene (TBG) shows a great variety of correlated states. Among the experimental observations, the cascades in the spectroscopic properties [1] and in the compressibility [2] happen in larger ranges of energy, twist angle and temperature than other effects, pointing to a hierarchy of phenomena. In this talk I will show that the spectral weight reorganization associated to the formation of local moments and heavy quasiparticles can explain the cascade signatures without invoking symmetry breaking orders [3]. Our results are based on Dynamical Mean Field Theory plus Hartree calculations. We reproduce the cascade flow of spectral weight, the oscillations of the remote band energies, the asymmetric jumps of the inverse compressibility, and the presence of resistive states. We predict a strong momentum differentiation in the incoherent spectral weight associated to the fragile topology of TBG. I will also show how strong correlations impact other measurements that can be performed in order to characterize the unconventional normal state of these moiré systems.

References

[1] D. Wong et al, Nature **582**, 198 (2020); Y. Choi et al, Nature **589**, 536 (2021).
[2] U. Zondiner et al, Nature **582**, 203 (2020).
[3] A. Datta, A. Camjayi, M.J. Calderón and E. Bascones, Nature Communications **14**, 5036 (2023)



Contour plot of the density of states obtained from the Dynamical Mean Field Theory plus Hartree calculations versus doping ν and energy ω. Cascades of incoherent spectral weight resemble scanning tunneling microscopy experiments [1]. The cascades at positive and negative energies are shifted in doping.

Field control of many-body phases in frustrated moiré bilayers

Laura Classen
Max Planck Institute for Solid State Research, Stuttgart, Germany
Technical University of Munich, Garching, Germany

We determine the ground states and excitation spectra of the paradigmatic four-flavour Heisenberg model with nearest- and next-nearest-neighbor exchange couplings on the triangular lattice in a field controlling the population imbalance of flavor pairs. Such a system arises in the strongly correlated limit of moiré bilayers of transition metal dichalcogenides in an electric displacement field or in-plane magnetic field, and can be simulated via ultracold alkaline-earth atoms. We argue that the field tunes between effective SU(4) and SU(2) symmetries in the balanced and fully polarised limits and employ a combination of mean-field calculations, flavour-wave theory, and exact diagonalisation to analyse the intermediate, imbalanced regime. We find different symmetry-broken phases with simultaneous spin and excitonic order depending on the field and next-nearest-neighbor coupling. Furthermore, we demonstrate that there is a strongly fluctuating regime without long-range order that connects candidate spin liquids of the SU(2) and SU(4) limit. The strong fluctuations are facilitated by an extensive classical degeneracy of the model, and we argue that they are also responsible for a strong polarisability at 1/3 polarisation that survives from the mean-field level to the exact spectrum.

2D Magnetic heterostructures: from artificial magnets to smart molecular/2D heterostructures

E. Coronado[1], **C. Boix-Constant**[1] **and S. Mañas-Valero**[1]

[1]*Instituto de Ciencia Molecular, Universitat de Valencia, Paterna, Spain*

The controlled assembly of 2D materials in van der Waals heterostructures provides the opportunity to design unconventional materials with novel properties. Here I will illustrate this concept through two examples:

1) Artificial magnets obtained by creating a twisted 2D heterostructure formed by two ferromagnetic monolayers of CrSBr twisted by an angle of 90º [1] Magneto-transport measurements in this new material show a multistep spin switching with the opening of hysteresis, which is absent in the pristine bilayer case (angle of 0º) [2], as a consequence of the competition between the inter-layer exchange interactions (which favour an antiparallel orientation of both spin layers), the local spin anisotropies (which tend to orient the spins along the easy axis of each monolayer, x and y) and an external magnetic field applied along one of these easy axes.

2) Smart molecular/2D heterostructures obtained by interfacing stimuli-responsive magnetic molecules with graphene, semiconducting layers (MoS_2 and WSe_2), a superconducting layer ($NbSe_2$), or the magnetic layer CrSBr. A tuning of the properties of the "all surface" 2D material is achieved *via* an active control of the hybrid interface. As smart-molecular systems, I will choose magnetic spin-crossover materials able to switch between two spin states upon the application of an external stimulus (temperature, light or pressure) [3]. This spin transition is always accompanied by a significant change of volume in the material (by ca. 10%). Hence, it can generate strain over the 2D material leading to a reversible change in its physical properties triggered by temperature or light upon the spin transition [4-6].

References

[1] C. Boix-Constant *et al.*, Nat. Mater.(2023) doi: 10.1038/s41563-023-01735-6
[2] C. Boix-Constant *et al.* Adv. Mater. **34**, 2204940 (2022).
[3] E. Coronado, *Nature Rev. Mater.* **5**, 87-104 (2020).
[4] R. Torres-Cavanillas *et al.,* Nat. Chem. **13**, 1101-1109 (2021).
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[6] M. Gavara-Edo *et al.,* Adv. Mater. **34**, 2202551 (2022).

Superconducting devices based on Bi_2Se_3 junctions

R. Gracia-Abad[1], S. Sangiao[1,2,3], G. Balakrishnan[4] and J. M. De Teresa[1,3]

[1] *Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, 50009, Spain*

[2] Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, Zaragoza, 50018, Spain

[3] *Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Zaragoza, 50009, Spain*

[4] Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

Superconductor-based devices have settled the basis for the development of quantum technologies [1], and hybrid devices combining superconductors and topological insulators represent an excellent opportunity for the study of the topological superconducting phase, which offers interesting features that might have significant implications in the development of quantum sensing and quantum computing [2]. On the other hand, the fabrication of new and complex devices can be enriched by the use of focused ion beam techniques, whose versatility enables to create sophisticated devices with high degree of customization [3]. Herein, we develop a novel approach for the fabrication of superconducting devices based on topological-insulator single-crystal Bi_2Se_3 in a geometry characteristic of a superconducting quantum interference device. The characterization of the devices shows that the superconductivity is induced in our crystal and the supercurrent is modulated by the application of an external magnetic field. One of the samples shows an unexpected behaviour with large modulation of the voltage with the magnetic field that cannot be explained with standard models. We propose a scenario in which this behaviour stems from the individual behaviour of one of the Josephson junctions with the interplay of the bulk states present in the crystal and the topological states that appear at the boundary between the crystalline and amorphous phases of Bi_2Se_3 created by the ion irradiation [4, 5].

References

[1] G. Wendin, Reports on Progress in Physics **80**, 106001 (2017)
[2] S. Das Sarma et al., NPJ Quantum Information **1**, 15001 (2015)
[3] K. Höflich et al., Applied Physics Reviews (2023), doi: 10.1063/5.0162597
[4] A. Bake et al., Nat. Commun. **14**, 1693 (2023)
[5] R. Gracia-Abad et al., submitted (2024)

Magnetic topological materials with electronic instabilities

Claudia Felser[1]

[1]*Max Planck Institute Chemical Physics of Solids, Dresden, Germany*
(e-mail: felser@cpfs.mpg.de)

Topology has emerged as a pivotal concept in condensed matter physics, solid state chemistry, and materials science, offering novel insights into the classification and properties of inorganic materials. Recent advancements have enabled the categorization of over 200,000 inorganic substances into either trivial or topological materials, encompassing varieties like topological insulators, and various semimetals (Dirac, Weyl, nodal-line) as well as topological metals [1]. A significant breakthrough was the identification of the first antiferromagnetic topological materials [2]. It's noteworthy that all band structure crossings in ferromagnets manifest as Weyl nodes or nodal lines. Materials with a Kagome lattice are particularly intriguing due to their unique topological characteristics, combining Weyl crossings with van Hove singularities and flat bands [3]. This has been experimentally demonstrated in materials like Mn_3Sn [4], FeSn and $Co_3Sn_2S_2$ [3]. Notably, non-collinear antiferromagnetic Weyl semimetals like Mn_3Sn and $YbMnBi_2$ [5] exhibit substantial anomalous Hall and Nernst effects. A versatile class of materials with the 1:6:6 composition (RET_6Z_6, where RE represents rare earth, T is a transition metal, and Z a main group metal) allows for flexible electronic structure design, further enhanced by charge density wave instabilities [6]. In the realm of real-space topology, skyrmions and antiskyrmions present promising avenues for next-generation data storage technologies [7]. Our research aims to discover novel quantum materials for efficient applications in spintronics, quantum computing, and energy conversion

1. Bradlyn *et al.*, Nature **547**, 298, (2017), Vergniory, *et al.*, Nature **566**, 480 (2019), Vergniory, *et al*., Science (2022).
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4. Kübler and Felser, EPL 120 (2017) 47002 and EPL108 (2014) 67001, Nayak, et al. Science Advances 2 (2016) e1501870
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7. Nayak et al., Nature 548 (2017) 561

Topological properties of altermagnets

R. M. Fernandes[1]

[1]*University of Minnesota, Minneapolis, MN 55455, USA*

Altermagnets are characterized by spin configurations that remain invariant under a combination of two symmetry operations: time reversal, which flips the spins, and a lattice rotation, which can be proper or improper. While altermagnetism is often considered in systems with negligible spin-orbit coupling (SOC), in this talk I will discuss interesting topological effects in altermagnets that are enabled by SOC. These include mirror-protected nodal lines and nodal points in the electronic spectrum, which have a significant impact on the properties of an altermagnet.

Yu-Shiba-Rusinov states in artificially constructed adatom structures: quantum spins, band formation and chirality

Lisa Rütten[1], Eva Liebhaber[1], Gaël Reecht[1], Jacob F. Steiner[2], Harald Schmid[2], Kai Rossnagel[3], Felix von Oppen[2], Katharina J. Franke[1]

[1]Fachbereich Physik, Freie Universität Berlin, Germany
[2] Fachbereich Physik and Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany
[3] Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany

Exchange coupled magnetic adatoms on superconductors constitute a versatile platform to construct artificial structures of correlated states. The magnetic adatoms induce Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap of the substrate. These states can be detected in scanning tunneling spectroscopy at the single-atom scale.
Here, we explore the quasi-two-dimensional superconductor 2H-$NbSe_2$ as a substrate for magnetic adatom structures. Fe adatoms induce four pairs of YSR states, associated to the singly-occupied crystal-field-split d orbitals. The spatial extent and symmetry of the YSR states is influenced by the Fermi surface of the substrate and the charge-density wave coexisting with superconductivity at low temperatures.
We place two magnetic Fe adatoms in close proximity to each other and investigate the interaction of their YSR states. We observe a shift and splitting of the YSR states, including a quantum phase transition from a screened-spin state to a free-spin state. The transition is driven by substrate mediated magnetic interactions (RKKY interactions) becoming possible in the free-spin state [2, 3].
We then deliberately build larger adatom structures, such as chains and triangles by adding individual Fe atoms with the STM tip. In each step we track the evolution of the YSR states. With increasing chain length, we find signatures of YSR band formation consistent with ferromagnetic coupling of quantum spins [2,4]. Triangular structures provide the unique opportunity to create structures with chiral YSR wavefunctions.

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Nonlinear topological thermoelectric currents as probes of interaction effects in Fermi liquids

J. Hofmann[1,2] and H. Rostami[3]

[1]*Department of Physics, Gothenburg University, 41296 Gothenburg, Sweden*
[2] *Nordita, Stockholm University and KTH Royal Institute of Technology, 10691 Stockholm, Sweden*
[3] *Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*

There is currently much interest in exploring ultraclean Fermi liquids in which electron interaction effects dominate over phonon and impurity scattering. In these systems, it has recently been established that a certain class of “odd-parity” Fermi surface deformations have anomalously slow relaxation rates that are suppressed as T^4 with temperature T, as opposed to the well-known T^2 scaling predicted by Fermi liquid theory. I this talk, I will argue that these long-lived modes, which are often hidden in linear response, have a significant impact on nonlinear transport by establishing a direct proportionality of nonlinear thermoelectric currents to the anomalously large relaxation time of odd-parity modes. These nonlinear currents exist in topological time-reversal invariant Fermi liquids, and their magnitude is characterised by new topological heat capacitance terms that we refer to as the Berry curvature capacity and the velocity-curvature capacity. I will discuss how to quantify the effect in Bismuth Telluride, which is an efficient thermoelectric and a topological insulator with a hexagonal Fermi surface. This highlights the potential to explore topological and many-body effects in Fermi liquids through nonlinear thermoelectric responses and will hopefully lead to experimental studies.

NanoSQUIDs for sensing magnetic fields on the nanoscale

D. Koelle

Physikalisches Institut, Center for Quantum Science (CQ) and Center for Light-Matter Interaction, Sensors & Analytics ($LISA^+$), Universität Tübingen, Germany

Magnetic properties of micro- and nanoscale objects, are currently a topic of intensive research. Their investigation requires the development of appropriate tools, e.g. for detection of the magnetization reversal of individual magnetic nanoparticles (MNPs) or for imaging magnetic field profiles on the nanoscale. Promising candidates for this task are strongly miniaturized superconducting quantum interference devices (SQUIDs) – so-called nanoSQUIDs. A SQUID consists of a superconducting loop, intersected by one or two weak links (Josephson junctions). SQUIDs are the most sensitive detectors for magnetic flux, and their sensitivity improves with shrinking size (inductance of the SQUID loop). As they enable direct detection of magnetization changes in small spin systems, that are placed close to the SQUID loop, nanoSQUIDs are very promising sensors for nanoscale applications. Moreover, if miniaturized SQUIDs can be brought in close vicinity to sample surfaces, they enable magnetic scanning probe microscopy on the nanoscale [1,2].

In this talk, I will review recent progress in the development and application of nanoSQUIDs, and I will present our approaches for developing sensitive Nb and $YBa_2Cu_3O_7$ (YBCO) nanoSQUIDs, which can be used for continuous measurements of magnetization loops of single MNPs in intermediate and strong magnetic fields up to the tesla range. Moreover, I will discuss recent developments in using nanoSQUIDs for scanning SQUID microscopy.

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Superconductivity in $KTaO_3$ Interfaces

Maria N Gastiasoro[1], Giulia Venditti[2], Maria Eleonora Temperini[3], Francesco Macheda[4], Paolo Barone[5], José Lorenzana[6]

[1]Donostia International Physics Center, Donostia–San Sebastian, Spain

[2]Department of Condensed Matter Physics, University of Geneva, Switzerland

[3]Department of Physics, Sapienza University of Rome, Italy

[4]Istituto Italiano di Tecnologia, Genova, Italy

[5]SPIN -CNR, Rome, Italy

[6]ISC-CNR and Department of Physics, Sapienza University of Rome, Italy

The discovery of superconductivity in $KTaO_3$ heterostructures, with critical temperatures an order of magnitude higher than that of $SrTiO_3$ heterostructures, has spurred significant interest in the last couple of years. The relevance of the polar modes for pairing, as well as the role of spin-orbit coupling are still under debate. I will present our theoretical results on the Rashba-like coupling between conduction electrons and soft transverse polar modes in $KTaO_3$, and the resulting pairing mechanism [1,2]. Superconductivity at these interfaces exhibits strong resilience against in-plane magnetic field and strongly violates Pauli limit. I will also propose two different mechanisms based on spin-orbit coupling to explain this resilience [3].

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Interplay between charge density waves, magnetism and superconductivity in transition metal dichalcogenides

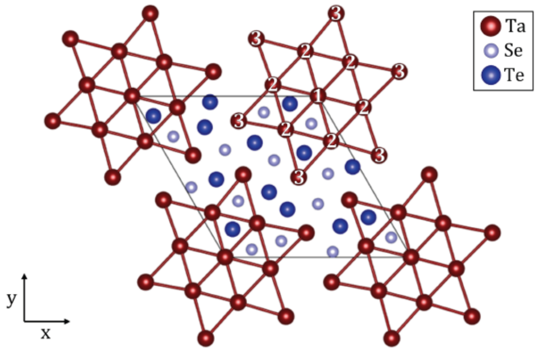
Víctor Pardo[1,2]

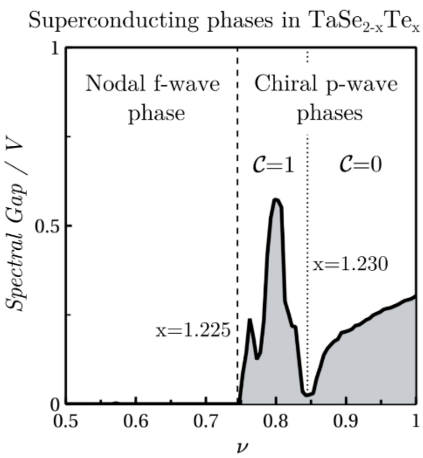
[1]*Instituto de Materiais iMATUS, Universidade de Santiago de Compostela, Santiago de Compostela, E-15782, Spain*

[2] *Departamento de Física Aplicada, Universidade de Santiago de Compostela, Santiago de Compostela, E-15782, Spain*

Charge-density waves are ubiquitous in low-dimensional materials, in particular in layered van der Waals systems. The interplay between structural distortions and, e.g. magnetism leads to very rich phase diagrams and the possibility of tuning and controlling the appearance of long-range magnetic order at higher temperatures.

In this talk, the family of Ta-based dichalcogenides TaX_2 (X=S, Se, Te) will be discussed in the monolayer limit, analyzed by means of ab initio calculations and effective models. TaS_2 and $TaSe_2$ in the so-called 1T structure have been shown to present a lattice distortion in the form of a peculiar charge density wave pattern with a $\sqrt{13} \times \sqrt{13}$ periodicity in the plane, leading to the so-called "star of David" that is depicted in the adjacent Figure. In this configuration, each star acquires a spin one-half, coupling weakly with each other. This lone spin arises from a very flat band near the Fermi level, that at half-filling becomes spin polarized.





In this talk, we will analyze how doping the system with Te leads to a charge transfer from the Te p bands (that become partly occupied) to the minority-spin Ta d flat band. Various ingredients come into play then: strong correlations in a very flat band, superconductivity, magnetism and topological properties, all resulting in the phase diagram shown in the adjacent Figure, where different triplet-superconducting phases coexist with a ferromagnetic ordering between stars.

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Cavity materials engineering: novel non-equilibrium phenomena in two dimensional heterostructures

Angel Rubio[1]

Max Planck Institute for the Structure and Dynamics of Matter,
Luruper Chaussee 149, 22761 Hamburg, Germany[1]

Center for Computational Quantum Physics Flatiron Institute,
Simons Foundation, 10010 NY, USA[2]

We present our recent studies on the thermodynamical stability, mechanical, electronic, structural and optoelectronic properties of 2D materials. We will discuss new states of matter that are optically induced and have no equilibrium counterparts, and we will identify the fingerprints of these novel states that will be probed with pump-probe spectroscopies. We will pursue the question whether it is possible to create those new states of materials. To this end we will show how the emerging (vaccum) dressed states resembles metastable states in driven systems. A particular appeal of light dressing is the possibility to engineer symmetry breaking with tailored optical cavities that can lead to novel properties of materials. We will discuss the potential to realize non-equilibrium states of matter that have so far been only accessible in ultrafast and ultrastrong laser-driven materials. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials, e.g coupling to circularly polarized photons leads to local breaking of time-reversal symmetry enabling the control over a large variety of materials properties (e.g.topology). We will illustrate the realisation of those ideas in molecular complexes and 2D materials and show that the combination of cavity-materials engineering and 2D twisted van der Waals heterostructures provides a novel and unique platform for the seamless realisation of a plethora of interacting quantum phenomena, including exotic and elusive correlated and topological phases of matter. For example, by controlling the Berry curvature in 2D layered materials (metal/insulator transition metal dichalcogenides, or TMD), a new class of quantum Hall states can be induced. In these states, the valley degree of freedom can be tuned with light. We will briefly introduce our new developed quantum electrodynamics density-functional formalism (QEDFT) as a first principles theoretical framework to predict, characterize and control the spontaneous appearance of those ordered phases of strongly interacting light-matter hybrids.

Polar vortex patterns in twisted freestanding oxides

G. Sánchez-Santolino[1], V. Rouco[1], V. Zamora[1], S. Puebla[2], H. Aramberri[3], F. A. Cuellar[1], C. Munuera[2,4], F. Mompean[2,4], M. Garcia-Hernandez[2,4], A. Castellanos-Gomez[2,4], J. Íñiguez[3,5], C. Leon[1,4], J. Santamaria[1,4]

[1]*GFMC. Dept. Fisica de Materiales. Facultad de Física. Universidad Complutense, 28040, Madrid*
[2]*Instituto de Ciencia de Materiales de Madrid ICMM-CSIC 28049 Cantoblanco, Spain*
[3]*Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Avenue des Hauts-Fourneaux 5, L-4362 Esch/Alzette, Luxembourg.*
[4]*Unidad Asociada UCM/CSIC, "Laboratorio de Heteroestructuras con aplicación en spintrónica"*
[5]*Department of Physics and Materials Science, University of Luxembourg, 41 Rue du Brill, L-4422 Belvaux, Luxembourg*

Recent studies on ferroelectric oxide materials have shown how complex polar topologies can be stabilized in epitaxial heterostructures [1]. However, the cube-on-cube structure of these materials forces the use of single crystalline substrates for their growth, limiting the electrical and mechanical boundary conditions that can be imposed to form such states. In recent years, advances in the manipulation of complex correlated oxides have made it possible to isolate them from their original substrate, opening the door to explore more complex boundary conditions [2].

In this work we show how an unconventional strain landscape can occur in twisted freestanding $BaTiO_3$ membranes leading to the formation of ferroelectric topological structures [3]. Here, we analyze the formation of such non-trivial structures as a function of the twisted angle and layer thickness by means of aberration-corrected scanning transmission electron microscopy in combination with density-functional theory calculations. These results show the possibility to create unique moiré assemblies with strong consequences in the ground-state and responses of complex correlated oxides.

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Topologically Enabled Superconductivity

Jörg Schmalian

Karlsruhe Institute of Technology

Static zero modes are a much sought-after consequence of one-dimensional topological superconductivity. Here, we show that zero modes accompanying dynamical instanton events strongly enhance - in some cases even enable - superconductivity[1]. We find that the dynamics of a one-dimensional topological triplet superconductor is governed by a θ term in the action. For isotropic triplets, this term enables algebraic charge-2e superconductivity, which is destroyed by fluctuations in nontopological superconductors. For anisotropic triplets, zero modes suppress quantum phase slips and stabilize superconductivity over a large region of the phase diagram. We present predictions of correlation functions and thermodynamics for states of topologically enhanced superconductivity. In addition we will discuss other one-dimensional superconducting structures, in particular instabilities in Josephson structures of topological superconductors [2,3].
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The emergent research landscape of altermagnetism: unconventional magnetism and its new connections

Jairo Sinova
Johannes Gutenberg University Mainz, Germany

Antiferromagnetic spintronics has been a very active research area of condensed matter in recent years. As we have learned how to manipulate antiferromagnets actively and their emergent topology, further surprises awaited. Turning off spin-orbit coupling, a new fresh view at the family of antiferromagnetic ordered systems reveals also an emergent new class, with properties characteristic of ferromagnets and antiferromagnets, as well as properties unique to itself. This third phase is characterized by compensated magnetic order and a spin-splitting momentum locking, suggesting its name altermagnetism. We show that this new phase is as abundant in nature as conventional ferromagnetism and antiferromagnetism. Its discovery as a distinct phase comes by using a non-relativistic spin-symmetry formalism which, counter to magnetic symmetries, delimits the phase uniquely. Material candidates occur in both three-dimensional and two-dimensional crystals, in diverse structural or chemistry types, and in conduction types covering the whole spectrum from insulators to superconductors. Altermagnets can have impact on prominent research areas, including spintronics, ultra-fast optics, neuromorphics, thermoelectrics, field-effect electronics, multiferroics, magnonics, valleytronics, magnetic topological matter, and unconventional superconductivity.

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Phase diagram of magic angle bilayer graphene

M. Sánchez Sánchez[1], I. Díaz,[1] J. González,[2] and T. Stauber[1]

[1]*Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), E-28049 Madrid, Spain*
[2]Instituto de Estructura de Materia (IEM-CSIC), E-28006 Madrid, Spain

The correlated insulator phases of magic angle bilayer graphene at even integer filling factor can be characterized by an U(4)-ferromagnet. But this approximate symmetry is broken in real samples and the way it is broken may lead to the asymmetry between the superconducting phases at electron and hole doping [1].

In order to address the phase diagram of realistic moiré systems, I will thus start from a microscopic tight-binding model and present two ways how to reduce the full density matrix in order to effectively describe the emergent flat bands. Implications for the correlated, superconducting and topological phases are discussed [2,3].

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Collective electronic states in a two-dimensional heavy-fermion system

Miguel M. Ugeda[1,*]

*mmugeda@dipc.org

[1]Donostia International Physics Center, P. Manuel de Lardizábal 4, 20018 San Sebastián, Spain.

Lowering the dimensionality of a material is an effective strategy to boost many-body correlations that fail to be captured by conventional pictures. In this arena, two-dimensional (2D) materials provide an ideal platform for the exploration of quantum collective phenomena arising from such strong interactions due to their simple synthesis and modelling. In this talk, I will review the rich physics that emerges in the family of transition metal dichalcogenide (TMD) metals when two layers of the T- and H- polytypes are vertically stacked. This simple heterostructure serves as an artificial 2D Kondo lattice platform, where strong electron correlations play a dominant role.

First, I will discuss the electronic structure of the two isolated building blocks in the prototypical $TaSe_2$, which we probe via scanning tunneling microscopy/spectroscopy (STM/STS) at low temperatures (340 mK). While the 1T-$TaSe_2$ layer hosts a 2D array of local magnetic moments, the 1H-$TaSe_2$ behaves as a normal metal, acting as a reservoir of conduction electrons [1]. When stacked together, our STM/STS measurements provide evidence for a coherent ground state of the spin lattice in the 1T/1H-$TaSe_2$ heterobilayer [2], which is distinct from the well-studied isolated-moment Kondo physics. Our observations in this system are only compatible with long-range antiferromagnetic order driven by indirect RKKY interactions and, more importantly, it does not condense into a Kondo insulator state as is commonly assumed for these bilayers. Lastly, I will describe our recent efforts to induce unconventional superconductivity in this type of heterostructures.

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Topological quantum chemistry and single particle Greens' function for correlated topological materials

Maia G. Vergniory
Max Planck for Chemical Physics of Solids, Dresden, Germany
Donostia International Physics Center, Donostia-San Sebastián, Spain

While there has been significant progress in classifying and predicting topological phases in weakly interacting materials using Bloch functions and Berry curvature, in strongly correlated systems, particularly where the quasiparticle picture breaks down, suitable alternative approaches are currently lacking. n this presentation, I will explore various methods for addressing this gap. In particular, I will elucidate how, under special circumstances, one can employ topological quantum chemistry to study heavy fermion systems. Additionally, by computing and scrutinizing the single-particle Green's function, I will delve into the topological Hamiltonian, the computation of Berry flux, and the role of zeros.

Electron correlations in moiré superlattices

Tim Wehling[1,2]

[1]I. Institute of Theoretical Physics, University of Hamburg, 22607 Hamburg, Germany

[2]The Hamburg Centre for Ultrafast Imaging, 22761 Hamburg, Germany

Controlling and understanding electron correlations in quantum matter presents an outstanding goal in materials engineering. In the past years a plethora of new correlated states have been found by carefully stacking and twisting two-dimensional van der Waals materials of different kind. Unique to these stacked structures is the emergence of correlated phases not foreseeable from the single layers alone. Here, we discuss the emergence of different flavors of correlated electron physics, namely Mott-Hubbard, heavy fermion and Hund physics, in moiré superlattices. We show how to switch between Mott-Hubbard and Hund physics in multiband moiré systems [1] and elucidate the interplay of (doped) Mott Hubbard and heavy fermion physics in 1T-1H TaS_2 bilayers [2] as well as magic angle twisted bilayer graphene [3]. With the latter system, we illustrate how the formation and ordering of local moments shapes electronic behavior of moiré quantum materials.

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Interplay of stripe and double-Q magnetism with superconductivity in $Ba_{1-x}K_xFe_2As_2$ under the influence of magnetic fields

K. Willa[1], R. Willa[2], F. Hardy[1], L. Wang[1], P. Schweiss[1], T. Wolf[1], and C. Meingast[1]

[1]*IQMT, KIT, Karlsruhe, Germany*
[2] *TKM, KIT, Karlsruhe, Germany*

At $x \approx 0.25$ $Ba_{1-x}K_xFe_2As_2$ undergoes a novel first-order transition from a fourfold symmetric double-Q magnetic phase to a twofold symmetric single-Q phase, which was argued to occur simultaneously with the onset of superconductivity [1]. Here, by applying magnetic fields up to 10 T, we investigate in more detail the interplay of superconductivity with this magnetostructural transition using a combination of high-resolution thermal-expansion and heat-capacity measurements. We find that a magnetic field suppresses the reentrance of the single-Q orthorhombic phase more strongly than the superconducting transition, resulting in a splitting of the zero-field first-order transition. The suppression rate of the orthorhombic reentrance transition is stronger for out-of-plane than for in-plane fields and scales with the anisotropy of the superconducting state. These effects are captured within a phenomenological Ginzburg-Landau model, strongly suggesting that the suppression of the reentrant orthorhombic single-Q phase is primarily linked to the field-induced weakening of the superconducting order. Not captured by this model is, however, a strong reduction in the orthorhombic distortion for out-of-plane fields, which deserves further theoretical attention.

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Unconventional High-Field Phases in Organic Superconductors

J. Wosnitza

Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden and
Institut für Festkörper- und Materialphysik, TU Dresden, 01062 Dresden, Germany

High magnetic fields either destroy superconductivity by orbital (screening currents) or spin effects. The latter appears for spin-singlet superconductors at the so-called Pauli limit, when the Zeeman energy becomes larger than the condensation energy. However, unconventional superconductivity beyond the Pauli limit is possible, for instance, in the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state forming a modulated superconducting order parameter. This state appears in quasi-two-dimensional (2D) organic superconductors with the magnetic field aligned precisely parallel to the superconducting layers. We have evidenced this by macroscopic specific-heat and microscopic nuclear magnetic resonance (NMR) measurements [1]. Further, we recently could resolve by NMR experiments in detail how the modulation amplitude of the superconducting order parameter evolves with temperature [2]. In addition, we studied the influence of orbital effects on the FFLO state by angular-resolved specific-heat measurements of the 2D organic superconductor κ-$(ET)_2Cu(NCS)_2$. Rotating the field away from the in-plane orientation leads to an increase of orbital effects and changes the nature of the transition from second to first order. Before orbital effects finally suppress the FFLO superconductivity, the specific-heat data evidence a transition to further superconducting states. With increasing the orbital contribution, our data are in line with theoretical predictions of a successive conversion of the FFLO order parameter into Abrikosov-like ones with higher-order Landau levels. The Abrikosov-like and FFLO states compete in 2D systems and represent a general phenomenology of 2D Pauli-limited superconductors [3].

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Heavy fermion systems: Recent surprises and new frontiers

G. Zwicknagl

Institute for Mathematical Physics,TU Braunschweig, Braunschweig, Germany

Since their discovery almost half a century ago, heavy fermion systems have been a continuous source of surprising discoveries often challenging the theoretical understanding at the time. For low temperatures, these materials exhibit a plethora of intriguing phenomena like quantum phase transitions, unconventional superconductivity and unusual magnetism that may eventually provide new functionalities. While heavy fermion systems in their “normal” state share common qualitative properties it is important to emphasize that there are different routes to heavy fermions such as geometric frustration, partial charge order, orbital-selective localization, and the Kondo effect. The focus of the present talk will be on intermetallic lanthanide (4f) and actinide (5f) compounds where the “heavy” quasiparticles arise due to the latter two effects. Starting from quasiparticle states calculated by the Renormalized Band method, I will discuss recently discovered novel Fermi surface instabilities and the interplay of superconductivity with these novel orders.

Abstracts of Posters

(in alphabetical order)

Tunneling spectroscopy through the magnetic phases of $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$

E. Herrera[1], M. Águeda[1], F. Martín-Vega[1], I. Guillamón[1], E. Mascot[4], B. Wu[1], J. Flouquet[2], J.P. Brison[2], G. Knebel[2], D. Aoki[3], D. Morr[4], H. Suderow[1]

[1] Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.
[2] Université Grenoble Alpes, CEA, INAC-PHELIQS, 38000 Grenoble, France.
[3] IMR, Tohoku University, Oarai, Ibaraki 311 - 1313, Japan
[4] Department of Physics, University of Illinois at Chicago, IL60607 Chicago, USA..

The magnetic entropy in a compound containing magnetic ions and itinerant electrons can be reduced to reach the ground state through two competing interactions. Either Kondo screening creates a spin-singlet nonmagnetic coherent state, or Ruderman-Kittel-Kasuya-Yoshida interactions produce magnetic order. $CeRu_2Si_2$ is an archetypical heavy fermion compound with a large electronic specific heat at low temperatures and no magnetic order. On the contrary, $CeRh_2Si_2$ presents AFM order below about 36 K. $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$ shows a combined behavior, with an antiferromagnetic phase (AFM) below 4.2 K, which vanishes above 2.5 T, and a metamagnetic transition at 5.5 T. The electronic properties of $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$ are highly susceptible to a magnetic field. Here we present atomically resolved tunneling spectroscopy studies in a millikelvin Scanning Tunneling Microscope across the magnetic phase diagram. We visualize directly atomic site dependent Kondo hybridization and its evolution across the different phases with applied magnetic field.

Universality of moiré physics in collapsed chiral carbon nanotubes

O. Arroyo-Gascón[1,2], **R. Fernández-Perea**[3], **E. Suárez Morell**[4], **C. Cabrillo**[3] **and L. Chico**[2]

[1]*Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain*
[2]*GISC, Departamento de Física de Materiales, Universidad Complutense de Madrid, E-28040 Madrid, Spain*
[3]*Instituto de Estructura de la Materia, CSIC, Serrano 123, E-28006 Madrid, Spain*
[4]*Departamento de Física, Universidad Técnica Federico Santa María, Casilla 110-V, Valparaíso, Chile*

The discovery of superconducting and correlated insulating behavior in twisted bilayer graphene (TBG) has shaken up the field of two-dimensional materials, reinvigorating the study of graphene-based systems. We demonstrate that one-dimensional moiré patterns, analogous to those found in TBG, can arise in collapsed chiral carbon nanotubes [1]. Performing a detailed study of the electronic structure of all types of chiral nanotubes, previously collapsed via molecular dynamics and validated against ab-initio modeling, we find that magic angle physics occurs in all families of collapsed carbon nanotubes [2]. Velocity reduction, flat bands, and localization in AA regions with diminishing moiré angle are revealed. Remarkably, all kinds of nanotubes behave the same with respect to magic angle tuning, giving rise to magic angles in full agreement with those of TBG.

Superconductivity in TBG was an unexpected phenomenon, so the quest for other systems which could be the one-dimensional analogues of TBG is of great interest. Moreover, nontrivial topological phases have been found in the magic angle regime and are closely related to flat bands. Therefore, chiral collapsed carbon nanotubes stand out as promising candidates to explore topology and superconductivity in low dimensions, emerging as the one-dimensional analogues of twisted bilayer graphene.

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Weyl-nodes and electronic correlations in $Ce_3Bi_4Pd_3$

M. Braß[1], J. Tomczak[1,2] and K. Held[1]

[1]*Institute of Solid State Physics, TU Wien, Vienna, Austria*
[2]*Department of Physics, King's College, London, United Kingdom*

The Kondo-Semimetal $Ce_3Bi_4Pd_3$ has been found to exhibit an unusually large spontaneous Hall effect, which in principle can be explained by a non-linear response to the electric field and the presence of Weyl-nodes close to the Fermi-energy [1]. However, first principle calculations within the single particle picture result in such nodes only far below the Fermi-edge [1], thereby indicating the necessity for a more accurate treatment of the electronic correlations of localized Ce-f electrons. I present DFT+DMFT calculations of the electronic structure which show that at low temperatures a single orbital out of the Ce-4f manifold dominates the low-energy physics. Hybridization with the conduction bands leads to a Kondo resonance and a strongly renormalized quasi-particle Hamiltonian which exhibits Type II Weyl-nodes within a few meV of the Fermi-energy. To pin-point these nodes in the Brillouin-zone I present a new numerical algorithm, which is efficient for models with many entangled bands.

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RIXS investigation of Cr-substituted $BaFe_2As_2$

<u>Marli R. Cantarino</u>[1,2]*, Wagner R. da Silva Neto[3], Juliana G. de Abrantes[2], Mirian Garcia-Fernandez[4], Claude Monney[5], Thorsten Schmitt[6], Fernando A. Garcia[2]

[1] European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France
[2] Universidade de São Paulo, 05508-090, São Paulo-SP, Brazil
[3] Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany
[4] Diamond Light Source, Harwell Campus, Didcot OX11 0DE, United Kingdom
[5] Département de Physique and Fribourg Center for Nanomaterials, Université de Fribourg, CH-1700 Fribourg, Switzerland
[6] Photon Science Division, Paul Scherrer Institut, 5232, Villigen PSI, Switzerland

* Contact: marli.cantarino@esrf.fr

Iron-based superconductors (FeSC) paved the way for investigating high-temperature superconducting (HTSC) materials beyond the framework of cuprates. The role of magnetic excitations in promoting or suppressing the different orders through the phase diagram is still under debate. The Cr-substituted $BaFe_2As_2$ (CrBFA) is a system with hole doping [1] where the superconducting (SC) ground state is absent. We employed high-resolution Resonant Inelastic X-ray Scattering (RIXS) to probe the magnetic excitations as a function of Cr content and direction over the 2D momentum space for these materials and found that the magnons are overdamped only for the Fe-Fe direction for 8.5% Cr substitution. We compare this trend with the case of Mn-substituted materials, where SC is also absent [2].
With ARPES and DFT+DMFT, we see a fractional scaling of the imaginary part of self-energy as a function of the binding energy, which is a signature property of Hund's metals [3], where the role of correlations is crucial [4]. We conclude that the spin density wave order is not only suppressed by the damping of (π, π) excitations but also by impurity scattering [5]. Finally, SC is lacking in CrBFA mainly because of magnetic pair breaking and scattering of the itinerant spin fluctuations that promote SC [6,7].

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Strain induced antiferromagnetic to altermagnetic transition in ReO_2

Atasi Chakraborty[1], Rafael González Hernández[2], Libor šmejkal[1,3], Jairo Sinova[1,3]

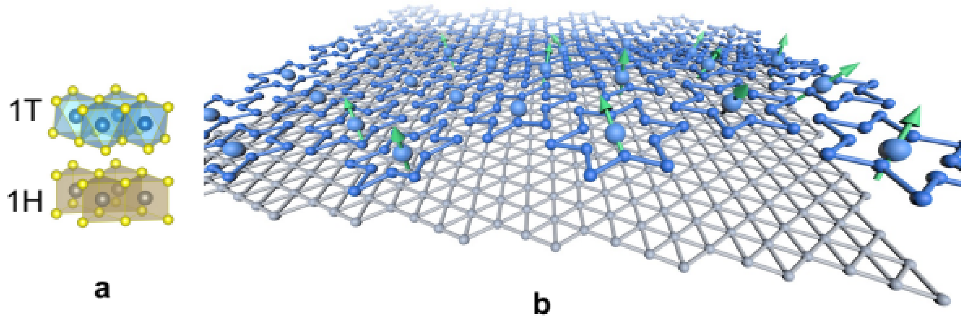
[1] *Institute, für Physik, Johannes Gutenberg Universität, Mainz, Germany*
[2] Departamento de Fisica y Geociencias, Universidad del Norte, Colombia
[3] Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic

The newly discovered altermagnets are unconventional collinear compensated magnetic systems, exhibiting even-parity-wave (d, g, or i-wave) spin-polarization order in the band structure, setting them apart from conventional collinear ferromagnets and antiferromagnets. Altermagnets offer advantages of spin polarized current akin to ferromagnets, and THz functionalities similar to antiferromagnets, while introducing new novel effects like spin-splitter currents. A key challenge for future applications and functionalization of altermagnets, is to demonstrate controlled transitioning to the altermagnetic phase from other conventional phases in a single material. Here we prove a viable path towards overcoming this challenge through a strain-induced transition from an antiferromagnetic to an altermagnetic phase in ReO_2. Combining spin group symmetry analysis and *ab initio* calculations, we demonstrate that under compressive strain ReO_2 undergoes such transition, lifting the Kramer's degeneracy of the band structure of the antiferromagnetic phase in the non-relativistic regime. In addition, we show that this magnetic transition is accompanied by a change in the non-trivial surface state topology from one phase to the other. We calculate the distinct signature of spin polarized spectral functions of the two phases, which can be detected in angle resolved photo-emission spectroscopy experiments.

Heterogeneous Ta-dichalcogenide bilayer: heavy fermions or doped Mott physics?

Lorenzo Crippa[1] ,**Hyeonhu Bae**[2], **Paul Wunderlich**[3], **Igor I Mazin**[4,5], **Binghai Yan**[2], **Giorgio Sangiovanni**[1], **Tim Wehling**[6,7], **Roser Valentí**[3]

[1] *Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany*
[2] *Department of Condensed Matter Physics, Weizmann Institute of Science, 7610001 Rehovot, Israel*
[3] *Institut für Theoretische Physik, Goethe Universität Frankfurt am Main, Germany*
[4] *Department of Physics and Astronomy, George Mason University, Fairfax, VA 22030*
[5] *Quantum Science and Engineering Center, George Mason University, Fairfax, VA 22030*
[6] *I. Institute of Theoretical Physics, University of Hamburg, Notkestrasse 9, 22607 Hamburg, Germany*
[7] *The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany*



Controlling and understanding electron correlations in quantum matter is one of the most challenging tasks in materials engineering. In the past years a plethora of new puzzling correlated states have been found by carefully stacking and twisting two-dimensional van der Waals materials of different kind. Unique to these stacked structures is the emergence of correlated phases not foreseeable from the single layers alone. In Ta-dichalcogenide heterostructures made of a good metallic "1H"- and a Mott-insulating "1T"-layer, recent reports have evidenced a cross-breed itinerant and localized nature of the electronic excitations, similar to what is typically found in heavy fermion systems.

Here, we put forward a new interpretation based on first-principles calculations which indicates a sizeable charge transfer of electrons (0.4-0.6 e) from 1T to 1H layers at an elevated interlayer distance. We accurately quantify the strength of the interlayer hybridization which allows us to unambiguously determine that the system is much closer to a doped Mott insulator than to a heavy fermion scenario.

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Topological Phase Transitions of Interacting Phases in Commensurate Magnetic Flux

<u>Axel Fünfhaus</u>[1,] and Marius Möller[1], Thilo Kopp[2] and Roser Valentí[1]

[1]Goethe Uni Frankfurt, Frankfurt am Main, Germany
[2] University of Augsburg, Augsburg, Germany

Lattice Hamiltonians in external magnetic fields provide a non-trivial magnetic translation algebra which results in Lieb-Schultz-Mattis (LSM) type theorems. The LSM theorems impose constraints on the topology of the system, in particuar on its Hall conductivity, and exclude trivial band insulating phases depending on the filling factor. We examine these constraints by taking into account the role of interaction driven spontaneous symmetry breaking of translation symmetry. Using exact diagonalization, we identify phase transitions from Hall insulating to topologically trivial charge density wave states for various flux quantum ratios and filling factors. Our findings demonstrate the importance of ”conventional” phase transitions in the study of topological phases as they may provide loopholes for properties otherwise protected by no-go LSM-type theorems.

Topology and disorder in a 2D semidirac material

Marta García Olmos,[1,2,*] Yuriko Baba,[3,2,†] Mario Amado,[1,‡] and Rafael A. Molina[2,§]

[1] *Nanotechnology Group, USAL—Nanolab, University of Salamanca Plaza de la Merced, Edificio Trilingüe, 37008, Salamanca, Spain.*
[2] *Instituto de Estructura de la Materia IEM-CSIC, Serrano 123, E-28006 Madrid, Spain*
[3] *GISC, Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain*

Semidirac materials in 2D present an anisotropic dispersion relation, linear in one direction and cuadratic in the perpendicular one. We study the topological properties and the influence of disorder in a 2D semiDirac Hamiltonian. Topological protection of edge states is anisotropic an occurs only in one direction and can be rigorously founded on the Zak phase of the one-dimensional reduction of the semiDirac Hamiltonian depending parametrically on one of the momenta. We explore the dependence on the disorder of the edge states and the robustness of the topological protection in these materials.

* mgarcia.o@usal.es
† yuribaba@ucm.es
‡ mario.amado@usal.es
§ rafael.molina@csic.es

2D lock-in analysis of ordered phases in superconductors

P. García Talavera[1], M. Águeda[1], J. A. Moreno[1], D. Navarro[1], M. Fernández-Lomana[1], F. Martín Vega[1], R. Sánchez-Barquilla[2], P. C. Canfield[3,4], E. Herrera[1], I. Guillamón[1] and H. Suderow[1]

[1] *Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049, Madrid, Spain*

[2] *Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, 03046, Cottbus, Germany*

[3] *Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA*

[4] *Department of Physics & Astronomy, Iowa State University, Ames, Iowa 50011, USA*

Unconventional superconductors usually present coexistence of different ordered phases, such as charge or pair density waves. These phases would present a non-uniform order parameter, and its spatial variations can be detected with techniques such as Scanning Tunneling Microscopy (STM). Here we implement the 2D lock-in technique to filter and analyze the different wavevectors of the ordered phases. We show the spatial variation of the amplitude and phase of these wavevectors. From the phase maps, we can detect topological defects, or dislocations, as points where the phase winds up 2π. Using topographies and spectroscopies obtained via STM, we analyze the appearance of these dislocations as a function of position and energy for different materials.

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Chiral quantum phase transition in moiré Dirac materials

A. García-Page[1] **and L. Classen**[1,2]

[1] *Max Planck Institute for Solid State Research, Stuttgart, Germany*
[2] *Department of Physics, Technical University of Munich, Garching, Germany*

Strong enough interactions induce a semimetal-to-insulator transition in Dirac materials, which can be viewed as the solid-state analogue of the chiral phase transition in quantum chromodynamics[1-4]. Moiré Dirac materials such as twisted bilayer graphene offer a new opportunity to study this transition because they facilitate tuning the effective interaction via a twist angle[5-6]. Motivated by this, we explore the quantum phase transition of a 2D Dirac material which spontaneously develops a gap that breaks an Ising symmetry[7]. We model it via an effective Gross-Neveu-Yukawa theory and employ the functional renormalization group method to map out the phase diagram. We analyze the quantum critical behavior at the transition and investigate the effect of a chemical potential which introduces a finite charge density.

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Towards hybrid van der Waals Josephson Junctions based on $NbSe_2$

<u>Celia González Sánchez</u>[1], J. Cuadra[1], E. Scheer[2], H. Suderow[1], A. di Bernardo[2], [3], E. J. H. Lee[1]

[1]Condensed Matter Physics Department, Universidad Autónoma de Madrid, Spain.
[2]Department of Physics 'E. Caianiello', Università degli Studi di Salerno, Italy.
[3]Department of Physics, Universität Konstanz, Germany.

The emergence of van der Waals heterostructures has paved the way for a "designer" approach, in which novel devices and new physics can be obtained by combining the properties of distinct two-dimensional materials. Among the many possibilities in this context, heterostructures based on superconducting few-layer $NbSe_2$ attract great interest for studying Josephson effects and the superconducting proximity effect in 2D systems [1]. Interestingly, recent work has reported on signatures of a topological superconducting phase in heterostructures based on $NbSe_2$ and 2D ferromagnets [2]. Moreover, first demonstrations of magnetic vdW Josephson junctions have been recently reported using a similar material combination [3, 4, 5, 6]. Motivated by the above developments, we present here our first results on nanodevices based on $NbSe_2$, including electronic transport and microwave measurements of Josephson junctions with and without ferromagnetic and antiferromagnetic tunnel barriers.

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Complex oxide memristors for cryogenic neuromorphic computing

T. Günkel[1,2*], A. Fernandez-Rodríguez[1], A. Barrera[1], J. Alcalà[1], L. Ballcells[1], N. Mestres[1], J. Suñe[2], A. Palau[1]

[1] *Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Spain.*

[2] *Dept. d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain*

*e-mail: tgunkel@icmab.es

Altough the memristor as a novel circuit element was proposed by Leon Chua already in 1971 [1], it took decades to implement these kinds of devices for real world applications. Nowadays memristors are the main building blocks in the emerging field of neuromorphic computing, which could tackle the continuously increasing demand on processing large sets of data [2]. Recent studies have demonstrated, that $YB_2C_3O_{7-\delta}$ (YBCO), besides its vast exciting properties, such as e.g. high-temperature superconductivity, also exhibits memristive properties. Originating from the charge carrier dependent properties of the YBCO, a voltage induced movement of oxygen vacancies might lead to a Metal-Insulator- or a Superconductor-Insulator transition inside the high-T_c superconductor, giving access to multiple resistive states [3].
In this study it is demonstrated, that complex oxide heterostructure made from the manganite $La_{1-x}Sr_xMnO_3$ (LSMO) and the cuprate YBCO are suitable candidates for neuromorophic devices, operating at cryogenic temperatures. Furthermore this might pave the way for a gate-tunable interaction between superconductors and ferromagnets and thus for novel superconducting electronic devices, based on superconductor-ferromagnet heterostructures [4].

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Characterizing the chemical structure of topological defects of graphene surfaces by ncAFM

H. Guo[1], E. Ventura-Macías[2], M. D. Jiménez-Sánchez[1], P. Pou[1,3], A. J. Martínez-Galera[4,5], J. Gómez-Herrero[1,3,5], R. Pérez[2,3] and I. Brihuega[1,3,5]

[1]*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[2]*Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[3]*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[4]*Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[5]*Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

Topological defects, whose structure is described by some topological invariant conserved upon local transformation, on two dimensional materials may strongly affect their pristine properties but can also induce the emergence of new correlated electronic phenomena. To fully understand the impact of such topological defects, development of imaging tools capable to resolve their intrinsic chemical structure is of paramount importance. Here, we show that by employing ncAFM, and without carrying out an explicit tip functionalization with CO molecules, we can resolve the chemical structure of different class of topological defects on graphene surfaces. We were able to characterize a variety of extended topological defects of graphene, like grain boundaries, divacancy reconstruction, and the so-called flower defect. Furthermore, the high-resolution imaging capability of our ncAFM has provided us with a direct tool to reveal a potential signature of tip-induced manipulation of the local strain and corrugation of the grain boundary regions.

Cold Atomic Excitons

F. Hirsch[1], O.K. Diessel[2], R. Ołdziejewski[3], and R. Schmidt[1]

[1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany
[2] ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138
[3]Max Planck Institute for Quantum Optics, Hans-Kopfermann-Straße 1, 85748 Garching, Germany
E-mail: hirsch@thphys.uni-heidelberg.de

We theoretically explore the prospect to simulate the physics of excitons and their dynamics using ultracold atoms in optical lattices. In recent years, study of optoelectronic properties of atomically thin transition metal dichalcogenides (TMD) has become a growing field in solid state physics. In these systems, the excitation of an electron from a filled valence band into an empty conduction band leads to formation of electron-hole pairs (excitons). At the same time, cold atom systems have emerged as versatile platforms for simulating such two-dimensional solid state structures. With all necessary experimental methods available and successfully utilized, we now investigate how excitons manifest under short range interaction, which can be realised e.g. using Rydberg atoms, dipolar atoms or ground states molecules.

Based on a combination of band structure calculation and variational many-body wavefunctions, we predict the existence of analogue atom-hole pairs (atomic excitons) in a system of single-component fermionic atoms with nearest neighbour interactions. Our 2D lattice has a hexagonal structure with two different lattice sites, leading to a band structure with nonzero bandgap. Analog to TMDs, we derive the energy spectrum of zero-momentum excitons which form around the K/K'-points. We show that excitonic effects can be found over a large range of system parameters, which also includes currently accessible regions of band gap, tunnelling rate and nearest neighbour interaction strength. Finally, using Fermis Golden Rule analysis, we propose experimental procedures to probe the states and their dynamics.

Fundamental laws of chiral band crossings

K. Alpin,[1] M. M. Hirschmann,[1,2] N. Heinsdorf,[1,3] A. Leonhardt,[1] W. Y. Yau,[1, 4] X. Wu,[1, 5] and A. P. Schnyder[1]

[1] Max Planck Institute for Solid State Research, Stuttgart, Germany
[2] RIKEN Center for Emergent Matter Science, Wako, Japan
[3] Department of Physics and Astronomy & Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver BC, Canada
[4] Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany
[5] Institute for Theoretical Physics, Chinese Academy of Sciences, Beijing, China

The number of surface states as well as the electric response of Weyl semimetals is determined to a large extent by the Chern number of the Weyl points, a property also referred to as their chirality. It is known [1,2] that rotation eigenvalues affect the value of the chirality.

We show that the previous works are applications of a local constraint [3], relating the Chern number with the exchange of rotation eigenvalues. This holds for arbitrary combinations of symmetries, as well as for chiral crossings comprising more than two bands. Using this constraint, we explain the chiralities of quadruple Weyl points, double Weyl points on two-fold rotation axes, and discuss the emergence of a Chern number 5 band within certain fourfold point crossings. Furthermore, with a global constraint stemming from the periodicity of the Brillouin zone, we can identify space groups with enforced topological nodal planes.

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The interplay between a charge density wave order and superconductivity in the kagome materials

S. C. Holbæk[1] **and M. H. Fischer**[1]

[1]*University of Zurich, Zurich, Switzerland*

In many superconductors, the superconducting state emerges on top of a charge density wave (CDW). An intriguing example is the AV_3Sb_5 (A=K,Rb,Cs) family of superconductors, where a 2×2 in-plane CDW ordered phase, potentially breaking time-reversal symmetry, appears at $T \approx 100$ K. To determine the microscopic origin and structure of the ordered phases, one often studies the CDW and superconductivity on the kagome lattice independently. However, it remains an outstanding question to understand the mutual influence of the different orders.

In our work, we present a phenomenological theory of CDW and superconducting orders based solely on symmetry arguments for the kagome lattice. For this purpose, we derive a Ginzburg-Landau free energy of possible 2×2 CDW order and superconductivity uncovering a rich phenomenology. In particular, we study the consequences of additional spatial or time-reversal-symmetry breaking of the CDW order, coupling to a pair density wave, and we discuss possible experimental consequences. Importantly, our work can inform future microscopic calculations on what order parameters to include.

Topology of SmB_6 revisited by means of topological quantum chemistry

Mikel Iraola[1,2], **Iñigo Robredo**[1,3], **Titus Neupert**[4], **Juan L. Mañes**[5], **Roser Valentí**[6] **and Maia G. Vergniory**[1,3]

[1]Donostia International Physics Center, Donostia-San Sebastian, Spain
[2] Institute for Theoretical Solid State Physics, Dresden, Germany
[3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
[4]Department of Physics, University of Zürich, Zürich, Switzerland
[5]Department of Physics, University of the Basque Country, Bilbao, Spain
[6]Institute for Theoretical Physics, Goethe University Frankfurt, Frankfurt am Main, Germany

The mixed-valence compound SmB_6 with partially filled samarium *4f* flat bands hybridizing with *5d* conduction bands is a paramount example of a correlated topological heavy-fermion system. In this study we revisit the topology of SmB_6 with the band theory paradigm and uncover previously overlooked aspects resulting from the formation of multiple topological gaps in the electronic structure. By invoking topological quantum chemistry we provide a detailed classification of the strong and crystalline topological features that derive from the existence of such topological gaps. To corroborate this classification, we calculate Wilson loops and simulate the surface electronic structure using a minimal tight-binding model, allowing us to describe its surface states and confirm the crystalline topology. We finally discuss its implications for experiments.

YBCO heterostructures for SQUID-on-Si-lever

K. Wurster[1], S. Koch[1], V. Harbola[2], Y.-J. Wu[2], R. Kleiner[1], J. Mannhart[2] and D. Koelle[1]

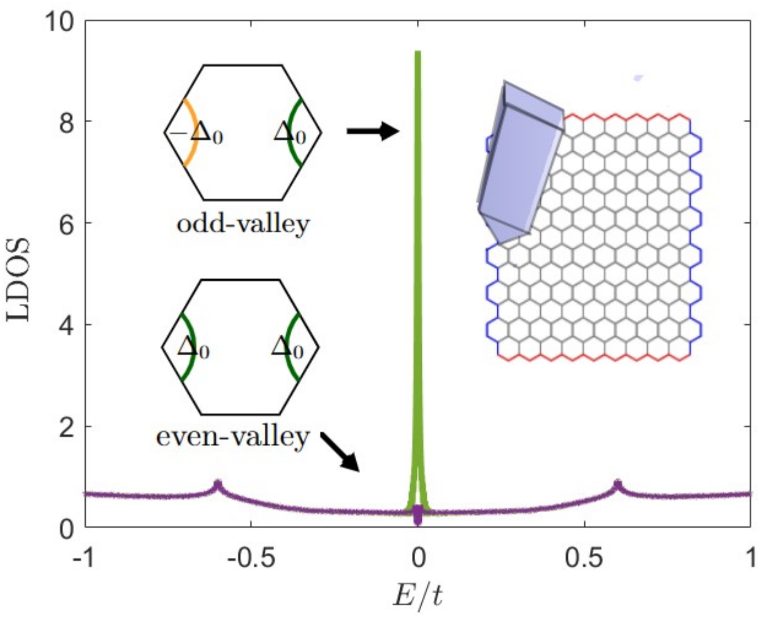
[1] *Physikalisches Institut, Center for Quantum Science (CSQ) and LISA⁺, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany*
[2] *Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany*

Scanning SQUID microscopy (SSM) is a powerful technique for imaging magnetic fields or dissipation processes. The use of the high-T_c cuprate superconductor $YBa_2Cu_3O_7$ (YBCO) combined with custom made Si AFM Cantilevers could enable SSM in the Tesla range and at temperatures up to about 80 K with a high spatial resolution.
However, YBCO has a complex crystal structure and a small coherence length, which leads to a high sensitivity to defects on the atomic scale. High quality YBCO films can only be obtained by epitaxial growth on lattice-matched substrates. Therefore, the challenge with this approch is the integration of YBCO thin films on Si wafers.
We intend to use $Sr_3Al_2O_6$ (SAO) or $Sr_2CaAl_2O_6$ (SCAO), which are lattice-matched to perovskite materials, such as $SrTiO_3$ (STO). SAO and SCAO can be dissolved in water, i.e. it can be used as a sacrificial layer for the realisation of free-standing single-crystalline perovskite thin films, including YBCO.
We present our process for the fabrication of YBCO heterostructures based on pulsed laser deposition (PLD) and discuss the optimization of growth conditions and properties of the used materials. Finally, we present our preliminary attempts to transfer YBCO films onto Si surfaces.

Spectroscopic signature of spin triplet odd-valley superconductivity in two-dimensional materials

Tim Kokkeler, Chunli Huang, Sebastian Bergeret, Ilya Tokatly

The poster presents a test to distinguish even-valley and odd-valley superconductivity in 2D materials whose Fermi surface consists of two valleys at $\pm K$-points. For odd-valley superconductivity, our low energy theory predicts the emergence of an almost flat band of edge states centered at zero energy for certain edge orientations. As a result, a prominent experimental signature of this type of superconductivity is the presence of a large zero-energy peak in the local density of states near those specific edges. Such peaks are absent if the pair potential is even-valley, and therefore provide a clear indication of odd-valley superconductivity. Our results are applicable to a wide range of materials and have been confirmed by analyses on specific microscopic tight-binding realizations of odd-valley superconductivity such as f-wave superconductivity on a honeycomb lattice in a ribbon geometry.



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Engineered topological and correlated states in van der Waals heterostructures

<u>F. Lüpke</u>

Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany

The assembly of van der Waals (vdW) materials into heterostructures enables the engineering of exotic quantum states by moiré and proximity effects. The resulting properties are typically well accessible on the heterostructure surfaces, such that scanning tunneling microscopy (STM) has become an important tool for their structural and electronic characterization. In my talk, I will summarize our developed vdW assembly methods for stacking air-sensitive vdW materials with atomically clean surfaces and internal interfaces [1], and will show results of engineered topological superconductivity in proximity heterostructures [2,3] and correlated states in twisted bilayers [4].

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Acknowledgements

The work was supported by the German Research Foundation's (DFG) Emmy Noether Programme and Priority programme 2244 ('2D Materials – Physics of van der Waals [hetero]structures', project nos. 443416235 and 422707584); the Alexander von Humboldt Foundation; Germany's Excellence Strategy - Cluster of Excellence Matter and Light for Quantum Computing (ML4Q); European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement no 824109 (European Microkelvin Platform); the Helmholtz Nano Facility; APVV-20-0425, VEGA 2/0058/20, Slovak Academy of Sciences project IMPULZ IM-2021-42, COST action CA21144 (SUPERQUMAP) and EU ERDF (European regional development fund) Grant No. VA SR ITMS2014+ 313011W856.

Skyrmion lattices in magnetic multilayers and lateral confinements

E. M. Jefremovas*, M. Fischer, K. Leutner, T. Winkler, T. Sparmann, R. Frömter, J. Sinova, and M. Kläui
***martinel@uni-mainz.de**
Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

Skyrmions are quasi-particle-like topologic spin textures extensively studied as promising candidates for information storage and information processing technologies [1, 2]. In the last years, magnetic skyrmions of micrometer size have been stabilized at room temperature in multilayers systems at relatively low magnetic fields (mT) with a high diffusion [3] thanks to the dipolar interactions (stray field). Nevertheless, the influence of such interactions in the skyrmion size and stability, resolved for isolated skyrmions [4], has not been elucidated yet for lattices, where the skyrmion-skyrmion interaction needs to be accounted. Aiming to resolve this contribution and its impact to dipolar interactions, we have designed a thin film material with skyrmion lattices and varied the dipolar interactions by (i) increasing number of repetitions in a magnetic multilayer stack; and (ii) geometric confinement, varying the size and shape of the patterned structures. Starting with the continuous films, a systematic decrease of the skyrmion size with increasing the number of repetitions has been observed. This behavior is opposite to the one predicted by the model for isolated skyrmions [4], resolving the crucial role of the skyrmion-skyrmion interaction. We propose a numerical model capable of reproducing the experimental behavior of these skyrmion lattices. Concerning the geometric confinements, both the area of the confinement and the angle of the confinement (shape) were found to play an important role on the skyrmion stability, periodicity, size and density. Below a certain area threshold, different for each symmetry, skyrmions are not stable, but a maze-domain configuration minimizes the energy of the system. This reveals the critical role of the stray field, reduced in the smaller geometries, where the reduced coordination in the edges leads to a reduced stray field. Concerning the angle, we have observed how skyrmions are stabilized in geometries with larger angles (octagons, heptagons) compared to smaller ones (squares or pentagons). This finding may be related to the skyrmion-edge repulsion, which is weaker in narrower angles. The presented work sheds light to the role of stray field in skyrmion lattices, allowing also to explore the different mechanisms (size reduction, angle dependency) to stabilize spin textures in magnetic multilayer stacks.

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Magneto optical response of bulk WTe_2

R. Mathew Roy[1] , F. Le Mardele[2], M. Orlita[2], C. Prange[1], M. Dressel[1], V. Hasse[3], C. Felser[3] and A.V. Pronin[1]

[1] 1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany
[2] Laboratoire National des Champs Magnétiques Intenses, CNRS-UGA-UPS-INSA-EMFL, 38042 Grenoble, France
[3] Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We report the bulk magneto-optical response of the type-II Weyl semimetal, WTe_2, in the energy range from 2 to 600 meV under an external magnetic field up to 32 T. The large non-saturating magneto resistance due to the perfect electron-hole compensation [1] as well as the highly anisotropic crystal structure of this compound stimulated our research interest in WTe_2. The anisotropy gives rise to the distinguishable optical properties along different crystallographic axes [2]. We observe substantial changes in the reflectivity spectra near the plasma frequency (around 55 meV) and anomalous absorption at a much lower frequency (below 20 meV). We compare our results with our zero-field temperature-dependent optical spectra and the temperature and field-dependent Hall conductivity. We also speculate on a possible relation between our observations and hydrodynamic electron behavior reported for this compound [3].

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Crossover from isolated YSR states to gapless superconductivity in 2H-$NbSe_{2-x}S_x$ at the atomic scale

<u>Jose A. Moreno</u>[1], Victor Barrena[1], Edwin Herrera[1], Antón Fente[1], Alberto Montoya[2], Samuel Mañas-Valero[2], Anita Smeets[1], Beilun Wu[1], Jazmín Aragón Sanchez[3], Yanina Fasano[3], Eugenio Coronado[2], Jose J. Baldoví[2], Isabel Guillamón[1], Hermann Suderow[1].

[1]*Laboratorio de Bajas Temperaturas, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.*

[2] *Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Catedrático José Beltrán 2, 49680, Paterna, Spain.*

[3]*Centro Atómico de Bariloche and Instituto Balseiro, CNEA, CONICET and Universidad Nacional de Cuyo, Avenida Bustillo 9500, 8400 San Carlos de Bariloche, Argentina.*

Anderson's theorem states that the superconducting gap of s-wave superconductors remains fully open even in presence of a large amount of non-magnetic impurities. A single isolated magnetic impurity leads to in-gap states, called Yu-Shiba-Rusinov (YSR) states. These states produce local density of states oscillations and have been extensively studied in pure 2H-$NbSe_2$ with a small number of magnetic impurities[1,2]. Here we study 2H-$NbSe_{2-x}S_x$ with highly diluted Fe impurities (0.02 at.%) and find that gapless superconductivity sets in over large areas[3]. The characteristic electron-hole asymmetry of the density of states of isolated YSR states is lost in the gapless regime. YSR oscillations exhibit wavevectors which differ from the ones found in pure 2H-$NbSe_2$, unveiling features in the electronic band structure such as the van Hove anomaly along the Γ-M direction. We show through density functional calculations that substitutional Se-S disorder leads to a band structure with enhanced quasi two-dimensional character. However, at the same time, the charge density wave of pure 2H-$NbSe_2$ is destroyed by in-plane disorder, leading to in-plane isotropic vortex cores in the gapless regime. Our experiments show that electronic correlations and disorder produce gapless superconductivity even with minute amounts of magnetic impurities.

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Microscopic model for the charge transfer in graphene/WS_2 heterostructure

Dilan Pérez-Paredes[1], Raul Perea-Causin[2], Samuel Brem[1], Ermin Malic[1,2]

[1]Philipps University Marburg, Department of Physics, Marburg, Germany
[2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Van der Waals heterostructures exhibit fascinating electrical properties such as ultrafast charge separation after photoexcitation. Nonetheless, the fundamental understanding of charge transfer in these materials remains unclear. Here we present a microscopic many-particle model to reveal the relevant microscopic charge transfer channels in WS2-graphene heterostructures. Based on a tight binding description around the K symmetry points, we unveil the origin of the experimentally measured charge-separated state. In particular, we reveal that the slow electron transfer can be traced back to the high energy barrier of this process and the fundamentally weak strength of this tunnelling process. Finally, we discuss how to extend our model to describe charge transfer in the whole Brillouin zone. Such a description would allow us to investigate the importance of other charge-transfer channels that might become relevant with finite twist angles.

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Transport properties of charged two-dimensional Dirac systems in hydrodynamic regime: the role of dynamical screening and plasmons

K. Pongsangangan[1], T. Ludwig[2], H.T.C. Stoof[2], and L. Fritz[2]

[1] *Institute of Theoretical Physics, TU Dresden, Germany*
[2] *Institute for Theoretical Physics, Utrecht University, The Netherlands*

Clean two-dimensional Dirac systems, for example, graphene, have received a lot of attention for being a prime candidate to observe hydrodynamical transport behavior of interacting electrons. In this talk, I will discuss the role of dynamical screening which gives rise to a collective mode, called plasmon, in the thermo-electric transport properties of those systems. We find that the plasmon is an additional low-energy degree of freedom which makes a sizeable contribution to the thermal conductivity and viscosity of graphene. In addition, we find that the form of the hydrodynamic equations as well as the definition of conserved quantities are not only constrained by symmetries of the kinetic energy but also by the interactions of the underlying system. We propose a novel type of hydrodynamics consisting of electrons, holes, and plasmons. Our result suggests that this is a generic feature of ultraclean two-dimensional electronic systems, also applicable to 2DEL, Bernal-stacked and twisted bilayer graphene.

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Dynamical correlations and order in magic-angle twisted bilayer graphene

Gautam Rai[1], Lorenzo Crippa[2], Dumitru Călugăru[3], Haoyu Hu[4], Luca de' Medici[5], Antoine Georges[6, 7, 8, 9], B. Andrei Bernevig[3, 4, 10], Roser Valentí[11], Giorgio Sangiovanni[2], Tim Wehling[1, 12]
[1]IUniversity of Hamburg, Notkestrasse 9, 22607 Hamburg, Germany
[2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany
[3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA
[4]DIPC, P. Manuel de Lardizabal 4, 20018 Donostia-San Sebastian, Spain
[5]LPEM, UMR8213 CNRS/ESPCI/UPMC, Paris, France
[6]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France
[7]CCQ, Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA
[8]Centre de Physique Théorique, Ecole Polytechnique, CNRS, Institut Polytechnique de Paris, 91128 Palaiseau Cedex, France
[9]DQMP, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève, Suisse
[10]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
[11]Goethe U Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany
[12]The Hamburg Centre for Ultrafast Imaging, 22761 Hamburg, Germany

In magic-angle twisted bilayer graphene, transport, thermodynamic and spectroscopic experiments pinpoint at a competition between distinct low-energy states with and without electronic order. In our work [1,2], we utilize Dynamical Mean Field Theory on twisted bilayer graphene to study the emergence of electronic correlations and long-range order in the absence of strain. We explain the nature of emergent insulating and correlated metallic states by three central phenomena: (i) the formation of local spin and valley isospin moments around 100K, (ii) the ordering of the local isospin moments around 10K, and (iii) a cascadic redistribution of charge between localized and delocalized electronic states upon doping. At integer fillings, we find that low energy spectral weight is depleted in the symmetric phase, while we find insulating states with gaps enhanced by exchange coupling in the ordered state. Doping away from integer filling results in distinct metallic states: a ``bad metal'' above the ordering temperature, where coherence of the low-energy electronic excitations is suppressed by scattering off the disordered local moments, and a ``good metal'' in the ordered states with coherence of quasiparticles facilitated by isospin order. Upon doping, there is periodic charge reshuffling between the localized and delocalized orbitals of the THF model that manifests itself in cascades of doping-induced Lifshitz transitions, local spectral weight redistributions, and periodic variations of the electronic compressibility ranging from nearly incompressible to negative. Our findings provide a unified understanding of the most puzzling aspects of scanning tunneling spectroscopy, transport, and compressibility experiments.

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Fabrication method for hybrid quantum devices involving topological insulators and superconductors using Focused Ion Beam Induced Deposition

<u>A. Sáenz-Hernández</u>[1], R. Gracia-Abad[1], S. Sangiao[1,2] and J.M. De Teresa[1]

[1]*Instituto de Nanociencia y Materiales de Aragón (INMA), Universidad de Zaragoza-CSIC, 50009, Zaragoza, Spain.*
[2] *Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, Spain.*

Superconducting nanostructures offer unique properties with promising applications. Josephson Junctions (JJs), consisting of two weakly connected superconductors, have raised interest for their possible implementation in quantum computing processors [1][2]. Other examples are Superconducting Quantum Interference Devices (SQUIDs), superconducting rings divided by two JJs, widely used in the development of high-precision sensors [3]. Additionally, Majorana states can be produced by the proximity effect of a superconductor and a topological insulator, which have been theoretically proven to be applicable in quantum processing [4].
For fabrication, we employ Focused Ion Beam Induced Deposition (FIBID), specifically focusing on tungsten devices. Previous studies on tungsten-based nanostructures deposited through FIBID have demonstrated superconductivity below 4-5 K [5], along with intriguing characteristics like vortex phenomena [6], tunable critical temperature T_c [7], and the potential for creating functional tungsten nano SQUIDs [8].
The present work deals with the fabrication of tungsten-based nanoscale single JJs and SQUIDs using topological insulators as weak links. We propose a new fabrication method using Ga^+ Focused Ion Beam Induced Deposition (FIBID) and $W(CO)_6$ as the gas precursor to study how superconductivity can be induced on a topological insulator.

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Evidence for ground state coherence in a two-dimensional Kondo lattice

Wen Wan[1], Rishav Harsh[1], Antonella Meninno [2,3,] Paul Dreher[1], Sandra Sajan[1, *], Haojie Guo[1], Ion Errea[1,2,3], Fernando de Juan[1,4] and Miguel M. Ugeda[1,2,4]

[1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain.
[2]Centro de Física de Materiales, Paseo Manuel de Lardizábal 5, 20018 San Sebastián, Spain. [3]Departamento de Física Aplicada, Escuela de Ingeniería de Gipuzkoa, University of the Basque Country (UPV/EHU), Plaza Europa 1, 20018 San Sebastián, Spain.
[4] Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain.

Email: sandra.sajan@dipc.org

Kondo lattices are ideal testbeds for the exploration of heavy-fermion quantum phases of matter. While our understanding of Kondo lattices has traditionally relied on complex bulk f-electron systems, transition metal dichalcogenide heterobilayers have recently emerged as simple, accessible and tunable 2D Kondo lattice platforms where, however, their ground state remains to be established. Here we present evidence of a coherent ground state in the 1T/1H-$TaSe_2$ heterobilayer by means of scanning tunnelling microscopy/spectroscopy at 340 mK. Our measurements reveal the existence of two symmetric electronic resonances around the Fermi energy, a hallmark of coherence in the spin lattice. Spectroscopic imaging locates both resonances at the central Ta atom of the charge density wave of the 1T phase, where the localized magnetic moment is held. Furthermore, the evolution of the electronic structure with the magnetic field reveals a non-linear increase of the energy separation between the electronic resonances. Aided by ab initio and auxiliary-fermion mean-field calculations, we demonstrate that this behaviour is inconsistent with a fully screened Kondo lattice and suggests a ground state with magnetic order mediated by conduction electrons. The manifestation of magnetic coherence in TMD-based 2D Kondo lattices enables the exploration of magnetic quantum criticality, Kondo breakdown transitions and unconventional superconductivity in the strict two-dimensional limit.

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Correlated insulators in magic-angle graphene at one magnetic flux quantum

Tobias Stauber and Miguel Sánchez[1]

[1]*Instituto de Ciencia de Materiales de Madrid ICMM-CSIC. Madrid (Spain)*

In the recent years, magic angle twisted bilayer graphene has been widely studied as an example of topology and strong interactions. The large moiré unit cell also allows to probe the Hofstadter regime, where the magnetic flux per cell is equal to the flux quantum, *h/e*. In this regime the flat bands and correlated insulators are reentrant. With a Hartree-Fock method, we study the correlated states at even fillings, and make connections with experiment[1].

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Spin-orbit coupled states arising in the half-filled t_{2g} shell

Marco Schönleber[1] and Maria Daghofer[1]

[1]*Institute for Functional Matter and Quantum Technologies , Stuttgart, Germany*

Strongly correlated and spin-orbit coupled t_{2g} systems have been extensively investigated. By coupling orbital and spin angular momentum into one quantity, spin-orbit coupling (SOC) tends to reduce orbital degeneracy, e.g. for the widely studied case of one hole in the t_{2g} shell. However, the opposite has to be expected at half filling. Without spin-orbit coupling, all orbitals are half filled, no orbital degree of freedom is left and coupling to the lattice can be expected to be small. At dominant spin-orbit coupling, in contrast, one of the j=3/2 states is empty and the system couples to the lattice. We investigate this issue. One finding is that the low-energy manifold evolves smoothly from the four S=3/2 states in the absence of SOC to the four j=3/2 states with dominant SOC. These four states are always separated from other states by a robust gap. We then discuss a relevant superexchange mechanism to assess the interplay between spin-orbit coupling and coupling to the lattice.

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Analog gravity in moiré Dirac materials

M. Tolosa-Simeón[1], Michael M. Scherer[1] and S. Floerchinger[2]

[1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

[2] Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, D-07743 Jena, Germany

Condensed matter systems can be used in various scenarios to emulate and study phenomena from a completely different field of physics, for example, elementary particle physics or gravity. Such analog condensed matter models provide a novel perspective to approach questions that are not directly accessible in the original systems as they can potentially be realized experimentally in a well-controlled setup.

In this project [1], we address the problem of cosmological fermion production in expanding universes using moiré Dirac materials as analog models. Recently, two-dimensional moiré Dirac materials, such as twisted bilayer graphene (TBG), have been established as highly tunable condensed matter platforms allowing us to manipulate electronic band structures and interaction effects in a controlled manner. A remarkable feature of moiré Dirac materials is the presence of fermionic low-energy excitations, described by a quasirelativistic Dirac equation where the velocity of light is replaced by the Fermi velocity. The Fermi velocity can be tuned dynamically over several orders of magnitude leading to a time-dependent metric for the Dirac fermions. In addition, we consider the presence of time-dependent Dirac masses that may originate from symmetry breaking and lead to a finite band gap in the energy dispersion. These ingredients allow us to construct an analog model for the phenomenon of cosmological fermion production in expanding universes, arising due to a time-dependent metric and conformal symmetry breaking.

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Nb constriction-Josephson-junction nanoSQUIDs on cantilevers patterned by He and Ne focused ion beams

J. Ullmann[1], T. Griener[1], S. Koch[1], S. Pfander[1], C. Bureau-Oxton[2], D. Jetter[3], A. Vervelaki[3], K. Bagani[3], U. Drechsler[2], O. Kieler[4], R. Kleiner[1], M. Poggio[3], A. Knoll[2] and D. Koelle[1]

[1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA+, Universität Tübingen, Germany
[2]IBM Research Europe – Zürich, Rüschlikon, Switzerland
[3]Department of Physics and Swiss Nanoscience Institute, University of Basel, Switzerland
[4]Department Quantum Electronics, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Nanopatterning of superconducting thin film structures with focused He or Ne ion beams (He/Ne-FIB) offers a flexible tool for creating constriction-type Josephson junctions (cJJs) which can be integrated into strongly miniaturized Superconducting Quantum Interference Devices (nanoSQUIDs) for magnetic sensing on the nanoscale. We present our attempts to use He/Ne-FIB for fabricating Nb nanoSQUIDs which shall provide ultra-low noise and high spatial resolution for their application in scanning SQUID microscopy (SSM). The nanoSQUIDs are designed as sensors for magnetic flux and dissipation. We address the possibility to implement multi-terminal, multi-cJJ SQUIDs that provide flexibility in SQUID readout on custom-made Si cantilevers, which will provide the possibility of simultaneous conventional topographic imaging by atomic force microscopy (AFM). We will discuss the status of this project and challenges that have to be met on the way to combine SSM and AFM on the nanoscale.

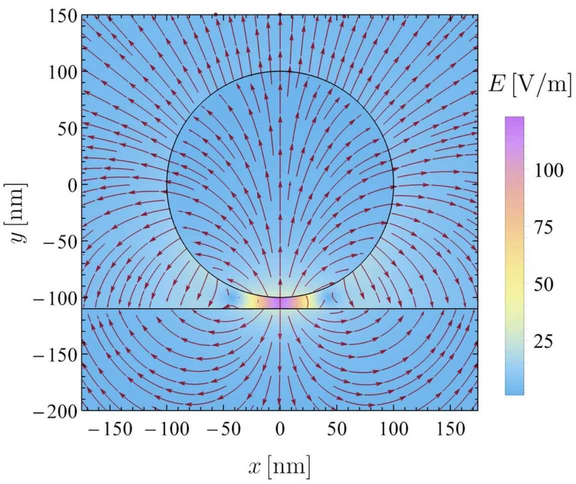
We acknowledge the European Commission under H2020 FET Open grant FIBsuperProbes (number 892427).

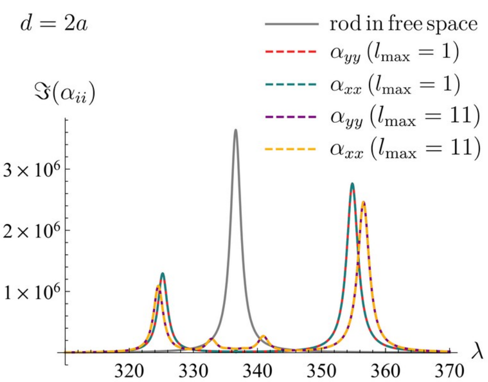
Plasmonic response of a nanorod in the vicinity of a planar surface

I. M. Vasilevskiy[1,2] and N. M. R. Peres[2,3]

[1]Instituto de Ciencia de Materiales de Madrid, Madrid, Spain
[2]University of Minho, Braga, Portugal
[3]International Iberian Nanotechnology Laboratory (INL), Braga, Portugal

This work belongs to the area of nanophotonics and is dedicated to the theoretical description of a composite system made of a cylindrical nanorod in the vicinity of a plasmonic semi-infinite metallic substrate. The complexity of this problem arises from the fact that the rod has axial symmetry, while the interface is planar. Solving the Laplace's equation with appropriate boundary conditions allows one to compute the eigenmodes corresponding to the excitation of surface plasmons. The bipolar system of coordinates represents a good choice to combine the two symmetries together in the solution of the Laplace's equation. Furthermore, it allows one to additionally consider a two-dimensional material, namely graphene, placed on the substrate.
The boundary integral method proposed by Eyges enables one to determine the electric field everywhere through the knowledge of the potential on the nanorod's surface in the presence of a uniform external electric field. After solving the integrals that connect the two symmetries, the problem is reduced to a linear algebra one, where all the terms in the system are known analytically. The computation of the scattered field is numerical, but an approximate analytical solution can be obtained for large distances between the rod and the planar surface. The polarizability of the system is computed through this method and the maxima of its imaginary part occur precisely at the frequencies predicted by the solution of the eigenmodes' problem[1].





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Tuning of the carrier localization, magnetic and thermoelectric properties in ultrathin $(LaNiO_{3-\delta})_1$ $/(LaAlO_3)_1(001)$ superlattices by oxygen vacancies

Manish Verma[1] **and Rossitza Pentcheva**[1]

[1]Department of Physics, Universität Duisburg-Essen, Duisburg, Germany

Email: manish.verma@uni-due.de

Understanding the role of defects on the complex behavior of transition metal oxides in bulk and the ultrathin limit is at the forefront of condensed matter physics. Using a combination of density functional theory calculations with an on-site Coulomb repulsion term (DFT+U) and Boltzmann transport theory within the constant relaxation time approximation, we explore the effect of oxygen vacancies on the electronic, magnetic, and thermoelectric properties in ultrathin $(LaNiO_{3-\delta})_1$ $/(LaAlO_3)_1(001)$ superlattices (SLs). For the pristine SL, an antiferromagnetic charge-disproportionated (AFM-CD) $(d^8\underline{L}^2)_{S=0}(d^8)_{S=1}$ phase is stabilized, irrespective of strain. At δ = 0.125 and 0.25, the localization of electrons released from the oxygen defects in the NiO plane triggers a charge-disproportionation, leading to a ferrimagnetic insulator both at a_{STO} (tensile strain) and a_{LSAO} (compressive strain). At δ = 0.5, an insulating phase emerges with alternating stripes of Ni^{2+} (high-spin) and Ni^{2+} (low-spin) and oxygen vacancies ordered along the [110] direction (S-AFM), irrespective of strain. This results in a robust n-type in-plane power factor of 24 $\mu W/K^2$ cm at a_{STO} and 14 $\mu W/K^2$ cm at a_{LSAO} at 300 K (assuming relaxation time τ = 4 fs). Additionally, the pristine and δ = 0.5 SLs are shown to be dynamically stable.

Broadband optical investigations of the antiferromagnetic kagome metal FeGe

M. Wenzel[1] and A. V. Pronin[1] and E. Uykur[2] and A. A. Tsirlin[3] and S. Pal[1] and R. Mathew Roy[1] and C. Yi[4] and C. Shekhar[4] and C. Felser[4] and M. Dressel[1]

[1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany
[3]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

Kagome metals became model compounds for studying the interplay of electronic correlations, non-trivial topology, and, in some cases, magnetism. Consisting of spatially separated metallic kagome planes, the itinerant carriers give rise to the peculiar kagome electronic band structure hosting dispersionless flat bands, saddle points, as well as linearly dispersing Dirac bands.
Here, we present a broadband optical spectroscopy study of antiferromagnetic FeGe down to 10 K. The contributions of itinerant and localized charge carriers to the optical spectra are discussed, and signatures of the emerging charge density wave state below approximately 100 K are unveiled. Aided by DFT calculations, we show that the low-energy interband transitions are very sensitive to subtle changes in the Fermi level and uncover a delicate interplay between phonons, charge order, and localized carriers.

Two-step growth of wafer-sized $NbSe_2$ film

S. Zahedi-Azad[1], V. R. Mantha[1], J. Martin[1]

[1]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489, Berlin, Germany
E-mail: setareh.zahedi-azad@ikz-berlin.de

Quantum computing promises to speed up computational tasks where classical computers reach their limits [1]. Currently, one of the most advanced quantum circuits are based on superconducting quantum bits (SC qubits). Recently, it has been shown that SC qubits could be built much more compact exploiting exfoliated $NbSe_2$ and hBN crystals [2]. Although exfoliation and layer transfer seem currently to be the state-of-the-art method to achieve the best performing devices, exfoliated flakes cannot be used in wafer-scale production.

Despite significant advancements in wafer-scale epitaxial growth of transition metal dichalcogenides [3] by chemical vapor deposition (CVD) not as much progress has been achieved for 2D-$NbSe_2$. A particular challenge is that $NbSe_2$ is chemically reactive in ambient conditions typically leading to the degradation of the surface [4]. Alternatively, physical vapor deposition (PVD)-methods could be applied to fabricate thin films of 2D-materials. Lin et al. [5] has demonstrated that $NbSe_2$ could withstand ambient and even harsher environments unharmed, as long as $NbSe_2$ was "never" exposed to oxygen during growth. Here, we will present first results in our quest to grow in-situ hetero-stacks comprising of $NbSe_2$ and $MoSe_2$ layers to provide the material for 2D-material based SC qubits. We are exploring a PVD-approach to grow $NbSe_2$ thin films on glass and sapphire substrates. Figure 1 schematically illustrates our deposition process. In the first stage, Niobium is deposited in a PVD chamber by an electron beam evaporator. In the second stage, the as-grown Nb-film is transferred in the selenization chamber without breaking the vacuum to modify it to $NbSe_2$. Our grown films were characterized by Raman, AFM and EDX. AFM-results indicate that even growing at high substrate temperatures the films are typically nano-crystalline.

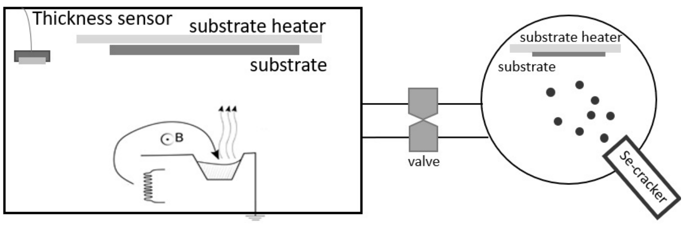

Figure 1. Schematic illustration of deposition chambers.

References

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