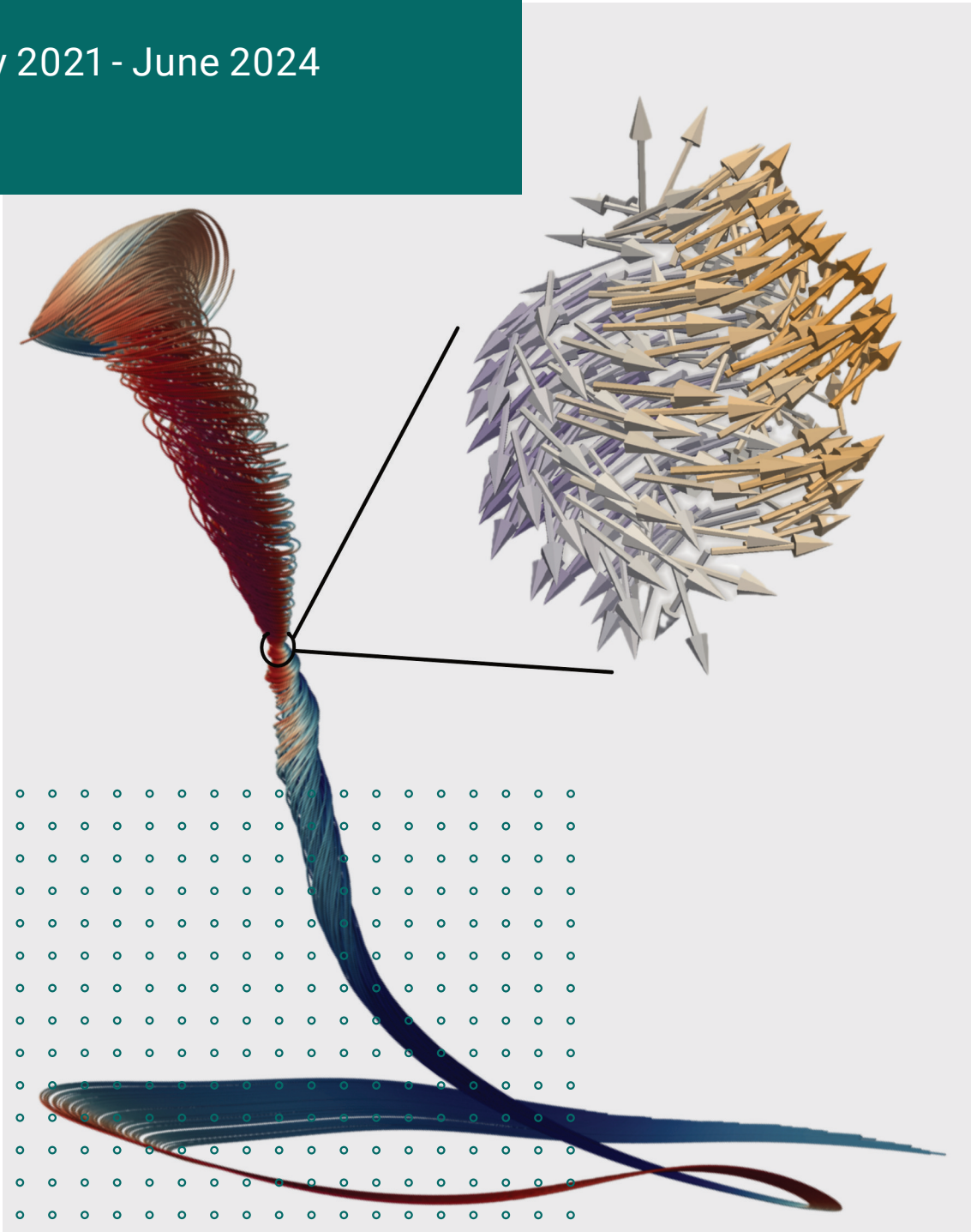




# STATUS REPORT

May 2021 - June 2024





**Max-Planck-Institut für Chemische Physik fester Stoffe**

**Max Planck Institute for Chemical Physics of Solids**

Nöthnitzer Str. 40, 01187 Dresden, Germany

## **Status Report**

May 2021 – June 2024

### **Institute Mission and Profile**

The core scientific goal of our Institute is to work at the forefront of modern solid-state chemistry and physics, and in particular to profit from strong interactions between departments to advance the interface of the two fields. By maintaining an open, collaborative atmosphere with minimal inter-group barriers, we profit from interdisciplinary expertise at a number of levels. Major open questions of particular interest to us include: understanding the interplay of topology and symmetry in modern materials; the identification and study of giant response functions at phase boundaries in materials at the borderline of standard metallic behavior; understanding the chemical nature and electronic structure of intermetallic and correlated materials through experimental, theoretical and computational investigations. Physicists and chemists are also encouraged to work together on the creation of new materials and the refinement of existing materials to world-leading levels of purity at which entirely new collective phenomena can emerge. Although we always strive to advance our in-house expertise, we also aim to be outward-facing, and maintain a network of collaborator groups, of appropriate quality, throughout the world.

Cover: X-ray magnetic tomography dataset reveals the structure of three-dimensional magnetic vortices, and singularities of the magnetisation.

<https://www.nature.com/articles/nature23006>

## IMPRESSUM

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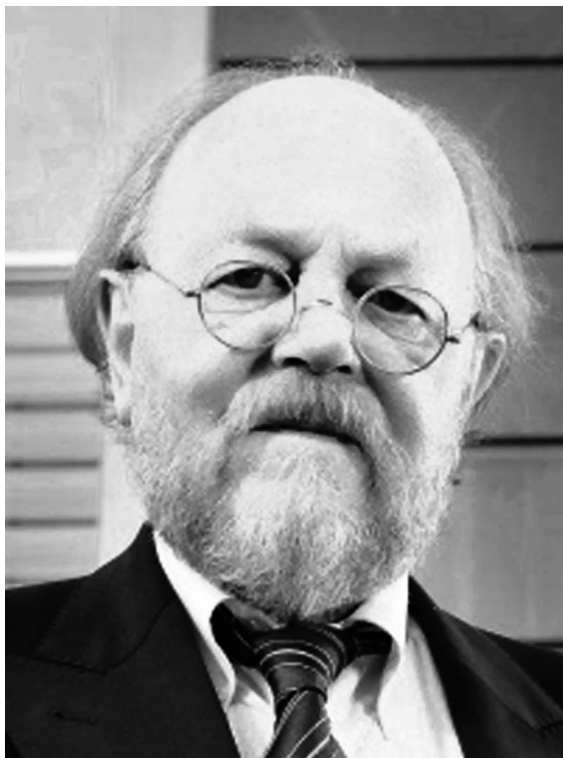
Peter Adler, Andrew P. Mackenzie, Petra Nowak, Helge Rosner, Claudia Schirmer, Liane Schröder, Ulrich Schwarz, Oliver Stockert, Liu Hao Tjeng, Ina Werner, Steffen Wirth

Web version adapted from the printed version of the status report

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**Prof. Dr. Dr. h.c. Rüdiger Kniep (\* 2 May 1945, † 26 October 2024)**



It is with great sadness that we have to announce the passing of Prof. Dr. Dr. h.c. Rüdiger Kniep, Emeritus Director of our institute.

Rüdiger Kniep was one of the leading experts in solid-state chemistry, who set new standards with his scientific research. He left a lasting mark on our Institute through his work and tireless commitment until his retirement in 2012. His pioneering spirit in building up the institute – he took up his post shortly after its founding – was both inspiring and motivating to our many employees.

Prof. Kniep's research field was interdisciplinary between chemistry, physics and materials science. This knowledge allowed him to synthesize new classes of compounds and materials with new chemical and physical properties, especially in metal-rich systems. His work on biorelevant systems has even found practical application. The scientific importance of Prof. Kniep is also reflected in the large number of awards he received.

For many of us, he will remain unforgotten as a mentor, supporter, and esteemed colleague. Our thoughts are with his family in these difficult times.

In silent remembrance

Claudia Felser, Juri Grin, Andy Mackenzie, Frank Steglich, and Hao Tjeng  
as well as all employees of the MPI CPfS



## Structure and Content of this Status Report

In the opening section 1 of this Report we provide an overview of the central theme of our work: our research activities and achievements. Each of the four departments: C. Felser, A. Mackenzie, L.H. Tjeng, and J. Grin; the Lise Meitner group of C. Donnelly, the MPRG of U. Vool, the Minerva / Boehringer Ingelheim group of E. Svanidze, and the Minerva / Schmidt group of B. Goodge; the work of the emeritus director F. Steglich, and the Max Planck Fellowship groups of M. Ruck, L. Molenkamp, J.C.S. Davis and since 2023 E. Hassinger are described in separate sections. Collaborative (inter-departmental/group) research is strongly encouraged in our Institute, so we highlight selected joint ventures in section 1.14.

In section 2 we describe the administrative and organizational structures that underpin this science, and some more summary performance statistics. Our aim was to keep this as brief as possible, and cross-reference to the more extensive set of data provided in the Addendum. In addition, we will provide (confidential) ‘Data, Facts, and Figures’ about personnel and finances during the Scientific Advisory Board site visit in February 2025. We cover all the points raised in the ‘Rules for Scientific Advisory Boards and Guidelines for Evaluation (2023)’ document of the Max Planck Society, but have altered the order from the one given there.

Rather than providing a comprehensive report on our scientific activities in a paper document running to hundreds of pages, we have striven to keep our written reporting concise and selective, concentrating on what we rate as our research highlights. The fuller background information is still available through longer reports that can be accessed from links in our main report, either on-line or using the USB drive appended to the back of the report booklet. In this way, we hope to ease the work of the readers, giving them access to the details, but only if they wish to read them.



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# 1. Institute's Research Program and Departments' Research Areas

## 1.1 Topological Quantum Chemistry

Director: Claudia Felser<sup>#</sup>

Group leaders: Sushmita Chandra, Erjian Cheng, Xiaolong Feng, Maia G. Vergniory, Jianfeng Ge, Edouard Lesne, Sergey Medvedev, Fabian Roman Menges, Yu Pan, Walter Schnelle, Chandra Shekhar, Xia Wang

The primary objective of the Topological Quantum Chemistry department is the design, synthesis, and physical characterization of innovative quantum materials with topological properties [1]. While the topological materials database serves as a crucial tool in discovering new stoichiometric materials, we have rigorously validated these predictions through experimental implementation. Notable examples of successfully realized topological quantum materials (TQMs) that have set new trends in condensed matter physics, resulting in numerous high-impact publications, include  $\text{Mn}_3\text{Ge}$ ,  $\text{Mn}_3\text{Sn}$ ,  $\text{Co}_2\text{MnGa}$ ,  $\text{Co}_3\text{Sn}_2\text{S}_2$ ,  $\text{Mn}_{1.4}\text{PtSn}$ ,  $\text{PdGa}$ ,  $\text{PtAl}$ ,  $\text{CoSi}$ , and  $\text{Ta}_8\text{Se}_8\text{I}$ . The first five compounds combine magnetism and topology [2], while the latter four blend chirality and topology, both key research areas for our team. Heusler compounds, a long-standing focus for over 25 years, are particularly significant, and our new insights into the hexagonally distorted versions of  $\text{Mn}_3\text{Sn}$  and  $\text{Mn}_3\text{Ge}$  have initiated two major global research directions: topological antiferromagnets with Berry curvature and metallic Kagome compounds.

Our research has concentrated on three highly interconnected areas: (i) advancing the study of magnetic topological materials, (ii) exploring the deep interconnections between chirality and topology, extending even beyond solid-state science, and (iii) investigating quantum effects at the boundary between 3D and 2D materials. At the core of topology in condensed matter systems are chiral electron states in the bulk, on surfaces, and at edges, where the spin and momentum of electrons are locked parallel or antiparallel to one another. Magnetic and non-magnetic Weyl semimetals,

for example, exhibit chiral bulk states that have enabled the realization of predictions from high-energy physics and astrophysics, such as the chiral anomaly, the mixed axial-gravitational anomaly, and axions.

With access to a diverse collection of unique crystals, we can explore their chemical, physical, and quantum properties through various transport measurements, including non-linear transport and light-matter interactions. Additionally, we can utilize these crystals as substrates for asymmetric absorption and catalysis, as shown in Figure 1.

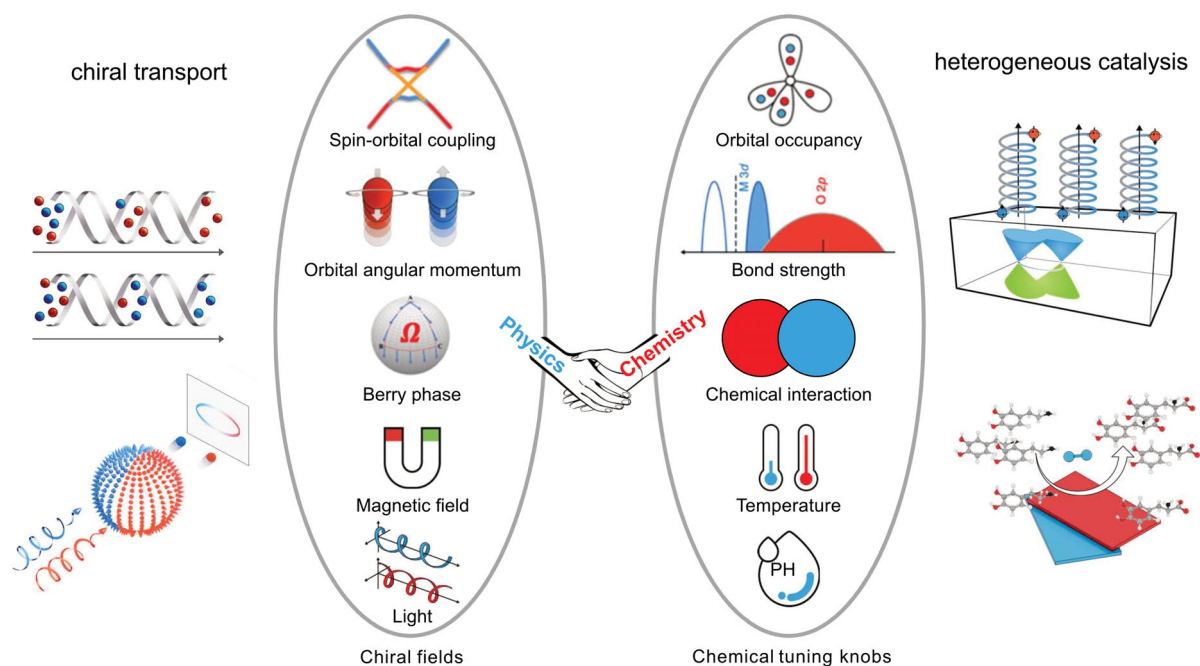
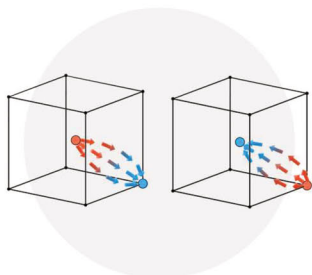
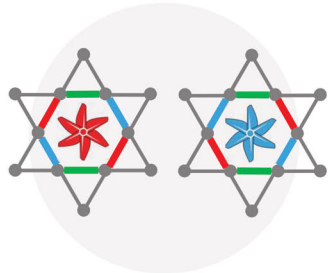


Fig. 1: The effect of chiral fields and chemical tuning on chiral transport and heterogeneous catalysis.

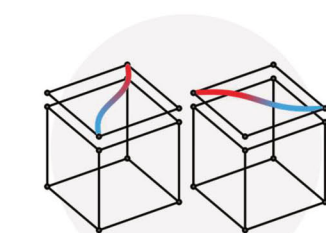
chirality in geometric phases



chiral charge density waves

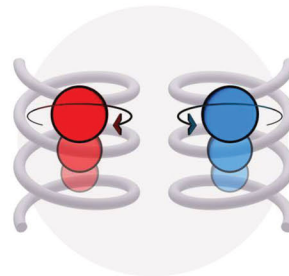


chiral structure and chiral spins



chiral surface states

chiral electrons



chiral phonons

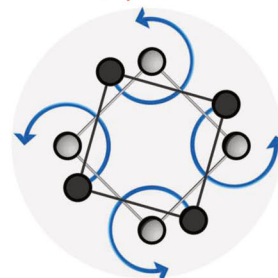


Fig. 2: The role of chiral fields on homochirality, chiral structure and chiral spins and the relation to the symmetry of the electrons, phonons, Berry phase, surface state and electronic instability.

Our research focuses on several key questions: How can we control chiral matter and the handedness of chiral molecules and solids? Is it possible to transfer chirality between different systems, such as from chiral electrons or chiral charge density waves to structural chirality? Or can we even understand the role chiral field on homochirality, connecting chirality as a quantum number to other chiral phenomena across different areas of science, including the asymmetry of matter and antimatter and the homochirality of life [3]?

A central challenge in chiral chemistry is that enantiomers often have indistinguishable physical properties. But current approaches lack sufficient tunability, limiting our understanding of the underlying mechanisms for homochirality and chiral molecule-matter interactions. In solid-state systems, the translation symmetry and corresponding  $k$ -space offer new opportunities beyond what is known from molecular systems. Topological materials, for instance, present not only structural chirality and chiral spin arrangements but also chiral surface states, chiral charge density waves, chiral electrons and phonons, and geometric phases such as the Berry phase (see Figure 2). As a research group operating at the intersection of chemistry and physics, we have the advantage of a wide array of tools, both chemical and physical, to fine-tune and investigate the properties of these materials (see Figure 1).

The foundation of our research in chirality and topology lies in the synthesis of high-quality homochiral crystals. However, achieving this, especially for inorganic crystals synthesized at high temperatures, remains an unresolved challenge. Over the past three years, we have successfully grown chiral crystals exhibiting homochirality using methods such as the laser floating zone furnace and Czochralski techniques, which rely on a seed crystal of the desired chirality. Nonetheless, it would be advantageous to explore whether chirality can be controlled or even altered during the growth process.

One promising approach is the use of chiral light, as the sensitivity of chiral crystals to such radiation suggests it could effectively control or modify handedness. A key experiment we plan to conduct, in collaboration with UC Santa Barbara, involves utilizing circularly polarized laser light to alter the handedness of a homochiral crystal during growth.

In contrast, the chemical vapor transport (CVT) and flux growth techniques have produced crystals with mixed handedness within the same batch or even in one crystal. To overcome this limitation, we are experimenting with alternative methods, such as the use of chiral transport agents, magnetic fields or other chiral fields and forces, and chiral fluxes, to improve control over the chirality of the crystals formed (see Figure 1).

## Topological Chiral Crystals

We have made significant progress in identifying the unique properties of chiral topological crystals, which can host higher-spin generalizations of Weyl quasiparticles, known as multifold fermions. These fermions have no high-energy counterparts. In each homochiral crystal, two multifold Weyl points appear at different energies, each characterized by distinct signs of large Chern numbers. These are accompanied by extensive chiral surface states, or Fermi arcs, that span the entire Brillouin zone. Theoretically predicted properties of these crystals have been confirmed in materials like PdGa and PtAl [4, 5]. Ideally, the quantized photogalvanic effect could also be observed, and preliminary evidence for this has emerged from a collaboration with UC Berkeley. Chiral topological crystals are also predicted to host orbital angular momentum monopoles, with spin-momentum locking around Weyl points [4, 5]. All these phenomena were recently confirmed in collaboration with Niels Schröter's team.

Despite the high conductivity of these crystals, making it challenging to measure intrinsic topological transport properties, we have succeeded in observing the chiral anomaly of multifold fermions in CoSi. This was achieved by working with Gotsmann's team, where a multi-terminal Hall bar was fabricated from a bulk single crystal using focused ion beam (FIB) techniques. Now that we have an FIB available within our own team, we have new opportunities to further investigate non-linear transport properties and quantum effects in the future.

For further reading see report [TQC\\_05\\_Shekhar](#).

## Topological Quantum Materials for Heterogeneous Catalysis

Topological catalysis leverages the unique interplay of spin, orbital, and topological properties in topological quantum materials to enhance catalytic reactions through unconventional quantum phenomena. The topological surface states of these materials, protected by time-reversal symmetry, are highly resilient to defects and impurities, while strong spin-orbit coupling locks electron spin to momentum. This precise control enables enhanced catalytic reactions such as hydrogen evolution (HER), oxygen evolution (OER), and oxygen reduction reaction (ORR). Additionally, the Berry phase amplifies charge carrier mobility and reactivity, while orbital angular momentum can be harnessed to generate chiral currents, offering potential applications in asymmetric synthesis. This dynamic responsiveness

enables real-time control over catalytic processes, paving the way for the design of smart, adaptable catalysts that can optimize reaction pathways and maintain high efficiency across varying conditions. Ultimately, topological catalysis presents a promising frontier for the development of next-generation catalytic systems.

Together with Bernevig's team we have developed a novel approach to identify efficient catalysts by locating active sites in crystalline materials with obstructed atomic insulators (OAI) that display metallic obstructed surface states (OSSs). Unlike traditional methods that modify surfaces for catalytic activity, this approach utilizes symmetry-protected OSSs, inherently present in certain materials, as active sites. Applying this method, 465 potential high-performance catalysts were identified, offering a streamlined way to design catalysts for various chemical reactions, such as water splitting and fuel cells. [6]

Recently Wang's team has focused on improving the efficiency of water splitting, a process crucial for clean energy production, by addressing a challenge known as the oxygen evolution reaction. The slow OER is caused by difficulties in the electron transfer process, which is influenced by the spin of electrons. The team explored materials called topological chiral semimetals (RhSi, RhSn, and RhBiS) that have unique electronic properties, specifically spin-polarized surfaces, to enhance this process. By using these chiral semimetals, the researchers managed to boost the spin-dependent electron transfer and overcome the performance limitations of conventional catalysts. They found that the strength of spin-orbit coupling (SOC), a key property linked to the material's ability to control electron spin, increases in the order of RhSi < RhSn < RhBiS, which directly correlates with improved OER performance. Among the materials studied, RhBiS showed exceptional performance, outperforming the widely used RuO<sub>2</sub> catalyst by over 100 times (see Figure 3) [7].

By applying electric or magnetic fields to TQMs, the energy levels of topological surface states can be modulated, inducing spin textures that further enhance catalytic activity, particularly in radical-driven reactions like CO<sub>2</sub> reduction.

The synthesis and separation of homochiral molecules present a significant challenge, as distinguishing between enantiomers requires a chiral catalyst or chiral light. However, due to the distinct Berry curvature and momentum-space (k-space) characteristics of the different enantiomers in our crystals, we may not only observe new transport and optical phenomena but also ad-

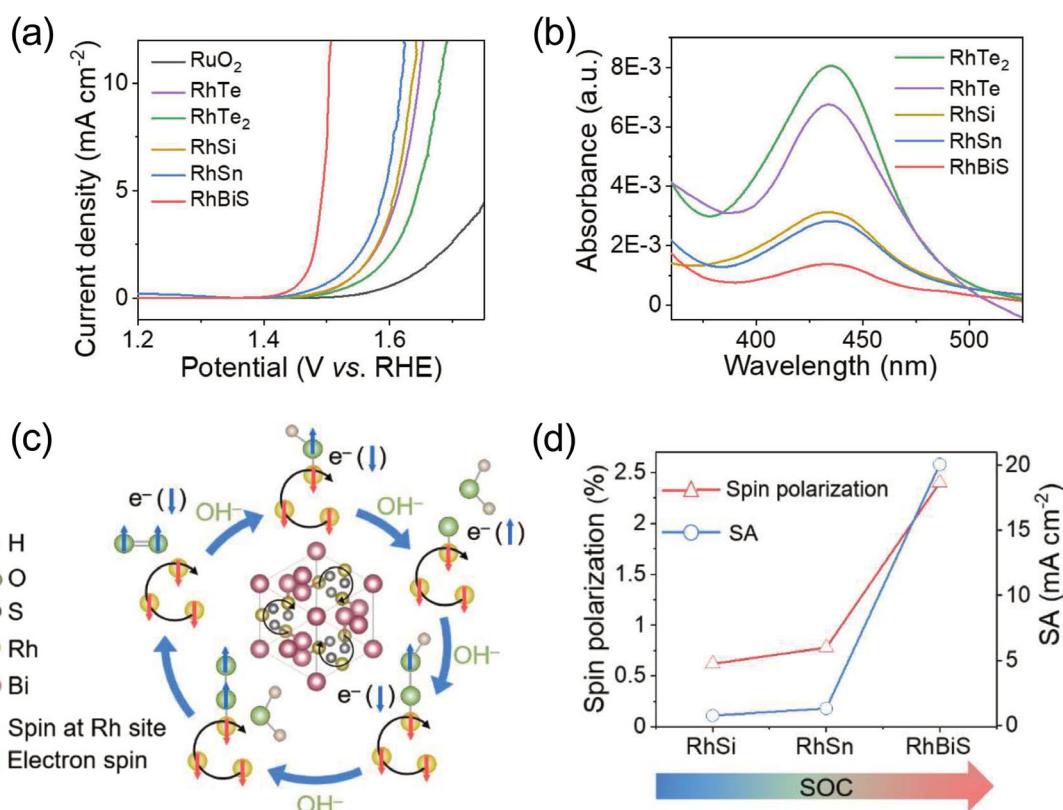


Fig. 3: (a) Catalytic activity of the topological chiral semimetals RhSi, RhSn and RhBiS. (b) The H<sub>2</sub>O<sub>2</sub> production is reduced and (c) Spin-polarization mechanism of the OER (d) The calculated spin polarizations (left axis) and corresponding specific activities (right axis) in the chiral crystals.

dress these challenges by providing a robust platform for asymmetric catalysis and molecular recognition.

Our first investigation on enantioselective processes has focused on PdGa homochiral single crystals, where distinct chiral lattice structures enable selective recognition of DOPA enantiomers via orbital angular momentum (OAM) polarization. The OAM is proportional to the Berry phase and therefore an indirect measure of the topology. PdGa crystals exhibit significant OAM polarization near the Fermi level, which differs based on crystal chirality, affecting the adsorption energies and bonding with DOPA enantiomers. This study suggests that OAM polarization in inorganic crystals could be a key factor in the natural development of homochirality and could open pathways for creating more efficient enantiomeric reactions [8].

Our future objective is to systematically explore the interactions between chiral crystals and chiral molecules, elucidating the underlying physics that govern these interactions. To achieve this, we will manipulate specific chemical and physical control parameters – such as electronic band structures, Berry curvature, spin dynamics, and electronic interactions (see Figure 1) – and correlate them with enantioselective molecule-matter interactions,

including adhesion, charge transfer, and spin transfer. For further reading see report [TQC\\_04\\_Wang](#).

### Topology and Crystalline Symmetry

Theory remains a crucial starting point for identifying materials with the desired quantum properties. However, only a few oxides are currently known to be topological, largely due to the limitations of density functional theory. To address this challenge, Vergniory's team has taken two approaches. First, they began incorporating correlations into the TCQ framework. Second, recognizing the structural similarities between Heusler and double perovskites, they systematically investigated these materials, leading to Chandra's team synthesizing several promising candidates. Another new direction explored was the study of topological properties of phonons in condensed matter systems. This approach proved particularly valuable when examining structural instabilities in the Kagome lattice and other systems.

Looking ahead, we will continue collaborating with Vergniory and Bernevig, with a new focus on 2D materials and the design of novel properties through twisting. For further reading see report [TQC\\_02\\_Vergniory](#).

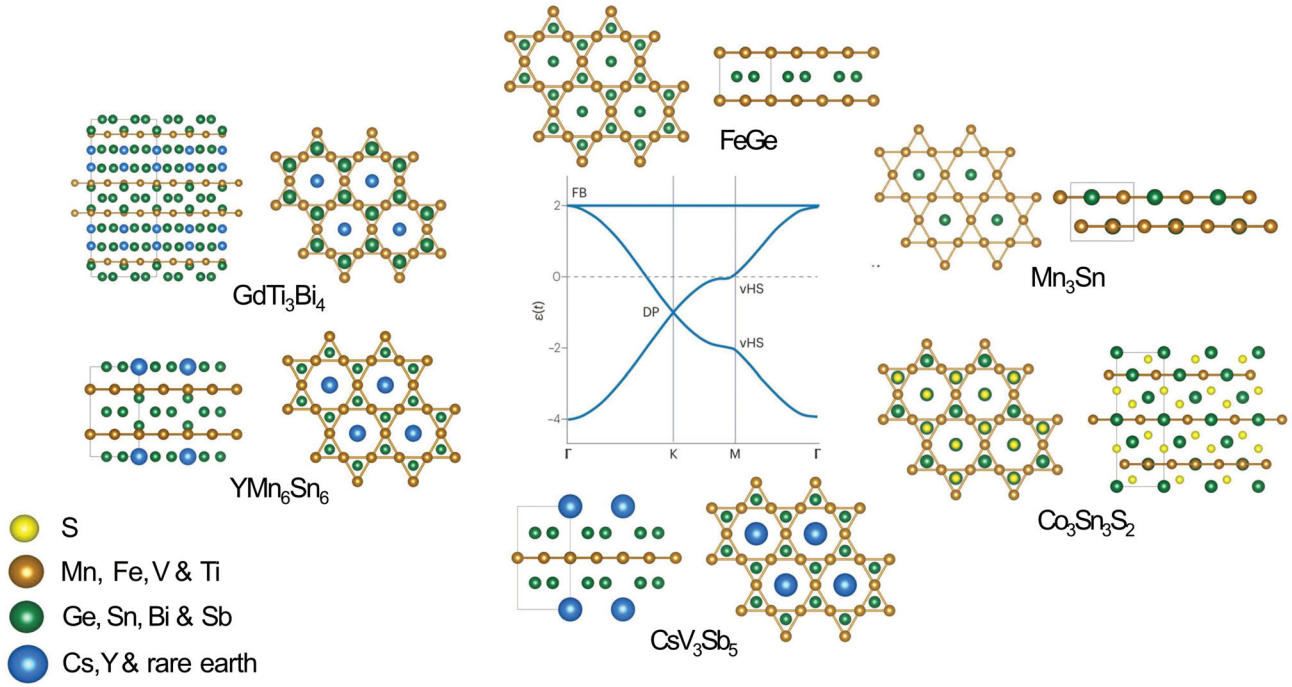


Fig. 4: Families of Kagome lattices, with transition metals as Kagome building blocks.

## Kagome Compounds

With  $\text{Mn}_3\text{Ge}$  and  $\text{Co}_3\text{Sn}_2\text{S}_2$  we have started the field of metallic and semi-metallic Kagome compounds. The Kagome lattice is of special interest, since it hosts van Hove singularities, Dirac or Weyl points and flat bands in their electronic structure and it is observed in a versatile family of crystal structures open nearly infinite tuning possibilities (see Figure 4). Flatband (FB) represents a highly degenerate dispersionless electronic state, and if located close to the Fermi energy, enables various emerging quantum phenomena, such as the high-temperature quantum Hall effect, fractional Hall effect, quantum anomalous Hall effect, unconventional superconductivity, unconventional magnetism such as non-collinear magnetism, charge density wave (CDW) instabilities, and other correlated effects might occur [9]. In twisted graphene and in Kagome lattices such flat bands were realized and several of the predicted physical effects were already observed. By leveraging solid-state chemistry, new Kagome materials, including superconductors, can be identified. A recent study used high-throughput DFT calculations on 293 Kagome compounds, revealing that 166 are stable, while others show phonon instabilities hinting at potential structural transitions. The introduction of magnetic order can eliminate some of these instabilities. In some cases, spin-phonon coupling is suggested as a cause for phenomena like CDW transitions, as seen in  $\text{FeGe}$ . The  $\text{LnTi}_3\text{Bi}_4$  family

also draws attention for its magnetic properties and coupling between magnetism and CDW behavior, particularly in  $\text{TbTi}_3\text{Bi}_4$ . This compound demonstrates magnetic plateaus and strong spin-charge coupling, although the underlying mechanisms still require investigation.

For further reading see report [TQC\\_03\\_Feng](#).

Motivated by the cascade of electronic instabilities in the Kagome lattice, the team grew single crystals of the superconductor  $\text{CsV}_3\text{Sb}_5$  and joined forces with physicists to explore whether the charge density wave instability in a charge density wave system could be controlled by external fields [10]. Typically, chiral transport – in which the electrical properties change depending on the “handedness” of the material – only occurs in materials whose atomic structure has no mirror symmetry. However, the team discovered a new way to control chiral transport in the Kagome metal  $\text{CsV}_3\text{Sb}_5$ , which has a symmetrical structure. At very low temperatures (below 35 K), they observed a strong chiral response when a magnetic field was applied in the plane. The handedness of the material's transport properties was simply changed by reversing the magnetic field. Recently, other materials with chiral charge-density wave instabilities have been identified, even at room temperature. The possibility of switching chirality in materials by external forces is an exciting idea, as it could lead to new possibilities in asymmetric chemistry and electronic devices. For further reading see report [TQC\\_02\\_Vergniory](#).

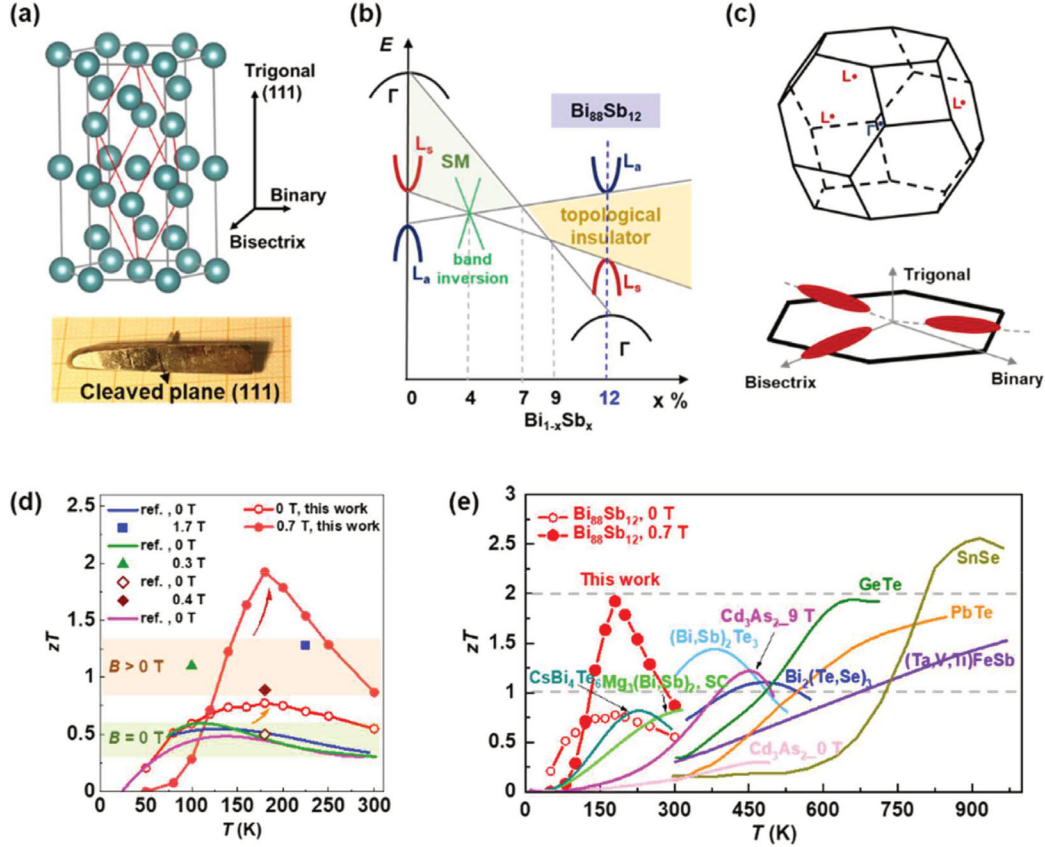


Fig. 5: High-performance single-crystalline  $\text{Bi}_{88}\text{Sb}_{12}$  alloy as thermoelectric material with improved properties under a magnetic field [12]

### Pressure-Induced Superconductivity in Topological Materials

Pressure can significantly alter the electronic band structures of the Kagome materials, influencing their behavior, as observed in  $\text{AV}_3\text{Sb}_5$  and  $\text{ScV}_6\text{Sn}_6$ . While in the past years our superconductivity research was mostly centered around transition-metal chalcogenides under high pressure, now materials with layered but also clearly three-dimensional structures with flat bands have come into focus. Several compounds with Kagome structure layers and rare-earth were already investigated by members of our group in this respect and we plan to extend research to some new Ni- and Cr-based systems and their high-pressure phases. It is well known that flat bands and van Hove singularities lead sequences of various ordered electronic states, however the role of dispersion remains to be investigated in more detail

We participate in the new consortium together with Bernevig, Millis etc. (SuperC) devoted to the finding of new candidates for superconductors with high critical temperature by high-throughput DFT and phonon calculations combined with machine learning. Our group, besides the Kagome materials, targets for the synthesis and investigation of Laves,  $\text{AlB}_2$ - and

$\text{ThCr}_2\text{Si}_2$ -type structure superconductors, which are of more three-dimensional character. In the last decade superconductivity has been discovered in compounds with large amounts of magnetic elements like Cr, Mn and Fe and we think there is potential to find more compound superconductors with such usually avoided elements at high pressure. Moreover, light-element compounds and their possibly superconducting phases at high pressure up to 100 GPa are of interest.

For further reading see report [TQC\\_08\\_Schnelle](#).

### Topological Materials for Thermoelectrics

Topological semimetals and insulators play a vital role in thermoelectrics. The interaction between magnetic properties and non-trivial band structures gives rise to exotic effects like substantial anomalous Hall conductivity (AHC), the topological Hall effect (THE), a large anomalous Nernst effect (ANE), and enhanced Seebeck effect in magnetic fields. Spin-orbit coupling and crystal symmetry are key to these phenomena. Our research shows significant AHC in materials with multiple mirror planes, such as Heusler compounds, which also have strong spin-orbit coupling. In single crystals, Berry curvature effects align well with experimental data.

Unlike traditional thermoelectric devices relying on the Seebeck effect, Nernst devices operate with a simpler transverse geometry. Antiferromagnets, previously thought to lack ANE due to their zero net magnetic moment, were recently found to exhibit ANE via Berry phase effects. This discovery was made in the antiferromagnet  $\text{YbMnBi}_2$ , where ANE values surpassed those in ferromagnets [11], revealing new potential for converting waste heat to energy. In the Kagome antiferromagnet  $\text{YMn}_6\text{Sn}_6$ , a large anomalous transverse thermoelectric effect ( $\approx 2 \mu\text{V K}^{-1}$ ) at room temperature, comparable to ferromagnets, was observed, attributed to Berry curvature near the Fermi level. In multiband topological semimetals, a large ordinary Nernst signal is expected, as seen in  $\text{WTe}_2$  and  $\text{TaAs}_2$ . The most exciting results come from the Weyl semimetal  $\text{Bi}_{88}\text{Sb}_{12}$ , which shows linear band dispersion and a strong magneto-Seebeck effect, with a dimensionless figure of merit ( $zT$ ) exceeding 2 in a magnetic field (see Figure 5). Pan's team discovered that applying a small magnetic field (less than 1 Tesla) to  $\text{Bi}_{88}\text{Sb}_{12}$  single crystals significantly enhanced their thermoelectric performance [12]. Specifically, they observed a high thermoelectric figure of merit ( $zT$ ) – a measure of efficiency – with values of 0.7 at 150 K (with no magnetic field), 1.9 at 180 K (with 0.7 Tesla), and approximately 1 at room temperature (300 K, with 1 Tesla). This improvement was due to the high mobility of electrons and a quantum effect called weak antilocalization, which helps reduce heat transfer while boosting electricity generation. Our finding shows that low magnetic fields can enhance thermoelectric performance in topological materials, making them more efficient at generating electricity from heat. Our approach can also be applied to other topological materials with similar electronic properties, opening new avenues for thermoelectric technology development.

Further reading: [TQC\\_06\\_He](#), [TQC\\_07\\_Shekhar](#).

### Quantum Materials in Reduced Dimensions

Beyond the synthesis of high-quality single crystals and using chemical and physical methods to discover new properties, reduced dimensions and designed interfaces offer unique opportunities to explore quantum and topological phenomena, relying on surface and interface states, as well as quantum confinement. The thin film lab, with expertise in magnetron sputtering of Heusler compounds, has expanded into molecular beam epitaxy, working on Half-Heusler and  $\text{Bi}_2\text{Se}_4$  films doped with magnetic ions to investigate quantum effects like the quantum spin and anomalous Hall ef-

fects. Future projects include Josephson devices with topological superconductors, leveraging new tools like the focused ion beam (FIB) for fabricating mesoscopic devices.

Exfoliation of van der Waals materials offers a promising avenue for studying the transition from 3D to 2D quantum Hall effects and creating artificial chiral materials for catalysis. Misfit layer compounds (MLCs), similar to twisted bilayer graphene, feature lattice mismatches that lead to Moiré patterns, and their potential applications span optoelectronics, catalysis, and energy storage. However, nanodevice fabrication using these crystals remains challenging. Topological semimetals like  $\text{ZrTe}_5$ , bismuth, graphite, and  $\text{YPtBi}$  show intriguing quantum Hall features, though their mechanisms are not fully understood. Recent studies have demonstrated promising results in the quantum anomalous Hall effect (QAHE) in some magnetic-element-doped topological insulators, with the goal of achieving it in bulk at higher temperatures. Researchers have also found evidence of anomalous Hall quantization in 3D magnetic compounds at temperatures in the tens of Kelvins, which could bridge the gap to high-temperature QAHE in thin films.

For further reading see report [TQC\\_09\\_Lesne](#).

### Photoemission and Tunneling Spectroscopy of Topological Materials

ARPES and STM are crucial for investigating the electronic structure of topological materials, particularly topological semimetals, which offer untapped physics. In the past we have performed ARPES measurement within our group but also in collaboration with Schröter and others. One example investigated by our team is  $\text{NbGe}_2$ , a superconducting material below 2 K with a chiral crystal lattice that hosts Kramers-Weyl fermions. ARPES has revealed chiral surface states, supported by band structure calculations, suggesting  $\text{NbGe}_2$  is an ideal platform for studying the interplay of chirality, topology, and superconductivity. Our current focus involves analyzing the band structures of these materials using ARPES and STM, but future research will emphasize their exotic quantum states.

Jacky Ge has joined the team as an independent group leader and an expert using STM to investigate topological superconductors. Topology coupled with superconductivity, these materials hold promise for error-resistant quantum computing. A key challenge in topological superconductivity is detecting Majorana quasiparticles, vital for quantum computing. Although elusive, new methods like local shot noise spectroscopy

offer a promising approach. This technique analyzes effective charge during tunneling to identify Majorana signatures. We recently used it with STM to image noise in the vortex lattice of NbSe<sub>2</sub>, aiding the study of pairing symmetries. Chiral topological superconductors may also host electron multiplets (quartets and sextets), leading to novel charge-4e and charge-6e superconductivity, which can be detected via shot noise spectroscopy.

For further reading see the report [TQC\\_10\\_Ge](#).

### Light-Matter Interaction and Topology

The Topological Quantum Chemistry department is advancing research on light-matter interactions, focusing on photoinduced magnetotransport and the novel use of laser-based techniques to probe topological transport phenomena. A key experiment involves ZrTe<sub>5</sub> crystals, where photovoltage maps revealed intricate spatial patterns, shedding light on how light affects topological materials. The group of Fabian Menges developed a cutting-edge experimental setup that uses cryogenic confocal laser scanning microscopy, allowing detailed visualization of transport dynamics in topological semimetals. This research emphasizes the open-system perspective in studying magneto-transport properties, particularly in non-homogeneous crystals, which challenge conventional closed-system models. Future work aims to explore hybridization of chiral fermion states and topological electromagnetic modes, broadening the understanding of quantum phases in topological materials.

For further reading see the report [TQC\\_01\\_Menges](#).

Our research aims to explore groundbreaking questions surrounding chirality and quantum materials. A central challenge is controlling chiral matter and understanding how handedness transfers between systems – such as from chiral electrons or charge density waves to structural chirality. These directions promise to reveal novel links between quantum phenomena and chiral fields, laying the groundwork for innovations across various scientific disciplines. The potential to connect

chirality as a quantum number to other chiral phenomena – ranging from the matter-antimatter asymmetry to life's homochirality – positions topological materials at the forefront of research.

Additionally, our research will focus on uncovering new quantum effects in reduced dimensions, especially at the intersection of 3D and 2D materials. Looking ahead, we will further expand into areas such as catalysis and reduced-dimensional studies to deepen our understanding of these complex systems.

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## 1.2 Physics of Quantum Materials

Director: Andy Mackenzie<sup>#</sup>

Group Leaders: Michael Baenitz, Manuel Brando, Ashley Cook, Elena Gati, Berit Goodge, Clifford Hicks<sup>†</sup>, Michael Nicklas, Hilary Noad, Helge Rosner, Veronika Sunko<sup>&</sup> and Haijing Zhang

**The goal of the Physics of Quantum Materials department is to perform work of lasting significance across the interlinked theme of unconventional behavior in superconductivity, electrical transport and magnetism, working wherever possible with materials of extremely high purity. A second key focus is the development of apparatus and experimental protocols that open new frontiers of investigation, both for us and for the field as a whole. We collaborate strongly within the department and broader institute, but also across the world. We perform many aspects of our work jointly with leading theory groups, to advance understanding as efficiently as possible.**

In the following pages we will outline our main achievements in the census period of May 2021 – June 2024 inclusive, but we begin by mentioning some particular highlights:

1. The demonstration and development of two new methods to probe the elastic properties of electronic matter at large uniaxial pressures. The first, the a.c. elastocaloric effect, was invented at Stanford University using uniaxial pressure cells introduced by our group, but we used it to perform the first extensive study of an unconventional superconductor, working at unprecedented levels of thermal precision [1]. The second, the measurement of the stress-strain relationship through a Lifshitz transition, was entirely our own development, and resulted in us making the first convincing observation of a conduction-electron-driven lattice softening first considered theoretically by Lifshitz over sixty years ago [2].

2. Using these and other thermodynamic measurements under high uniaxial pressure to essentially disprove the hypothesis that signatures of time reversal symmetry breaking in  $\text{Sr}_2\text{RuO}_4$  result from the behaviour of a bulk, homogeneous order parameter. Our work also sheds strong doubt on whether the bulk order parameter of  $\text{Sr}_2\text{RuO}_4$  even has two components. We believe that the significance of our findings goes beyond that of helping unravel the ‘ $\text{Sr}_2\text{RuO}_4$  order parameter mystery’ (interesting though that is in its own right). Our findings [1–5] also question whether results from muon spin relaxation and ultrasound spectroscopy are misleading the entire field of unconventional superconductivity.

3. Intense research, in collaboration with the Max Planck Fellow group of Prof. Elena Hassinger, on another unconventional superconductor,  $\text{CeRh}_2\text{As}_2$ . For this material, which was discovered in our department,

there *is* strong thermodynamic evidence for a two-component order parameter [6] (see also Perspective by A. Pourret and G. Knebel, Science 373 (2021) 962, <https://dx.doi.org/10.1126/science.abj8193>). Here, the focus has been on understanding the relationship between superconductivity, magnetism and proposed quadrupolar order [7–10].

4. Observation and understanding of new classes of non-local transport in ultra-pure delafossite metals, including the concept of ‘directional ballistics’ in resistivity, magnetoresistance, and microwave conductivity, in which Fermi surface faceting plays a dominant role [11–13]. The data also highlight the contribution of a viscous contribution to the transport, whose origin we believe we have now understood.

5. Insights into the strange metal problem, which continues to generate widespread theoretical interest but on which definitive experiments are harder to conceive. Our contributions have included a review article which we hope has helped give the field improved definition [14], transport and thermodynamic measurements on  $\text{PdCrO}_2$  [15, 16], and novel spatially-resolved diffusivity experiments on ruthenates [17].

We will expand on each of these below, setting them in the context of our broader program of research.

### 1. Thermodynamics under uniaxial pressure

*The a.c. elastocaloric effect (Gati, Nicklas, Noad, Hicks, Mackenzie)*

Thermodynamics tells us that for any material whose entropy is dependent on an external tuning parameter, there will be a caloric effect in which the temperature of a sample changes as a function of changes to the tuning parameter, if the experiment is performed under quasi-adiabatic conditions. A well-known example is

the magnetocaloric effect which is used, for example, in adiabatic demagnetization cooling. The strain equivalent is the elastocaloric effect, traditionally employed as a tool for studying materials such as shape memory alloys with a huge strain dependence of the entropy.

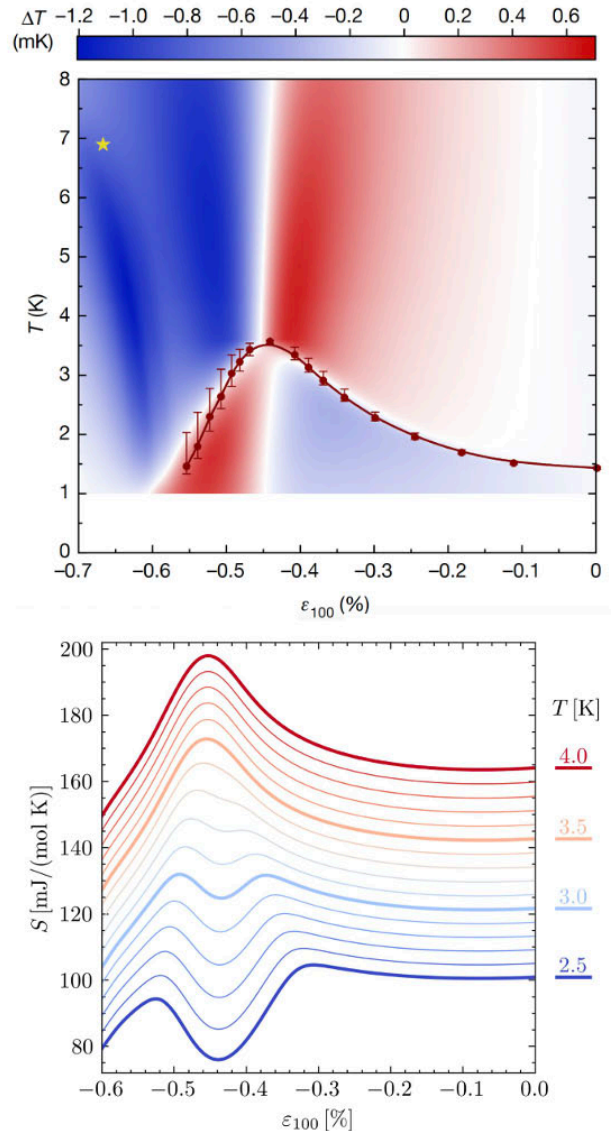
For most superconductors and quantum materials, the elastocaloric signal is predicted to be so small that applying the technique with the usual ‘d.c.’ methods is unlikely to yield high resolution information. However, our colleagues in the group of Ian Fisher at Stanford University realized that the piezo stacks that we use to apply uniaxial pressure in our Dresden-designed cells might also respond to a.c. voltages, and demonstrated that excitation at frequencies of up to 10 kHz is possible, providing a.c. pressure and strain. By locking into the temperature modulation at the excitation frequency, they demonstrated that a huge increase in sensitivity can be achieved, opening a wide range of new measurement possibilities.

A major attraction of the a.c. elastocaloric effect is its simplicity: the only quantity to measure is the a.c. temperature change. Using a low temperature transformer with a superconducting input circuit to read the voltage from a thermocouple, we achieved a measurement resolution of  $1 \mu\text{K}(\text{Hz})^{-1/2}$ , and showed that this enables the acquisition of exquisitely precise thermodynamic information from  $\text{Sr}_2\text{RuO}_4$  [1] (see Figure 1). Further, careful calibration and numerical data analysis allows determination of the full entropy landscape as a function of strain and temperature, in absolute units, with a measurement efficiency that is orders of magnitude better than that available by traditional techniques.

We believe that this is a substantial breakthrough in experimental quantum materials research, with the possibility of replacing a number of traditional methods for probing thermodynamic properties. We have already begun to apply it to heavy fermion compounds [18],  $\text{YBa}_2\text{Cu}_3\text{O}_7$  [19] and a number of magnetic systems (work in progress), and have ambitious plans to go even further.

#### **Determining stress-strain relations (Gati, Nicklas, Noad, Hicks, Mackenzie)**

While the elastocaloric effect is sensitive to first derivatives of the entropy, the elastic constants measured by stress-strain experiments are sensitive to the second strain derivative of the free energy. This means that in principle they yield more information, such as condensation energies of thermodynamic phases. The signal-to-noise ratio (at least with current measurement tech-



*Fig. 1: (Top): Raw elastocaloric data as a color plot defining the phase diagram of  $\text{Sr}_2\text{RuO}_4$ . Note the tiny experimental signal of approximately  $\pm 1\text{mK}$ , resulting from an a.c. strain of order  $10^{-6}$ . We could work to these exacting experimental demands because of  $1 \mu\text{K}(\text{Hz})^{-1/2}$  thermal precision developed for a.c. heat capacity measurements. The heat-capacity-derived  $T_c$  obtained from the same sample is shown by the dark red symbols. After years of development to obtain those data, the full phase diagram mapping by the a.c. elastocaloric effect, at higher experimental resolution, took only two weeks [1]. The yellow star shows the observation of magnetic order by muon spin rotation; the contours of the magnetic phase are seen in dark blue. (Bottom): Quantitative deduction of the entropy from the elastocaloric data, in absolute units. The conversion of the Van Hove peak in the normal state entropy to a pronounced dip within the superconducting state places strong constraints on the order parameter [3].*

nology) is much poorer than that of the a.c. elastocaloric effect, so measuring the Young’s modulus of  $\text{Sr}_2\text{RuO}_4$  across the Lifshitz transition was a challenging experiment, but one which we really wanted to try. Successfully executing it (see [2]) came with the reward of a big surprise: the huge softening at the Lifshitz transition (Figure 2). After considerable thought, as part of a collaboration with the Karlsruhe theory group that also played an important role in our elastocaloric work, we understood its origin. The basic physics had been considered by Lifshitz himself in 1960, but the size of the effect he predicted was a thousand times smaller than our observation, so this aspect of his work had been largely forgotten.

Eventually, we were able to understand the way in which two-dimensionality, high material purity and details of the electronic hopping in  $\text{Sr}_2\text{RuO}_4$  combine to give the signal we observe. The work highlights the physical utility of stress-strain measurements under elevated uniaxial pressure and work is in progress in the department to increase the signal-to-noise ratio of the experiments. Again, the fun of this project has been to go into entirely unexplored experimental territory and again, we will work intensively to extend and improve the technique in the coming years.

For further reading see the following reports:

- [PQM\\_02\\_Nicklas](#)
- [PQM\\_03\\_Gati](#)
- [PQM\\_04\\_Noad](#)

## 2. Unconventional superconductivity

### *The thorny issue of the order parameter of $\text{Sr}_2\text{RuO}_4$ (Hicks, Nicklas, Mackenzie)*

Fully understanding the superconducting state of  $\text{Sr}_2\text{RuO}_4$  remains a benchmark problem for the field of unconventional superconductivity. In the last census period we reported on our contribution to overturning the received wisdom that  $\text{Sr}_2\text{RuO}_4$  is a spin triplet superconductor. Continuing with our work on the issue, we first ruled out various proposals for mixed order parameters with modest triplet fractions [4]. Next, we carefully performed and analyzed uniaxial pressure experiments for pressures applied along each of the three principal axes of  $\text{Sr}_2\text{RuO}_4$ , attaining record pressures and experimental resolutions in the process [1, 3, 5]. Unexpectedly, our results rather strongly support a hypothesis of a single-component order parameter, and rule out nodes along the [100] direction.

We also mapped out a magnetic phase, likely to be a spin density wave, in proximity to the superconducting

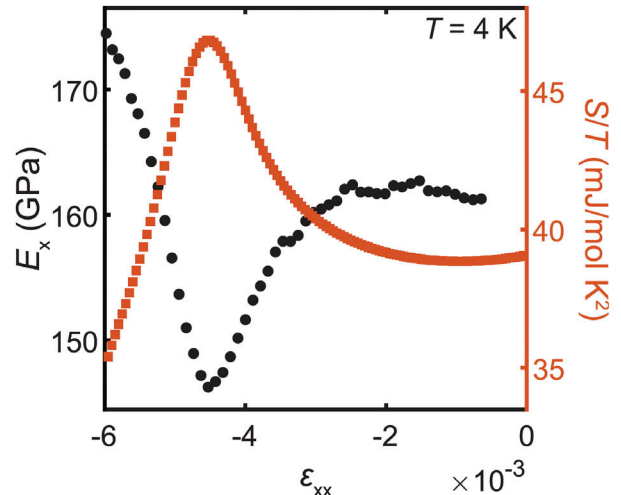


Fig. 2: Young’s modulus  $E_x$  (black dots) shows a pronounced dip, representing a lattice softening, as  $\text{Sr}_2\text{RuO}_4$  is tuned through its Lifshitz transition at 4K. Complementary entropy data (red squares) obtained from elastocaloric measurements prove that the effect is driven by conduction electrons, because filled valence bands have no electronic entropy, and the phonon contribution is negligible in  $\text{Sr}_2\text{RuO}_4$  at this low temperature [2].

dome. The simplest ‘Occam’s Razor’ interpretation of our findings is a  $d_{x^2-y^2}$  order parameter in a phase diagram similar to that of most other unconventional superconductor families. Further investigations are in progress, and will continue in the next assessment period.

Beyond its superconductivity,  $\text{Sr}_2\text{RuO}_4$  continues to surprise and delight as a platform for studies of normal state correlated electron physics in bulk [20–22] and at surfaces [23], and even shows promise as a transparent conductor [24] and a water-splitting catalyst [25]!

### *The superconductivity and correlated electron phase diagram of $\text{CeRh}_2\text{As}_2$ (Khim, Brando)*

In contrast to  $\text{Sr}_2\text{RuO}_4$ , which is nearing its 30<sup>th</sup> birthday,  $\text{CeRh}_2\text{As}_2$  is a young material, whose superconductivity was discovered in our department only a few years ago [6]. It has generated considerable attention in the community, both for its intriguing two-phase superconductivity (see Figure 3) and for the richness of the phase diagram describing the metallic state from which the superconductivity condenses. As is the case with most young superconductors, crystal quality still plays a strong role, particularly regarding the observation of magnetism and the characteristics of an intri-

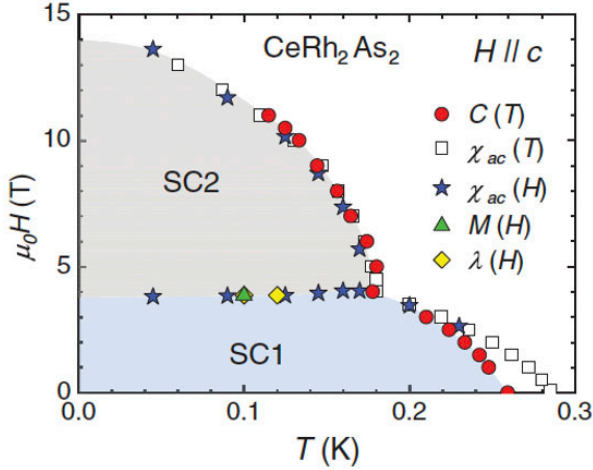


Fig. 3: The empirically-derived superconducting phase diagram of  $\text{CeRh}_2\text{As}_2$ , including thermodynamic evidence for a phase transition between the SC1 and SC2 phases. The existence of this phase boundary can be elegantly explained in terms of local inversion symmetry breaking producing two inequivalent Ce layers with Rashba spin-orbit coupling of opposite signs, but in an overall inversion-symmetric crystal in which parity remains a good quantum number [6].

going phase transition outside the superconducting state. Over the assessment period, our main focus has been on improving crystal quality and on classifying and understanding the signatures of magnetism and a proposed quadrupole density wave in the process [7–10] (see also the report of Prof. Hassinger in [section 1.10](#)). Research on this fascinating system will continue to be a focus of the department moving forward, with comparison with the physics of  $\text{UTe}_2$  [26] likely to be informative.

For further reading see the following reports:

- [PQM\\_02\\_Nicklas](#)
- [PQM\\_05\\_Brando](#)
- [PQM\\_06\\_Khim](#)

### 3. Unconventional transport

#### *Non-local transport and electrostatics in delafossite metals (Mackenzie)*

The non-magnetic delafossite metals  $\text{PdCoO}_2$  and  $\text{PtCoO}_2$ , with their astonishing in-plane mean free paths of tens of microns, offer the opportunity to access entirely new regimes of non-Ohmic electrical transport.

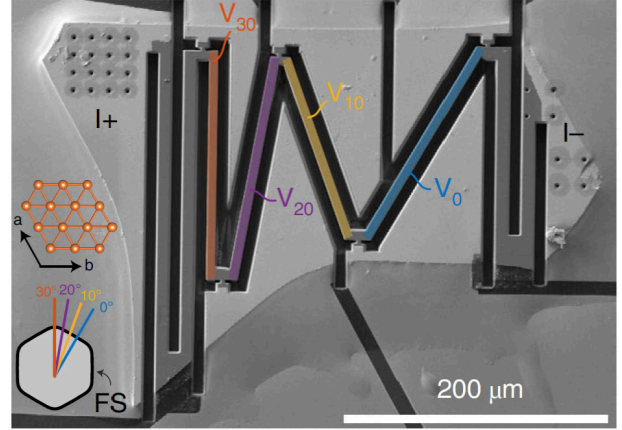


Fig. 4: The FIB-sculpted device used in an explicit demonstration of directional ballistic transport in  $\text{PdCoO}_2$ . The four color-coded tracks range from the directions subject to most ( $30^\circ$ ) to least ( $0^\circ$ ) boundary scattering. The scattering is lowest for the  $0^\circ$  orientation because  $1/3$  of the quasiparticles first injected into the track, or emerging from bulk scattering events, are moving parallel to the walls. The effect is large (at least a factor of two), and would be banned by the lattice symmetry for ohmic transport [11].

Over the assessment period, our main focus has been on classifying and understanding the phenomenon of ‘directional ballistics’, in which the electrical transport in mesoscopic devices depends on the orientation of the device relative to the directions of facets in the hexagonal Fermi surfaces of the materials. Working first with focused-ion-beam sculpted devices, we demonstrated strong anisotropies of in-plane resistivity and magnetoresistivity in oriented tracks [11] (Figure 4) and mesoscopic squares [12] (Figure 5), modelling the data with Boltzmann transport simulations and, separately, Landauer-Büttiker analyses. We then extended the work to high-frequency electrodynamics in a unique broadband microwave experiment in which the mesoscopic restriction comes from the skin depth rather than any device fabrication, and can therefore be continuously tuned [13] (Figure 6).

Analyzing these experiments motivated the development of a full electrodynamic Boltzmann transport code, which we have used to advance understanding of non-local transport in general, including the relationship between ballistic and viscous contributions to transport in ultra-pure metals. In particular, we identified small-angle scattering from out-of-plane defects as the source of the signatures of viscosity that we observe.

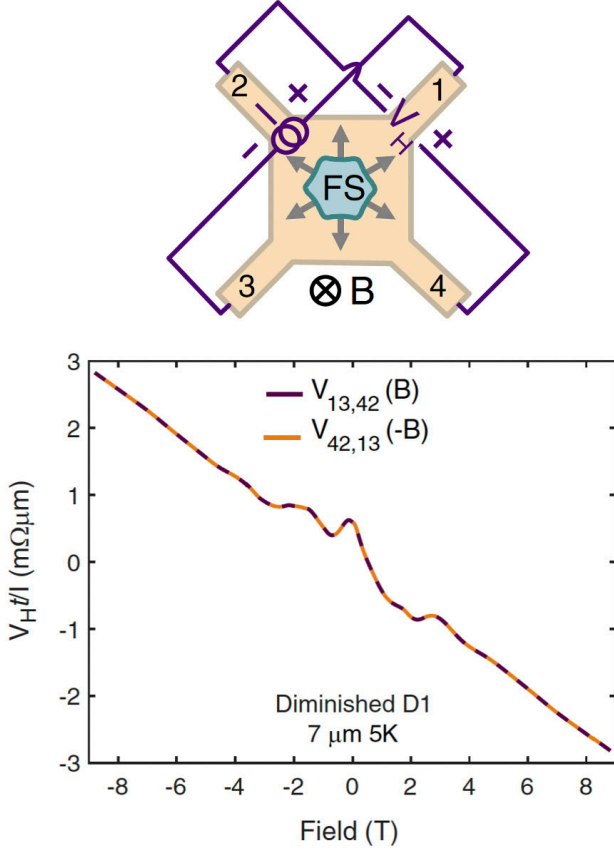


Fig. 5: ‘Text-book’ demonstration of the power of the Büttiker generalization of the Onsager relations to non-local transport. The combination of the hexagonal Fermi surface of  $\text{PtCoO}_2$  and the square-shaped mesoscopic device results in a low-symmetry overall situation. The non-local ‘Hall effect’ is strongly asymmetric in field, but this does not imply the breaking of time reversal symmetry. Rather, it can be explained perfectly within Büttiker’s theory, considering the combination of time reversal symmetry and the overall symmetry of the Fermi surface-device geometry [12].

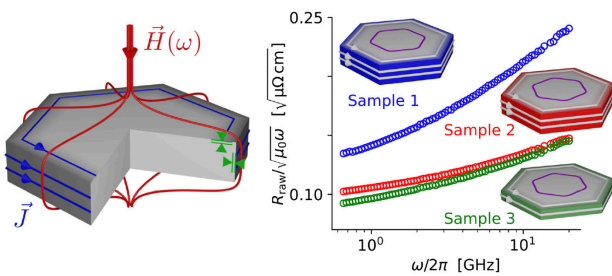


Fig. 6: Remarkably, directional ballistic effects, tuned by varying the skin depth in a broadband microwave experiment on  $\text{PdCoO}_2$ , change not just the value but also the frequency dependence of the microwave conductivity.

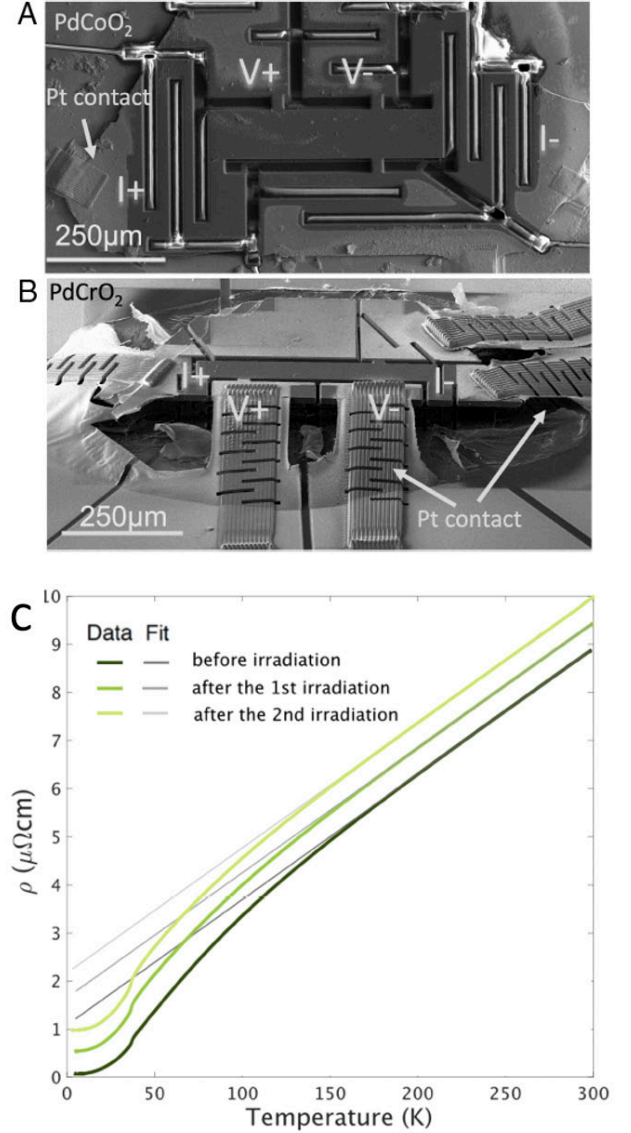


Fig. 7: Working with FIB-sculpted devices of  $\text{PdCrO}_2$  we could show that the temperature-dependent resistivity above 150 K precisely saturates the putative scattering rate bound  $k_B T / \hbar$ . This then provided the opportunity to study the effect of point disorder on this ‘strange metal’ transport, by irradiating the device with 2.5 MeV electrons produced at a special accelerator in Paris. To do so, we had to develop a multi-step protocol that produced floating devices attached to the substrate only by special stress-relieving FIB-deposited Pt structures [15]. Successful implementation of a demanding experiment showed that point disorder simply adds a temperature-independent component to the overall scattering rate, which for this material can be explained by a special form of magneto-elastic scattering originating in a Kondo coupling between Mott insulating magnetic  $\text{CrO}_2$  layers and the conducting Pd planes [16].

### ***Strange metals and Planckian dissipation (Mackenzie, Sunko, Rosner)***

There is large and on-going theoretical interest in the behaviour of strongly correlated metals, particularly the possibility of a bound of  $k_B T/\hbar$  on their scattering rate. Analysis of transport data across a large and growing number of materials gives good evidence that the bound is approximately satisfied, but in most materials, knowledge of the quasiparticle properties is insufficiently detailed to enable a precise analysis. Given this freedom in terms of established experimental facts, theoretical treatments of the problem are diverse, imaginative, and often divergent. A priority during the assessment period was to co-author a review article aiming to discuss and contextualize the many approaches found in the literature, in as didactic and dispassionate style as possible [14].

Experimentally, we focused our attention on a magnetic delafossite,  $\text{PdCrO}_2$ , for which the quasiparticle parameters are well enough known to allow a degree of control that is inaccessible in most other compounds. The scattering rate bound is obeyed with high precision [15] (Figure 7), motivating a concrete theory for what is going on in that particular material [16]. A second point that has become clear is that both quasi-elastic electron-phonon scattering and inelastic electron-electron scattering can both, in principle, saturate the scattering bound. The distinction is important because only electron-electron scattering could be discussed in terms of dissipation. In an effort to identify the mechanism at play in ruthenates and cuprates, we employed a novel spatially-resolved optical technique to investigate high temperature thermal transport, concluding that it has to be dominated by electron-electron scattering [17].

As described separately in the report of our Minerva Group Leader Berit Goodge ([section 1.8](#)), transport in the doped nickelates bears a strong resemblance to that in the cuprates, motivating further experiments on that material class.

### ***Hall effect in ionic liquid gated and uniaxially pressurized crystals (Zhang, Baenitz, Noad, Hicks, Cook, Mackenzie)***

The Hall effect is now understood to be sensitive to a rich variety of background physics, ranging from standard Boltzmann transport to Berry curvature effects in both real and momentum space. Since all this physics combines to give only a single experimentally accessible voltage, definitive interpretation can be

challenging. Our approach to this has been to study the Hall effect in systems of interest which we can continuously tune using electrostatic gating [27] and uniaxial pressure [28–31]. In each case, the response to tuning helped in identifying the underlying mechanism responsible for the measured signal.

For further reading see the following reports:

[PQM\\_01\\_Baenitz](#)  
[PQM\\_04\\_Noad](#)  
[PQM\\_07\\_Zhang](#)  
[PQM\\_08\\_Mackenzie](#)

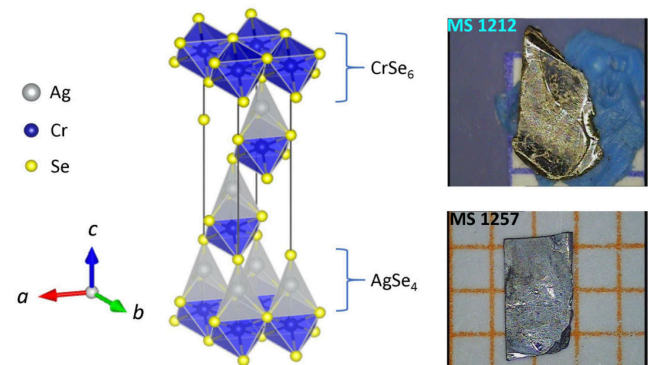
### **4. Unconventional magnetism (Baenitz, Brando, Gati, Nicklas, Rosner)**

Partly due to intrinsic interest and partly to identify promising materials for pressure tuning and thermodynamic study as described in section 1 above, we retain an interest in novel magnetic systems.

During the assessment period we introduced  $\text{AgCrSe}_2$  as a platform for research on layered triangular lattice magnetism in metals [27, 32, 33] (Figure 8), and extended our activities to an organic salt [34]. We further studied pressure- and magnetic-field tuning of unusual magnetic systems [35, 36] and even spatially modulated magnetism resulting from electronuclear entanglement [37].

For further reading see the following reports:

[PQM\\_01\\_Baenitz](#)  
[PQM\\_02\\_Nicklas](#)  
[PQM\\_03\\_Gati](#)  
[PQM\\_05\\_Brando](#)  
[PQM\\_09\\_Rosner](#)



*Fig. 8: Crystal structure and sample single crystals of  $\text{AgCrSe}_2$ , an inversion-symmetry breaking layered triangular lattice magnet [32] that supports an anomalous Hall effect [27].*

## 5. Microstructuring Laboratory

One of the foundational infrastructure developments associated with the establishment of the Physics of Quantum Materials Department in 2013 was the establishment of a microstructuring facility, consisting of a bespoke cleanroom, electron beam lithography and focused ion beam sculpting. This laboratory has now reached a mature steady state, in which the majority of the department's graduate students and post-doctoral fellows learn the appropriate protocols and perform their own sample preparation. The system for using the facility, involving electronic booking and the potential for 24 hour a day running, is highly efficient, and has become integral to our operation. While we no longer list new microstructuring activities as standalone achievements, microstructuring played an important role in the success of experiments described in each of sections 1–4 above. It is much more than a source of attractive figures such as Figures 4, 7A and 7B above: in most cases the published results simply could not have been obtained without its use.

The efficient mode of operation of the facilities has made it possible to share them on collaborative projects both internal and external to the Institute. Internally, the group of Dr. Claire Donnelly uses the laboratory for 3D printing of nanostructures (see her contribution in [section 1.5](#) of this report), and Dr. Berit Goodge has used them in a collaboration with the group of Prof. Julia Mundy from Harvard University. More broadly, we offer them to collaborators in the Dresden area, notably the groups of Dr. Toni Helm from the Helmholtz Center in Rossendorf and Dr. Audrey Grockowiak from the IFW Dresden, and further afield, such as the group of Jens Müller at the Goethe Universität Frankfurt.

## 6. Future plans

Although we thrive in the Max Planck Society environment where research decisions are taken in the present rather than having to be predicted years in advance, we have a clear idea of some of our future research priorities. We believe that our work on thermodynamics under uniaxial pressure will be of lasting significance, so we plan to extend it in two ways. We will study exotic magnetic systems and a much wider range of unconventional superconductors, and work to develop new techniques for studying elastic properties in high magnetic fields and with ever-increasing resolution.

One of the frontiers of magnetic physics is the realization of the existence of class of magnets, altermagnets, that are group theoretically distinct from either ferro- or antiferromagnets. We have attracted the leading young theorist in this new field, Libor Smejkal, to lead a Max Planck Research Group jointly between our Institute and the neighbouring Physics of Complex Systems Institute, and have already begun the investigation of some promising altermagnet candidates, in discussion with him. Altermagnetism comes hand in hand with piezo-magnetism, and we believe that we already have some unique tools with which to study it, and ideas for further development at the uniaxial pressure–optics interface.

As well as moving into new areas, we will opt for strategic continuation in areas where we believe we can make a difference. These will include the physics of  $\text{Sr}_2\text{RuO}_4$  and  $\text{CeRh}_2\text{As}_2$  and nickelates, high temperature investigation of the strange metal problem and non-local transport in ultra-pure metals (but moving on from delafossites as our main platform).

A further continuing priority will be to help our group leaders with their career development. Two of them currently hold faculty offers from the USA, while Veronika Sunko has accepted one from IST Austria, and Elena Gati has been promoted to a W2 position in our Institute combined with an Honorary Professorship at TU Dresden. These and other potential promotions will obviously lead to perturbations to the department's activities, but the long-term benefits to the field outweigh short-term inconvenience to the department!

## External Cooperation Partners

Our main collaboration partners, in alphabetical order, are Felix Baumberger (University of Geneva); Erez Berg (Weizmann Institute for Science); Stuart Brown (UCLA); Debanjan Chowdhury (Cornell); Toni Helm (Helmholtz Zentrum Rossendorf); Markus Garst (Karlsruhe Institute of Technology); Sean Hartnoll (University of Cambridge); Bernhard Keimer (MPI for Solid State Research); Phil King (University of St Andrews); Philip Moll (MPI for Structural Dynamics); Carsten Putzke (MPI for Structural Dynamics); Thomas Scaffidi (UC Irvine); Jörg Schmalian (Karlsruhe Institute of Technology); Anna Tamai (University of Geneva); Jochen Woznitza (Helmholtz Zentrum Rossendorf).

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## 1.3 Physics of Correlated Matter

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Our aim is to understand how electrons in transition-metal, rare-earth and actinide based materials interact to produce the extraordinary and often unexpected quantum phenomena observed in these systems. Due to the limitations of *ab-initio* calculations and the inaccessibility of exact many-body solutions, we seek to develop approximations that capture the essential physics governing these phenomena – specifically, to find routes from a generic high-energy Hamiltonian to the appropriate low-energy one. To achieve this, we are advancing state-of-the-art x-ray spectroscopic techniques combined with material-specific many-body model calculations. This may lead to, for example, the identification of coherent spectral weights and various forms of satellites, which can be associated with quasi-particles and their dressing, respectively. Our experimental efforts also focus on materials development, synthesizing new materials in both bulk and thin film forms to tune the relevant interactions and potentially uncover novel phenomena. Our department’s research is driven by a collaborative team of researchers, each bringing their own expertise, working together to explore the complex behaviour of correlated materials.

Members of our Department coauthored 293 publications in the census period of May 2021 – June 2024 (for comparison, we have 224 publications in 2018–2021, 187 in 2015–2018, and 161 in 2012–2015).

### CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub>: A high Kondo-temperature oxide

Transition metal oxides exhibit a wide range of remarkable physical properties, including superconductivity, metal-insulator transitions, spin-state transitions, unusually large magnetoresistance, orbital ordering phenomena, and multiferroicity. Notably, heavy-fermion or Kondo behavior is rarely observed in oxides. While common in rare-earth and actinide intermetallics, evidence for heavy-fermion physics in oxides is limited, with perhaps only LiV<sub>2</sub>O<sub>4</sub> showing such indications. The discovery of the transition metal oxide CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub> (CCRO), which displays Kondo-like properties, therefore generated significant excitement. However, this Kondo interpretation has been met with strong skepticism. For instance, it has been argued that the specific heat coefficient  $\gamma$  does not deviate significantly from the band structure value, suggesting that electronic correlations play only a minor role.

Here, we address the CCRO problem from a different perspective. Figure 1 shows the magnetic susceptibility of CCRO together with that of CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> (CCTO), as reproduced from literature. One can observe that CCTO follows, far above its 25 K Néel temperature, almost a textbook Curie-Weiss law for paramagnetic  $S = 1/2$  Cu<sup>2+</sup> ions. In contrast, CCRO shows a completely different behavior with a magnetic susceptibility that is an order of magnitude smaller. There are also no indications at all for magnetic order in CCRO.

In our combined x-ray spectroscopy and LDA + DMFT study [1], we first established, through x-ray absorption spectroscopy (XAS) and resonant photoelectron spectroscopy (PES), that the Cu in CCRO is divalent, rather than monovalent or low-spin trivalent. This confirms that the Cu ions are paramagnetic. Additionally, the Cu 2*p* core-level PES spectra revealed a double main-peak structure, indicating the presence of a screening process by conduction electrons.

By utilizing the strong energy dependence of photoionization cross-sections in hard and soft x-ray PES, we successfully identified the Cu 3*d*, Ru 4*d*, and O 2*p* contributions to the valence band. These findings were

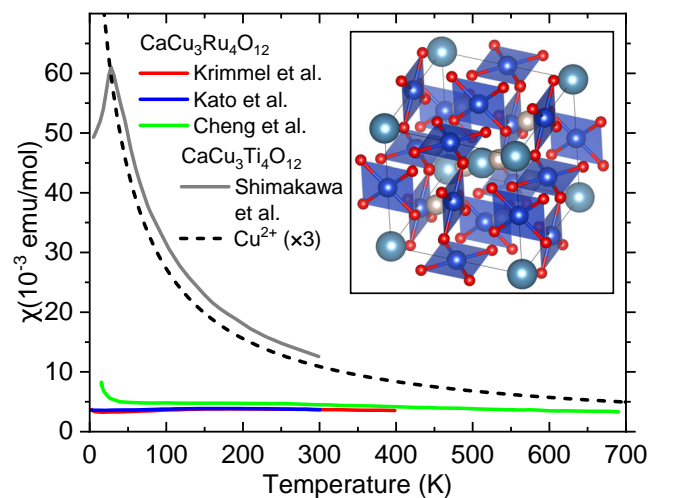


Fig. 1: Magnetic susceptibility of CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub> and of CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub>, as well as of a  $S = 1/2$  Cu<sup>2+</sup> ion scaled by a factor of 3. Inset: Crystal structure of CaCu<sub>3</sub>Ru<sub>4</sub>O<sub>12</sub> with the blue, red, gray, and indigo blue spheres representing Cu, O, Ru, and Ca, respectively.

used to refine the double-counting correction and other parameters in the LDA+DMFT calculations. The calculated spin and charge susceptibilities then confirmed that CCRO is a Kondo system, with a Kondo temperature in the range of 500–1000 K. This high Kondo temperature implies that the contribution of the Kondo screening process to the low-temperature specific heat is modest. This explains why band structure calculations appear to reproduce the experimentally observed  $\gamma$  value of the specific heat, as the main contribution originates from the uncorrelated Ru-O-derived bands.

### Paramagnetic LaCoO<sub>3</sub>: A highly inhomogeneous mixed spin-state system

LaCoO<sub>3</sub> has been the focus of intense and continuous research for more than 50 years. It exhibits a fascinating gradual transformation from a nonmagnetic insulator at low temperatures to a paramagnetic semiconductor at approximately 50–100 K, followed by an insulator-to-metal transition around 450–550 K. The interest in LaCoO<sub>3</sub> stems from the long-standing and ongoing debate about the nature of these transitions, as well as the considerable potential of Co-oxide-based materials for applications in battery technology and catalysis.

It has long been speculated that LaCoO<sub>3</sub> in the paramagnetic phase is an inhomogeneous spin-state system, where nonmagnetic low-spin (LS) Co<sup>3+</sup> ions and magnetic high-spin (HS) Co<sup>3+</sup> may even form an ordered state, possibly on a short-range dynamical scale. This speculation arises from the fact that the effective ionic radius of LS Co<sup>3+</sup> is smaller than that of HS Co<sup>3+</sup>, as illustrated in Figure 2, which shows the ionic 3d charge density for both cases. In the CoO<sub>6</sub> octahedra of LaCoO<sub>3</sub>, the steric repulsion between Co and O along the bond axes is greater when the  $e_g$  orbitals are occupied, compared to when no  $e_g$  electrons are present. Consequently,

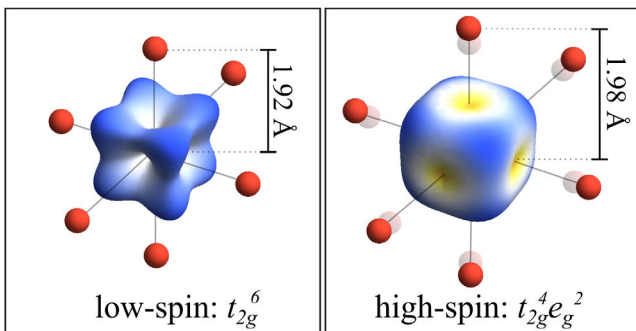


Fig. 2: Local ionic Co<sup>3+</sup> 3d charge density in the CoO<sub>6</sub> octahedron: low-spin  $t_{2g}^6$  (left) and high-spin  $t_{2g}^4 e_g^2$  (right). The  $t_{2g}$  electron density is shown in blue and the  $e_g$  in yellow. Red dots mark the oxygen positions (faint dots in the right denote the low-spin positions).

the Co–O bond lengths are strongly dependent on the spin state of the Co ions.

Structural studies, however, have not detected any evidence of such ordering or of Co sites with different bond lengths in the paramagnetic state. Consequently, most experimental and theoretical investigations of the electronic structure of LaCoO<sub>3</sub> assume either equivalent Co atoms or spin-state inequivalent Co atoms based solely on electronic considerations. Although there is no direct proof of structurally distinct Co sites to date, this issue cannot be ignored. For instance, the temperature dependence of the spin-state transition remains an unresolved problem, and it is unclear how well LaCoO<sub>3</sub> functions as a metal at high temperatures. These challenges are, in fact, common to many transition metal compounds that exhibit phase transitions.

We investigated LaCoO<sub>3</sub> using bulk-sensitive hard x-ray PES (HAXPES) and XAS at the O-*K* edge, combined with configuration-interaction calculations that incorporate full atomic-multiplet theory [2]. The enhanced bulk sensitivity allowed us to observe a pronounced temperature dependence and obtain spectra with unprecedented detail. We found that the energy gap decreases by approximately 0.6 eV across the spin-state transition, from 80 to 650 K. However, the intensity near the Fermi level remains low, classifying LaCoO<sub>3</sub> as a bad metal even in its metallic phase. Our analysis interprets the spectra as incoherent sums of LS and HS Co<sup>3+</sup> contributions. Furthermore, we discovered significant differences in the energy parameters for the two Co sites, indicating that paramagnetic LaCoO<sub>3</sub> is a highly inhomogeneous system with spin-state-specific local lattice relaxations. This finding provides insight into the long-debated temperature dependence of activation energies and the observed bad metal behavior.

See [PCM\\_01\\_Tjeng](#) for our spectroscopic studies on other transition metal compounds.

### Direct imaging of valence orbitals using hard x-ray photoelectron spectroscopy

PES is one of the most powerful experimental methods for studying the electronic structure of crystalline materials. The capability to detect band dispersions through angle-resolved PES (ARPES) has firmly established its significance in fields such as high-T<sub>c</sub> superconductivity and topological insulators. More recently, the development of HAXPES has opened new research avenues due to its greatly increased probing depth. In the following we describe how we utilize HAXPES to bring to application a long-sought complementary aspect of photoelectron spectroscopy: the ability to image the key

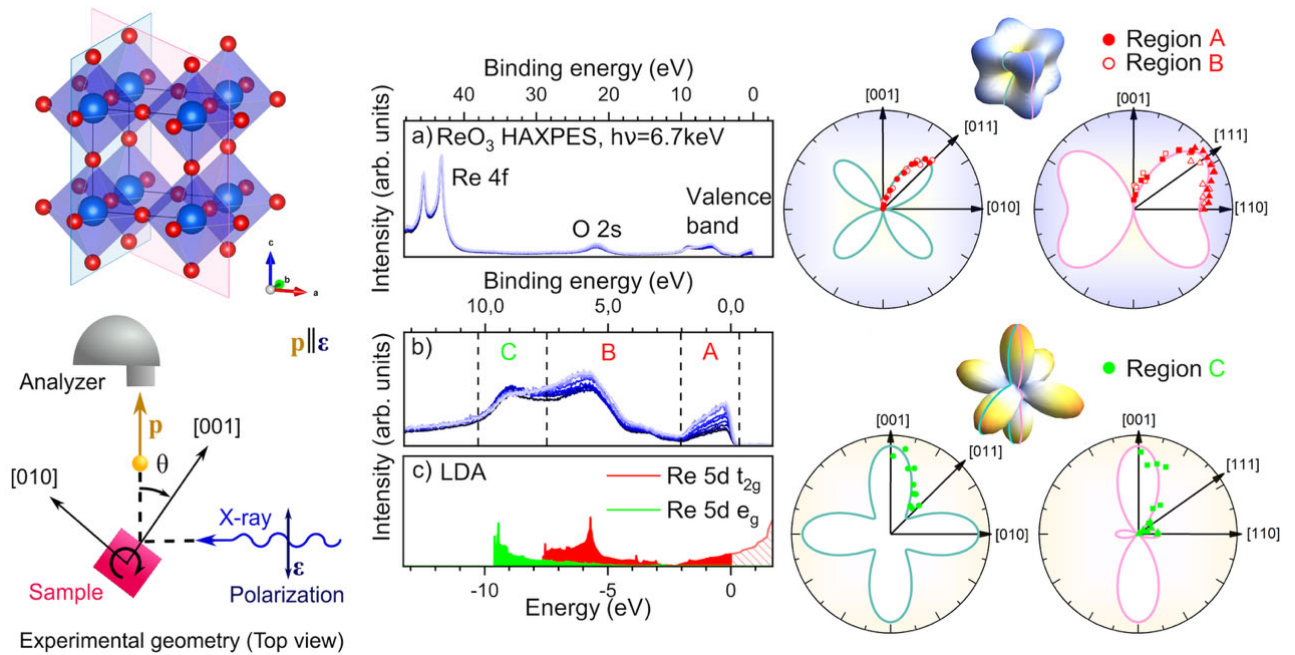


Fig. 3: Left panels: Crystal structure of  $\text{ReO}_3$  and experimental geometry; Middle panels: Orientation dependent HAXPES spectra and LDA calculations; Right panels: Polar plots of the HAXPES intensities in regions A, B, and C from middle panel (b) together with the 3D plots of the  $t_{2g}$  (in blue) and  $e_g$  (in yellow) charge densities.

orbitals that contribute to the valence band structure of crystalline solid-state materials.

In the early 1980s, Goldberg, Fadley, and Kono [Solid State Commun. 28, (1978) 459; J. Electron Spectrosc. Relat. Phenom. 21, (1981) 285] calculated the photoionization cross-sections for atomic orbitals with fixed spatial orientation. They found that these cross-sections are directly proportional to the probability distribution of the initial state orbital when the experiment is conducted in a specific geometry where the polarization of the light and the direction of the measured photoelectrons are parallel. Figure 3 illustrates this geometry. By rotating the sample and measuring the orientation dependence, the experiment could potentially create a direct spatial image of the occupied orbital. This method represents a real-space type of imaging that is calculation-free. However, what holds true for freestanding atoms may not be applicable to solids. In solids, electron scattering is significantly stronger, leading to well-known phenomena such as photoelectron diffraction effects, which disturb the measurements.

In Ref. [3], we present our experimental as well as theoretical efforts to implement the Goldberg, Fadley, and Kono idea for crystalline solids. As a model system we investigated  $\text{ReO}_3$ , an oxide with a simple but remarkable crystal structure, namely, a simple cubic arrangement of interconnected  $\text{ReO}_6$  octahedra; see Figure 3. In terms of properties,  $\text{ReO}_3$  is an atypical and fascinating oxide: It is one of the best conducting oxides, with a conductivity comparable to that of Cu or Ag metal.

The middle panel of Figure 3 shows a selection of spectra obtained with different crystal orientations while keeping the measurement geometry fixed. A key innovation in our approach is normalizing the spectra to the shallow  $\text{Re } 4f$  core level. This normalization effectively removes intensity variations caused by sample and beam spot inconsistencies. More importantly, it significantly mitigates the pronounced angular dependence arising from x-ray photoelectron diffraction (XPD) processes. The shallow  $\text{Re}$  core levels and the  $\text{Re}$  valence band states exhibit similar XPD effects due to their nearly identical kinetic energies, while the fully filled core levels possess spherical symmetry, resulting in no initial-state orientation dependence. By normalizing the spectra to the shallow core levels, we can isolate the desired initial-state orientation dependence of the partially filled valence band orbitals.

The right panel of Figure 3 displays polar plots showing the orientational dependence of the photoemission intensities from regions A, B, and C of the valence band. These intensity variations clearly indicate that regions A and B exhibit  $t_{2g}$  character, while region C is  $e_g$ -like, a finding supported by LDA band structure calculations. We note that our analysis assumes the ability to subtract an isotropic angular background from the polar plots, an assumption validated by *ab initio* one-step photoemission calculations. This approach allows us to create direct images of the orbitals contributing to the band structure of the material. The images are energy-specific and reveal the role of each orbital in chemical bond-

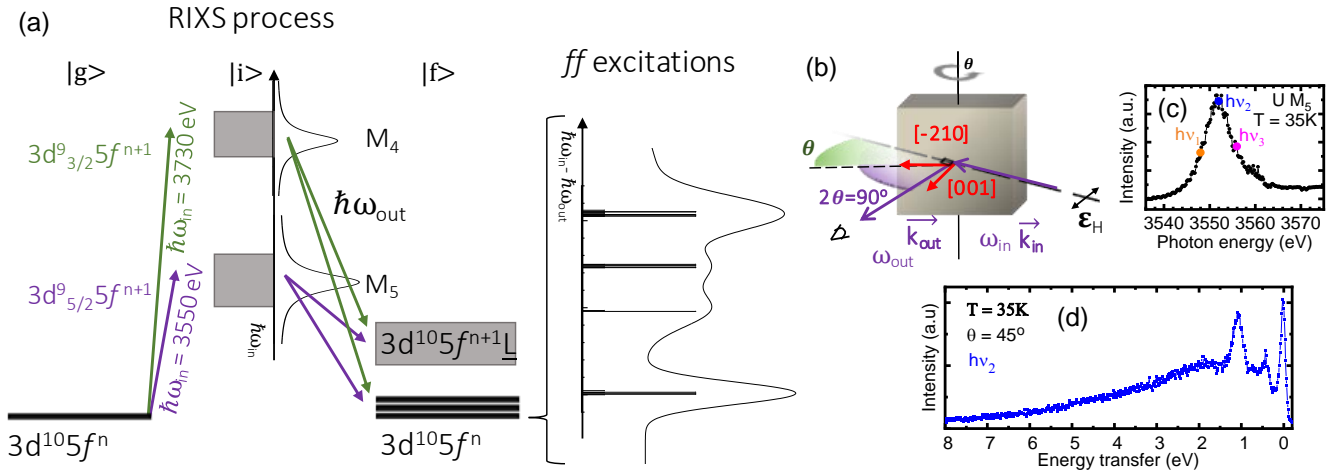


Fig. 4: (a) RIXS process at  $UM_{4,5}$  edges for a  $5f^n$  ground state. (b) Scattering geometry of RIXS experiment with scattering angle  $2\Theta = 90^\circ$ . (c) Fluorescence-yield  $M_5$  XAS spectrum of  $UGa_2$ , dots marking the incident photon energies for RIXS ( $h\nu_1$ ,  $h\nu_2$ ,  $h\nu_3$ ). (d)  $M_5$  RIXS data of  $UGa_2$  acquired with  $h\nu_2$  and a sample angle  $\theta = 45^\circ$ .

ing and Fermi surface topology. This orbital imaging information complements data obtained from ARPES, thereby enhancing our understanding of the electronic structure. This new method is applicable to a wide range of crystalline materials.

### Multiplets and singlet magnetism in intermetallic $UGa_2$ unveiled by inelastic x-ray scattering

Actinide intermetallics exhibit a wealth of fascinating phenomena, including heavy-fermion behavior, hidden order, unconventional magnetism, and unconventional superconductivity, as well as orbital multicomponent or spin-triplet superconductivity with potential topological properties. It is generally understood that these complex emergent properties arise from the intricate interplay of band formation and correlations involving the  $5f$  electrons. However, it remains unclear how to quantitatively describe the electronic structure of these systems. For instance, it is debated whether an itinerant approach or an embedded impurity model that explicitly incorporates local degrees of freedom serves as the better starting point. A major challenge is that many intermetallic uranium compounds, with the possible exception of  $UPd_3$ , do not exhibit local excitations in their inelastic neutron scattering data. In fact, there is a lack of spectroscopic data to confirm the presence of remnants of atomic-like states, let alone to identify which multiplet and/or crystal-field state is actually occupied.

Not long ago, we discovered that atomic-like multiplet states exist in the core-level spectra of  $UM_2Si_2$  ( $M = Ru, Pd, Ni, Fe$ ) [4, 5]. This finding was based on non-resonant inelastic x-ray scattering (NIXS or x-ray Raman scattering) measurements that utilized beyond-dipole transitions. This approach enabled us to access atomic-

like final states with high quantum numbers and, consequently, low energies, making them highly excitonic and resistant to broadening from continuum states. These discoveries motivated us to search for multiplet excitations without the presence of a core hole, specifically low-energy intra-valence-band excitations that fall within the energy range covered by Raman, optical, or neutron scattering experiments. To this end, we have invested in the development of a new instrument at PETRA III to conduct high-resolution resonant inelastic x-ray scattering (RIXS) measurements in the tender x-ray range, targeting the strong  $UM_{4,5}$  edges (ca. 3730 eV and 3552 eV, respectively). Figure 4 shows the experimental setup and the principles of the spectroscopic method [6]. The energy resolution at the  $UM_5$  edge has recently been improved from 150 meV to 70 meV.

We investigated  $UGa_2$  as a representative case of metallic U compounds where the balance between itinerancy and localization is a key issue.  $UGa_2$  crystallizes in the hexagonal  $A1B_2$  structure (space group  $P6/mmm$ ), with U-U distances significantly exceeding the Hill limit. It exhibits ferromagnetic ordering below the Curie temperature ( $T_C$ ) of 125 K, with moments of approximately  $3\mu_B$  aligned in the  $ab$  plane. Previous attempts to explain the magnetism have been based on local  $f^2$  or  $f^3$  charge configurations, as well as itinerant models.

Figure 4 shows a representative RIXS spectrum that displays sharp peaks below 2 eV, superimposed on a broad feature likely arising from charge-transfer excitations. The sharp peaks are characteristic of local atomic-like excitations. By comparing the spectra to full atomic-multiplet calculations, we find that the multiplet excitations in RIXS exhibit the characteristic fingerprint of the  $5f^2$  configuration. Thus, the  $5f^2$  configuration is crucial for understanding the correlated nature of this fer-

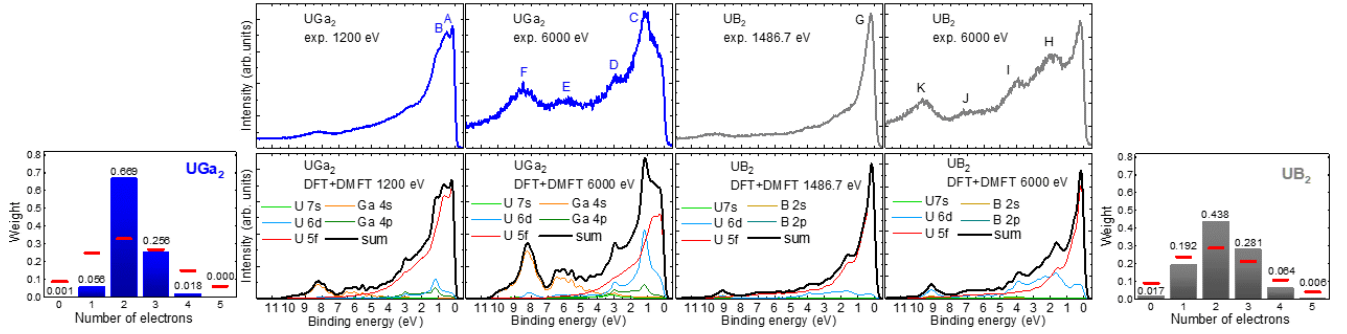


Fig. 5: Top panels: Experimental hard and soft x-ray valence band spectra of  $UGa_2$  and  $UB_2$ . Middle bottom panels: DFT + DMFT calculations for  $U_{ff} = 3$  eV,  $J = 0.59$  eV, and  $\mu_{dc} = 4.25$  eV, weighed with photoionization cross-sections. Left and right bottom panels: Atomic  $U 5f^n$  configuration histograms of  $UGa_2$  and  $UB_2$ , respectively. The red ticks indicate the uncorrelated statistical distribution.

romagnet. The orientation and directional dependence of the spectra indicate that the ground state consists of a  $\Gamma_1$  singlet and/or a  $\Gamma_6$  doublet symmetry. Given that the ordered moment lies in the  $ab$ -plane, we infer that the magnetism originates from the higher-lying  $\Gamma_6$  doublet, which mixes with the  $\Gamma_1$  singlet due to intersite exchange. This qualifies  $UGa_2$  as a true quantum magnet [6].

Here we note that induced quantum magnetism in singlet ground state systems has been well explored in  $4d^4/5d^4$  transition metal or  $4f^2$  Pr materials. In these cases the presence of multiplets is clear. Singlet magnetism is however rarely recognized so far in U compounds, but with the ability to establish that the  $U 5f^2$  configuration might be quite common, we may find many more U compounds to belong to this class of singlet magnets, all requiring theories beyond mean-field.

### Quantifying the $U 5f$ covalence and degree of localization in U intermetallics

As mentioned earlier, uranium intermetallic compounds exhibit a wide range of fascinating physical phenomena arising from the intricate interplay between atomic-like correlations and the band formation of  $U 5f$  electrons. Describing these materials requires approaches that go beyond mean-field theory. Recent developments combining DFT with DMFT offer an exciting opportunity to capture certain aspects of both low- and high-energy properties. While these calculations yield promising results, they often encounter challenges, such as how to appropriately subtract correlation effects already included in both the DFT and DMFT components, as well as how to determine the actual magnitude of these correlations. Consequently, accurately reproducing experimentally observed quantities, such as spectra in electron spectroscopy, can be difficult when aiming for truly *ab initio* calculations. As a result, the community faces conflicting findings from different spectroscopic techniques re-

garding the extent of correlations and the occupancy of the  $U 5f$  shell.

In this study, we aim to establish a procedure to empirically reduce or even eliminate the uncertainties in DFT + DMFT. Material specific parameters can be obtained by tuning the calculations to accurately reproduce the valence band spectra measured with various photon energies [7]. The changes in the spectra, originating from the energy dependence of the photoionization cross-sections of the atomic subshells involved, enable DFT + DMFT to be more specific about the various subshell spectral line shapes and energy positions.

We consider isostructural  $UGa_2$  and  $UB_2$  as model materials [7] that are at the opposite sides of the localization spectrum.  $UGa_2$  is expected to exhibit more atomic-like behavior, while  $UB_2$  is anticipated to be more delocalized. This distinction arises because the shortest U–U distance in  $UGa_2$  is well above the Hill limit, whereas in  $UB_2$ , it is significantly below it.

The top panels of Figure 5 display the experimental valence band spectra of  $UGa_2$  and  $UB_2$  measured with soft x-rays ( $h\nu = 1200$  eV and 1486.7 eV) and hard x-rays ( $h\nu = 6000$  eV). Using soft x-rays, the  $U 5f$  spectral weight is enhanced relative to the non- $U 5f$ , while with hard x-rays the contribution of the  $U 5f$  is more comparable to those of the non- $U 5f$ . The bottom middle panels of Figure 5 show the DFT + DMFT spectra calculated with parameters that are tuned to match best the experiment: Hubbard  $U_{ff} = 3$  eV, Hund's  $J = 0.59$  eV, and double counting correction  $\mu_{dc} = 4.25$  eV.

Based on the excellent agreement, we can now reliably address the issue of covalence and localization. The left and right panels of Figure 5 depict the atomic  $U 5f^n$  configuration histograms for  $UGa_2$  and  $UB_2$ , respectively. The mean  $U 5f$  filling was calculated to be 2.24 for  $UGa_2$  and 2.20 for  $UB_2$ , indicating almost the same filling despite their vastly different properties. However, the distribution of configurations differs significantly: it is

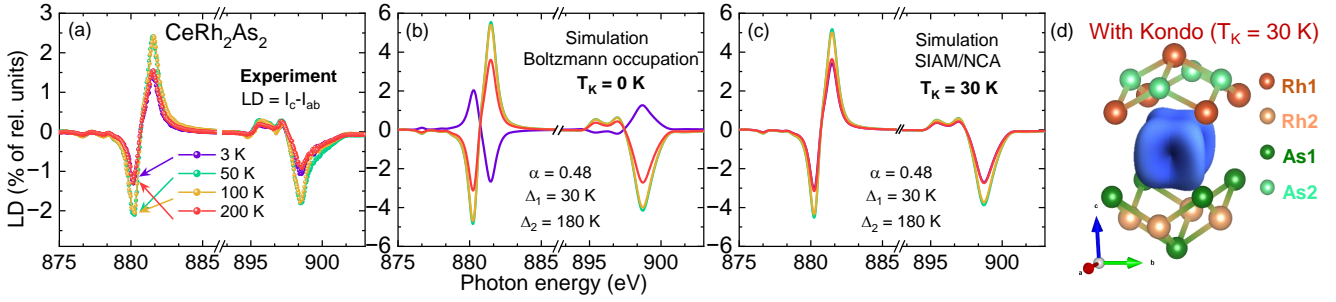


Fig. 6: (a) Temperature dependence of the linear dichroism of  $\text{CeRh}_2\text{As}_2$ , (b) simulated with thermal occupation of crystal-field states, (c) with occupations from an Anderson impurity calculation with a Kondo temperature of 30 K, and (d) Ce charge density of the Kondo-mixed ground state with its nearest neighbors.

narrow for the "localized"  $\text{UGa}_2$  and nearly statistically broad for the "itinerant"  $\text{UB}_2$ . This variation is primarily due to the very different  $U\ 5f-5f$  hopping integrals, rather than a difference in the  $U_{\text{ff}}$  value, which remains constant at 3 eV. With these parameters, we can also quantitatively reproduce the satellites in the  $U\ 5f$  core-level spectra and explain the presence and absence of intra- $5f$  multiplet excitations in the RIXS spectra. These findings allow us to address the longstanding question of why different spectroscopic techniques yield seemingly divergent values for the  $U\ 5f$  valence in intermetallic U compounds.

### Spectroscopic evidence of Kondo-induced quasi-quartet in $\text{CeRh}_2\text{As}_2$

$\text{CeRh}_2\text{As}_2$  is a new multiphase superconductor, with indications of an additional itinerant multipolar ordered phase. Modeling the low-temperature properties of this heavy-fermion compound requires a quartet  $\text{Ce}^{3+}$  crystal-field ground state. However, the Ce ions are locally coordinated in a tetragonal structure without inversion symmetry, and the admixture of  $5d$  states is negligible. Therefore, one would typically expect three Kramer's doublets for the  $4f$  electrons. The goal of our study [8] is to identify a mechanism via spectroscopy that allows for the formation and existence of a quasi-quartet state arising from two doublets.

We first performed bulk-sensitive HAXPES on the Ce  $3d$  core level and XAS at the Ce  $M_{4,5}$  edges ( $3d \rightarrow 4f$ ). This allowed us to observe satellites in the spectra, indicating the presence of Kondo hybridization in  $\text{CeRh}_2\text{As}_2$ . Next, we conducted polarization-dependent XAS measurements to determine the orbital occupation. While the linear dichroism (LD) is small, it exhibits a distinct temperature dependence, as shown in Figure 6(a). A full multiplet analysis simulation, based on a crystal-field model that reproduces the macroscopic data, unambiguously reveals the influence of Kondo physics in coupling the Kramer's doublets into an effective quasi-

quartet. Notably, assuming thermal occupation of states alone cannot account for the temperature dependence of the LD, see Figure 6(b). In contrast, the state occupation derived from an Anderson impurity model calculation using the non-crossing approximation (SIAM/NCA) successfully reproduces this dependence, see Figure 6(c). Our findings also align with the entropy of  $R \ln(4)$  observed in specific heat measurements, confirming that an essential ingredient for multi-orbital ordering – a fourfold degenerate ground state – is present in  $\text{CeRh}_2\text{As}_2$ . Additionally, we determined the in-plane orientation of the quasi-quartet state utilizing the beyond-dipole transitions in non-resonant inelastic x-ray scattering spectroscopy at the Ce  $N_{4,5}(4d \rightarrow 4f)$  edges. The final result is shown in Figure 6(d), where the ground state  $4f$  charge density of the Ce ion is plotted in relation to the nearest neighbor Rh and As ions.

See [PCM\\_02\\_Severing](#) for our spectroscopic studies on other  $4f$  and  $5f$  electron systems.

### X-ray spectroscopic study on transition metal oxide based catalysts and battery materials

Over the past three years, we have intensified our efforts to study transition metal oxide-based catalysts and battery materials using synchrotron-radiation based spectroscopies. Our goal is to determine the electronic states of the transition metal ions during various operational processes. We leveraged our long-standing expertise in soft-XAS, which encompasses not only the experimental acquisition of reliable and accurate data but also the nuanced analysis of the spectra. This is further supported by our extensive database of energy-calibrated reference spectra, collected over the last 30 years.

We collaborated closely with partners who specialize in catalyst and battery research. We selected systems for study that align with our specific expertise in soft-XAS and transition metal compounds. In most cases, we were able to extract detailed information about the charge, orbital, and spin state of the ions.

We analyzed the spectra using configuration-interaction (CI) calculations that include the full atomic-multiplet theory. CI is essential for accurately describing covalency in these strongly correlated systems, as covalency reflects the presence of ligand hole states that play a dominant role during catalytic processes and the charging-discharging cycles of batteries. Including full atomic multiplet theory is necessary not only to accurately represent the energy structure of the soft-XAS final states but also to derive the correct total energy level diagram for the ground/initial state problem. Relying solely on the diagonal terms of the Coulomb matrix could lead to significant errors.

Another invaluable aspect of CI is that the spectra can be reproduced using well-defined values of the Racah parameters or Slater integrals. This allows the tunable parameters in the calculation to directly fix the ligand-to-transition metal charge transfer energy and transfer integrals, providing valuable information about the ligand hole states. These calculations treat the ground/initial state and the soft-XAS final state problems on equal footing by employing atomic-like basis functions that appropriately include local Coulomb and exchange interactions. This approach ensures optimal accuracy for the simulations, resulting in a reliable and detailed description of the ground/initial state.

Our activities in this field have resulted in over 130 publications during the 2021–2024 census period, a significant increase from the 40 publications in the 2018–2021 period. This surge reflects the growing interest within the community to utilize our expertise. It’s worth noting that, while catalysis and battery research is a highly popular field with a large community, 30 of these 130 publications appeared in journals with an impact factor greater than 20, plus 14 in Nature Communications.

A project that exemplifies our contribution to this field is titled “Unusual double ligand holes as catalytic active sites in LiNiO<sub>2</sub>” [9]. Traditionally, theoretical descrip-

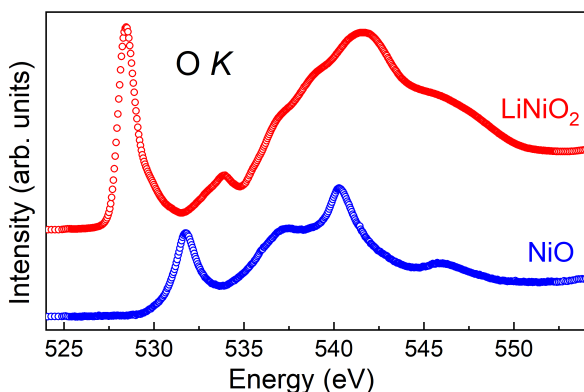


Fig. 7: O–K edge x-ray absorption spectrum of LiNiO<sub>2</sub> and the NiO reference.

tions of the oxygen evolution reaction (OER) focus on charge-transfer steps at the metal sites. However, recent evidence suggests that lattice-oxygen-vacancy sites play a significant role, particularly in late 3d transition-metal oxides with high oxidation states. To investigate this hypothesis, we utilized LiNiO<sub>2</sub> as a pre-catalyst, given its edge-shared Ni-O-Ni network, which is more stable than the corner-shared networks found in RNiO<sub>3</sub> or RSrNiO<sub>4</sub> (R = rare earth). Our goal was to determine the valence of the metal ions and the presence of O 2p ligand hole states. The LiNiO<sub>2</sub> material was prepared in our Dresden laboratory.

While divalent Ni oxides are known to have large positive charge transfer energies, making them rather ionic, the situation is quite different for formally trivalent Ni compounds. In these compounds, the charge transfer energy can become small (though still positive), resulting in significant hybridization between the Ni 3d<sup>7</sup> configuration and the 3d<sup>8</sup> $\underline{L}$  state. In cases where the charge transfer energy becomes negative, we use the notation Ni<sup>III</sup> instead of Ni<sup>3+</sup> to indicate that the dominant electronic configuration is 3d<sup>8</sup> $\underline{L}$ , where  $\underline{L}$  represents a hole in the O 2p ligand. Figure 7 shows that the pre-edge peak in the O-K XAS spectrum of LiNiO<sub>2</sub> is very strong and located at a much lower energy than that of NiO, providing clear evidence for the strong presence of O 2p ligand hole states.

Figure 8 displays the Ni-L<sub>2,3</sub> XAS spectrum of the catalyst material before and after the oxygen evolution reaction (OER). These spectra differ significantly from that of the Ni<sup>2+</sup> reference, NiO. The LiNiO<sub>2</sub> spectrum prior to the OER can be explained using a Ni 3d<sup>8</sup> $\underline{L}$  Ansatz, corroborating the findings from the

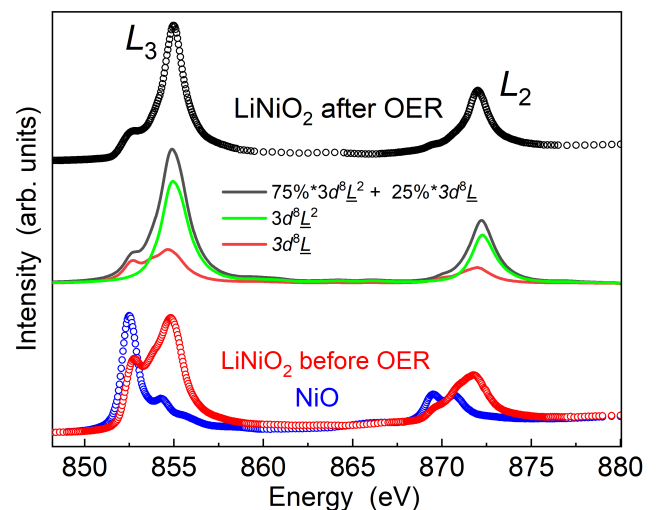


Fig. 8: Ni-L<sub>2,3</sub> edge x-ray absorption spectrum of LiNiO<sub>2</sub> before and after the oxygen evolution reaction (OER) together with the NiO reference and simulations.

O-K XAS. After the OER, the Ni- $L_{2,3}$  XAS spectrum changes substantially. The excellent simulation, which begins with the  $3d^8\bar{L}^2$  configuration and includes some  $3d^8\bar{L}$  contributions, provides strong evidence for the formation of double ligand hole states during the catalytic process. Our XAS data and analysis indicate that a significant fraction of the Ni ions undergoes a voltage-dependent valence state transition from Ni<sup>III</sup> to Ni<sup>IV</sup>, which drives the OER activity.

See [PCM\\_03\\_Hu](#) for an overview of our spectroscopic studies on catalysts and battery materials.

### Other activities

Our group continues to search for new transition metal compounds that could host unconventional magnetic states. One notable discovery is the observation of 1/3 magnetization steps in the non-triangular lattice pyroxene CoGeO<sub>3</sub> [10], which is described and explained in [PCM\\_04\\_Komarek](#).

We have started a new project focused on the synthesis and structural characterization of correlated rare-earth nitride thin films. Our objective is to achieve high-quality materials through epitaxial growth, enabling us to identify and understand potentially interesting properties through careful spectroscopic studies. The initial results on HoN [11] and SmN [12] are detailed in [PCM\\_05\\_Altendorf](#).

Electronic inhomogeneities are of significant interest, both from a fundamental perspective and for practical applications, such as in sensors and spintronics. We highlight our research on two types of electronic inhomogeneity: the formation of topologically non-trivial surface states in the Kondo insulator SmB<sub>6</sub>, achieved through systematic manipulation of its surface conductivity [13], and nanoscale phase separation due to the formation of magnetic polarons in Eu<sub>5</sub>In<sub>2</sub>Sb<sub>6</sub> [14], a material that exhibits colossal magnetoresistance. Further details can be found in [PCM\\_06\\_Wirth](#).

We continued our research on heavy-fermion systems near magnetic quantum criticality, focusing on the effects of geometrical frustration on quantum-critical behavior. Additionally, we initiated detailed investigations of compounds near structural quantum criticality, monitoring the relevant phonon softening [15]. For more information, see [PCM\\_07\\_Stockert](#).

### External Cooperation Partners

Andrea Severing (University of Cologne); Atsushi Hariki (Osaka Metropolitan University); Jan Kuneš (Technical University Vienna); Arata Tanaka (Hiroshima University); Takashi Mizokawa (University of Tokyo); Jan Minar (University of West Bohemia); Hlynur Gretarsson, Andrei Gloskovskii (DESY); Bernhard Keimer (Max Planck Institute for Solid State Research); Maurits W. Haverkort (Heidelberg University); Eric D. Bauer (Los Alamos National Laboratory).

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## 1.4 Chemical Metals Science: (25 years) From Preparation and Characterization to Chemical Bonding and Property Analysis of Intermetallic Compounds

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Intermetallic compounds represent one of the most fascinating family of inorganic materials. Due to the peculiar type of atomic interactions between the mostly metallic components, intermetallic compounds adopt compositions which can be considered unusual from the traditional chemical viewpoint. The crystal structures cover a range from a single to thousands of atoms in the unit cell. The structural and bonding complexity gives rise to unique combinations of chemical and physical properties of these materials, from catalysis via superconductivity and magnetism to thermoelectricity and other electrical and thermal transport properties. The chemical aspects of intermetallic compounds and their properties were in the focus of the research of the Department of Chemical Metals Science for the last decades.

Studies on the chemical nature of intermetallic compounds started at the MPI CPfS already in 1998 within a W2 research group as part of the Department of Inorganic Chemistry. Since 2001, this research direction was in the focus of the Department of Chemical Metals Science. Mainly being composed of metallic elements close to, and left of, the Zintl line in the Periodic Table, intermetallic compounds form and exist under conditions of valence electron deficiency. Therefore, the traditional chemical concepts fail in explaining compositions and crystal structures of those substances. This was the starting point for the research on chemical metals science at the MPI CPfS. The present report is a brief summary of the department's development and some current results.

Because of the non-predictable composition of the synthesis products (lack of valence rules), the precise preparation of materials with a specific target composition of the intermetallic compounds is experimentally challenging. In order to overcome this problem several experimental steps were performed. From the very beginning, the traditional preparation techniques including arc- and HF-melting were transferred into protective atmospheres in order to avoid contamination with non-metallic components. A side-product of this development was the construction of an arc-melter for glove-box applications.

At the same time, the specialized laboratory of high safety standards was constructed and developed to enable chemical experiments based on Be, U, Th, Hg, Os and other elements with enhanced toxicity, in accordance with the modern safety rules (see [1] and [CMS\\_02\\_Leithe-Jasper](#)). On the basis of this technology, chemistry and physics of the intermetallic compounds of mercury with the rare-earth and alkaline-earth

metals as well as thorium and uranium were studied in collaboration with the newly-created REALM research group (see report of E. Svanidze in [section 1.7](#)).

The technique of centrifugation-aided separation of reaction products from a liquid-metal medium was expanded to temperatures exceeding 1100 °C. This development paved the way for preparing single crystals of noble-metal and transition-metal compounds with aluminum and gallium [2–4]. The current progress is going towards the use of lithium as reaction environment. Beside plenty of mm-sized crystals of nitrido-metalates (see [CMS\\_09\\_Hoehn](#)), this development led to the discovery of a new family of intermetallic compounds of alkaline-earth metals with noble metals and lithium. A striking example is the compound family  $AELiAu(H)$  ( $AE$  = alkaline earth metal). The chemical bonding in these rather unusual materials is characterized by high ionicity of the multi-atomic interactions. Moreover, an in-depth analysis shows that these

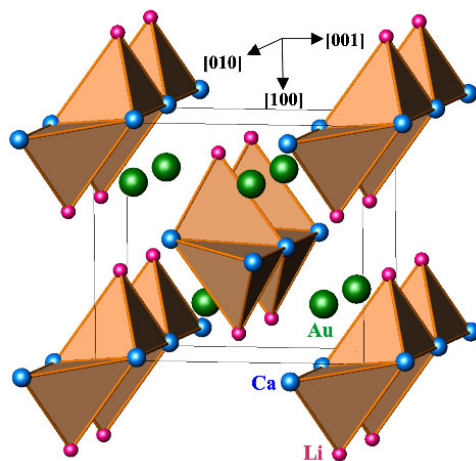


Fig. 1: Arrangement of Au anions and edge-condensed [CaLi] polycations in the crystal structure of CaLiAu.

are so-called ‘electron-excess’ compounds, where one part of electrons, which are not used in the bonding with gold, is employed to form four-atomic edge-condensed polycations  $[\text{Ca}_3\text{Li}] = [\text{CaLi}]$  (Figure 1), i.e. they can be schematically described by the electronic balance  $\text{Ca}^{2+}\text{Li}^{1+}\text{Au}^{1-} \times 2e^-$  or – in polyanionic form –  $[\text{CaLi}]^{1+}\text{Au}^{1-}$ . Alternatively, they can be used for the formation of a hydride  $\text{CaLiAuH}$ .

The adaptation of traditional redox-reactions for the synthesis of intermetallic compounds did not only result in the discovery of a new modification of germanium some years ago [5], but, more recently, also allowed to obtain a new sodium gallide  $\text{Na}_2\text{Ga}_7$  (see [CMS\\_03\\_Baitinger](#)). Due to the very small liquidus window in the phase diagram and a composition which is very close to the already known sodium tetragallide, the phase  $\text{Na}_2\text{Ga}_7$  was not recognized in the binary system for decades (Figure 2). Only the oxidation of Na-rich  $\text{Na}_7\text{Ga}_{13}$  by gaseous  $\text{NH}_3$  revealed the existence of this new phase, which was confirmed to be thermodynamically stable [6].

The achieved progress in preparation techniques paved the way to the specific preparation of single-phase compounds like the already mentioned  $\text{Na}_2\text{Ga}_7$  and  $\text{NaGa}_4$  (22.2 and 20.0 at.% Na, respectively) or  $\text{Be}_7\text{Ru}_4$  and  $\text{Be}_{12}\text{Ru}_7$  (63.6 and 63.2 at.% Be, respectively [7]).

Further adaptation of gas-solid redox reactions for the preparation of intermetallic compounds led to the development of a technique for manufacturing boride-based catalysts for electrochemical energy conversion. The production of hydrogen for energy purposes requires the use of large scale electrolyzers with  $\text{m}^2$ -sized electrodes for water decomposition. One of the ways to apply a catalyst on the surfaces of such size are gas-solid reactions. The discovered reaction of boron halides with metal surfaces allows to deposit a thin layer of a boride-containing catalyst on the electrode surface in an optimal way [8] and [CMS\\_10\\_Antonyshyn](#).

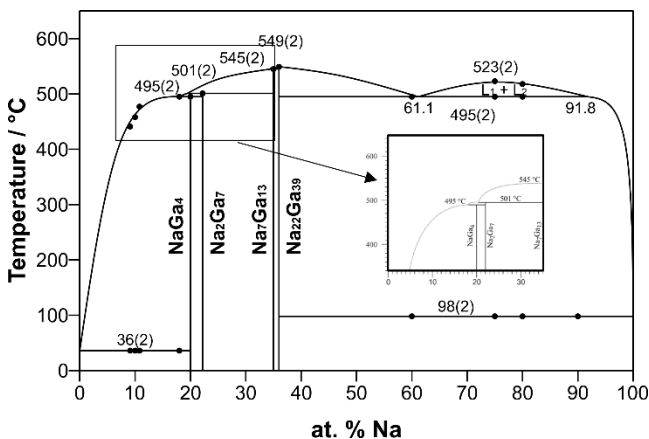


Fig. 2: Re-investigated phase diagram of the Na-Ga system.

Together with chemical composition and temperature, pressure is a state variable for completing the spectrum of preparation techniques for intermetallic compounds. Several dozens of materials were prepared by controlled application of high pressure at elevated temperatures in the past (see [CMS\\_01\\_Schwarz](#)). The proper adjustment of experimental parameters enabled the recent preparation of single crystals under extreme conditions. This, in turn, made the determination of complex crystal structures of hp-phases possible. As a result, the crystal structure of the ‘hp- $\text{Mg}_2\text{Ge}$ ’ –  $\text{Mg}_9\text{Ge}_{5.1}$  was successfully reinvestigated resulting in a new model with complex crystallographic features describing a modulated, partially disordered structure [9].

X-ray powder (PXRD) and single-crystal diffraction (SCXRD) are the traditional characterization techniques for intermetallic compounds. Improving the experimental procedures and data evaluation allowed striking results in the interpretation of local translational symmetry violations in crystal structures. A combination of X-ray diffraction results with findings of atomic-resolution transmission electron microscopy (AR-TEM) – a second key technique for the characterization of intermetallic compounds – was found to be especially efficient. Initial exploitation of the Technai F30 setup (operating voltage 300 kV) showed that its resolution (nominal point resolution 2.0 Å) is by far not sufficient to resolve the atomic arrangements in intermetallic compounds. Therefore, in the year 2014, a JEM-ARM300F, called the Dresden Grand Atomic Resolution Microscope (G-ARM), was installed. It was worldwide the first commercial high-end setup, considered the best TEM at that time. The improved capabilities allowed resolutions down to 0.66 Å for the TEM and 0.40 Å for the STEM mode, respectively (see [CMS\\_05\\_Simon](#)). Such a technical development allowed to understand the real structure of intermetallic clathrates and its importance for phonon transport properties [10]. It also enabled the visualization of violations of translational symmetry in the intermetallic catalyst  $o\text{-Al}_3\text{Co}_4$  [11]. The local atomic disorder in  $\text{Mg}_{29-x}\text{Pt}_{4+y}$  with a crystal structure of approx. 400 atoms per unit cell was resolved using diffraction data in combination with atomic resolution TEM imaging [12]. The local violation of the translational symmetry in the real structure of  $\text{Be}_2\text{Ru}$  was also resolved by combining single-crystal X-ray diffraction analysis with AR-TEM applications [13]. In this apparently simple atomic arrangement (structure type  $\text{Fe}_2\text{P}$ ), three different structure motifs coexist on the atomic level: The parent  $\text{Fe}_2\text{P}$  as a majority and two minority pat-

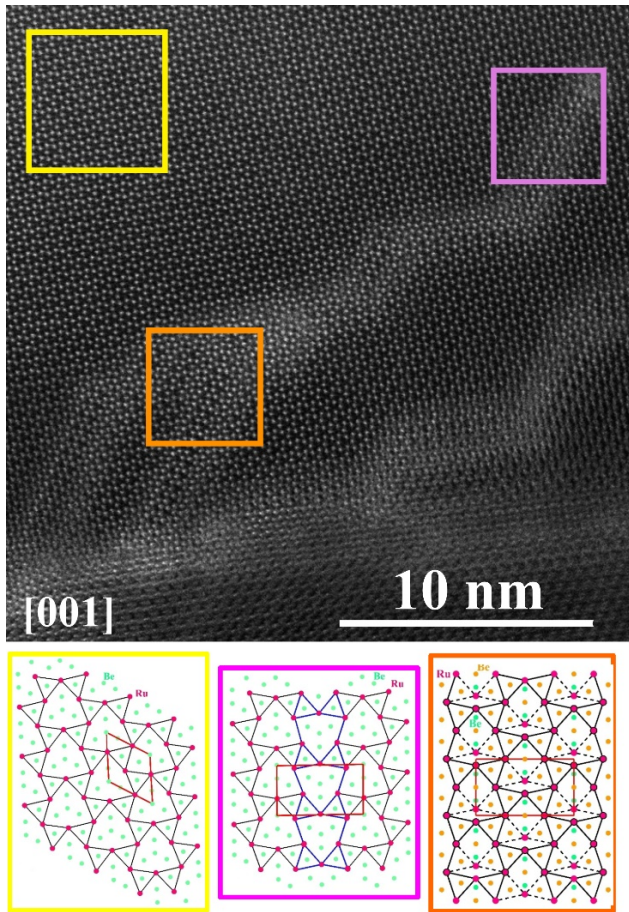


Fig. 3: Local violation of translational symmetry in  $Be_2Ru$  from atomic-resolution TEM and the according atomic arrangements (after [13]).

terns, NbRhB and a new one hitherto not observed among intermetallic compounds (Figure 3). The harsh preparation conditions (cf. high-pressure synthesis above) and/or the formation reactions without participation of a liquid phase make the preparation of single crystals of the desired compound exceedingly challenging if not impossible at all. In this case, using the focused-ion beam technology (FIB) for preparation of  $\mu\text{m}$ -sized single-crystalline specimens from multiphase polycrystalline samples with the electron tomography diffraction experiment allows to develop the primary model of the studied atomic pattern and to perform structure refinement using powder X-ray diffractions data. This approach was applied to the investigation of the new clathrate-VIII  $Na_8B_ySi_{46-y}$  ( $y$  between 3 and 5), whereby the local substitutional disorder was resolved [14], and  $Ge_{32}Co_{9-x}$  [15] with – for an intermetallic compound unusual – chair-like  $Ge_6$  groups as structural units (Figure 4).

Often, the combination of two experimental techniques is not sufficient for the understanding of a material, and involving chemical bonding analysis is necessary to

make further progress. With this approach, i.e. combining three techniques, the chemically unusual mixed occupation of the same crystallographic position by Mg and Pt in  $Mg_{29-x}Pt_{4+y}$  was confirmed [12], the formation of  $Ge_6$  ‘molecules’ in  $Ge_{32}Co_{9-x}$  (Figure 4) could be recognized [15], and the chemical reasons for the complexity of diffraction pattern and real atomic arrangements in  $Ba_6Li_8Ga_8N$  were studied in-depth (see [CMS\\_07\\_Prots](#)).

The importance of the microstructure for the properties of bulk materials is one of the corner stones of material science. An outstanding example here is the influence of the microstructure on the mechanical properties of superalloys operating at temperatures close to their melting points. Thus, at the beginning, optical metallography was used for the analysis of the phase composition during material preparation. Implementation of the electron backscatter diffraction (EBSD) technique into the toolbox of the metallography group was an essential step, allowing to interlink surface properties and bulk crystal structure. In consequence, the determination of the crystallographic orientation of a CaAg catalyst surface, in combination with the bonding analysis, enabled insight into the unusual chemical stability of this material under the conditions of an ethylene epoxidation reaction [16]. Further progress in metallographic analysis was achieved by implementing the enantiomorph assignment technique using EBSD data. The verification of the developed technique (together with A. Winkelmann, AGH Krakow) was brought about by applying SCXRD [17]. This paved the way for the assignment of  $\alpha$ -Mn enantio-

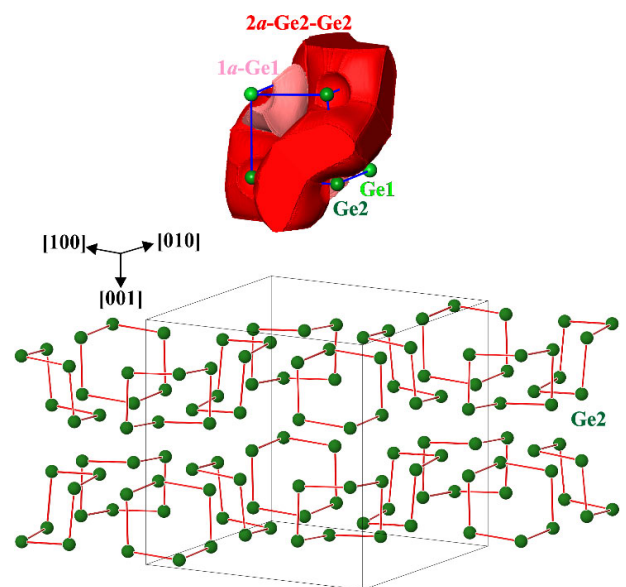


Fig. 4: ELI-D bonding basins and arrangement of chair-like  $Ge_6$  groups in  $Ge_{32}Co_{9-x}$  (after [14]).

morphs in the microstructure, which was impossible by traditional diffraction techniques. Here, the combination of metallography and X-ray diffraction was required to solve the problem [18]. The most recent progress was achieved in the analysis of the microstructure of single crystals of the *non-centrosymmetric* Weyl semimetal CoSi [19]. First, the presence of different enantiomorphs within one crystallite was established by EBSD. The complete analysis of the situation was performed combining this data with the results of SCXRD, AR-TEM, electron tomography and chemical bonding analysis showing and confirming extended regions of both CoSi enantiomorphs in the same crystallite (see [CMS\\_06\\_Burkhardt](#)). In addition, the presence of nm-sized regions of the intermediate *centrosymmetric* atomic arrangement similar to that of KHg was established. The resulting picture resembles a ‘two-phase’ single crystal albeit with huge majority of the ‘main phase’ (Figure 5).

The presented examples underline that the study and the use of the results of the chemical bonding analysis are inseparable parts of chemical research on intermetallic compounds [CMS\\_04\\_Wagner](#). The inherent challenge is the low number of electrons in the outermost shell of the components (hereafter labelled as ‘valence electrons’) forming intermetallic materials. The developed schematic picture can be applied to understand the nature of intermetallic compounds from the point of view of chemical bonding. If a sufficient amount of valence electrons is available in a system, all short interatomic contacts in the crystal structure can be considered as 2c–2e covalent bonds. If the number of valence electrons is reduced, the covalent 2c–2e bonds can be considered only in the anionic part of the structure, and the cations donate their valence electrons to the anionic substructure. In this situation, the Zintl concept applies. Further reduction of the amount of valence electrons requires the conceptual implementation of multi-center interactions (e.g., Wade-Mingos-Lipscomb electron counting schemes). In many intermetallic compounds, the average number of valence electrons is very small, often around two or even less. Nevertheless, or precisely because of this, they often form complex crystal structures with hundreds of atoms in the unit cell and local atomic configurations which resemble (filled) deltahedral clusters with a number of vertices larger than 12. This does not allow for the application of straight forward chemical concepts based on the 8–N rule and 2c–2e or 3c–2e bonds, i.e. the usual orbital picture of chemical bonding. This was the main motivation to study chemical bonding in intermetallic compounds using one-electron functional electron density (ED) [20].

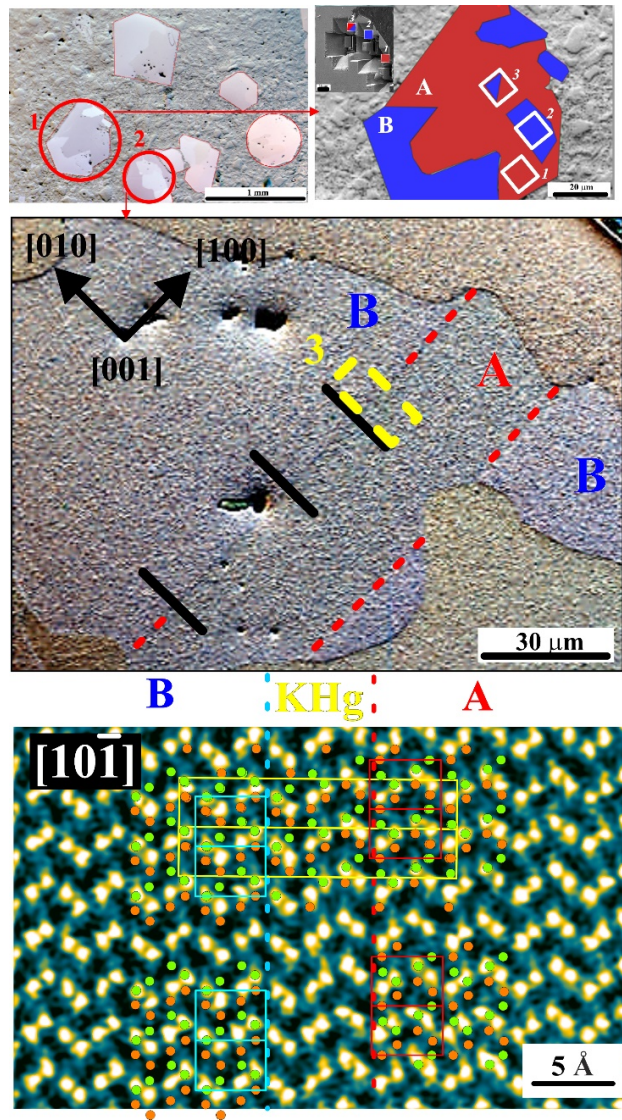


Fig. 5: Enantiomorph assignment in CoSi : (Top left) Crystallites 1 and 2 containing both enantiomorphs; (Top right) Single crystals for SCXRD cut from different regions of crystallite 2; (Middle) Specimen cut for AR-TEM along  $[10\bar{1}]$ ; (Bottom) Coexistence of the CoSi enantiomorphs A and B with the intermediate KHg-like structure in the same crystallite from AR-TEM (after [19]).

This quantity is measurable and – according to the Hohenberg-Kohn theorems – determines the total energy and potential of a system, and thus its properties. In order to look for the link between chemical bonding and properties, the chemical bonding has also to be defined on the basis of the electron density. First attempts to proceed in this direction were made by the analysis of effective atomic charges and charge transfer in intermetallic compounds using the so-called QTAIM (Quantum Theory of Atoms in Molecules of R. F. Bader) approach, e.g., for the systematic analysis of charge transfer in Al–Pt, Y–Ga in the past or, recently, Be–Ru

[21] compounds. To obtain further information about the atomic interactions, the two-electron functional – Electron Localization Function – was used at first. Subsequently, this was replaced by the Electron Localizability Indicator (ELI). The strategy of combining ED and ELI for developing new categories for the description of atomic interactions – the position-space approach – was established. Within this approach a series of quantitative bonding descriptors were derived based on the topological analysis of ED and ELI: atoms as the ingredients for chemical bonding, their effective charges (after Bader), charge transfer, bond participants (atoms contributing to the bond basin) and their contributions to the given bond [20], etc. Based on that measure, the bonding polarity is quantified between one (ionic bond or close-shell situation) and zero (covalent non-polar bond) [22], and ELI-based oxidation numbers (ELIBON) were derived. The last step in the development of the position-space approach was the implementation of the Interacting Quantum Atoms Method (IQA) for crystalline solids. It provides a position-space energy decomposition of crystals. Thereby, all energy components are physically meaningful. The new package *ChemInt* enables users to compute intra-atomic and inter-atomic energies, as well as electron population measures used for the quantitative description of chemical bonds in crystals with different types of bonding [23]. As a general advantage of the position-space approach, all bonding descriptors are derived from the same source (ED) and therefore can – without informational losses – be compared and discussed in a concerted fashion.

The conceptual interpretation of the results of quantum chemical calculations is important because it enables a conceptual use of those quantities. The introduced penultimate shell correction (PSC0) for the electronic occupation of the valence basins represents an important ingredient in this procedure. It paves the way from the effective charges via ELIBON to the (formal) Zintl charges as exemplified for the compound  $\text{La}^{\text{III}}_2\text{M}^{\text{II}}\text{Ge}_6$  and its binary analogous [24]. Thus, it represents a way to the Zintl concept from the quantum chemical point of view.

In the schematic picture mentioned above, the border region between the Zintl count and the Wade-Mingos-Lipscomb one is particularly interesting because it introduces a qualitatively new descriptive category – 3c–2e bonds. In Zintl phases, the octet rule (the basis of the Zintl counting scheme) plays a key role for the polyanions following the 8–N rule, such that a unique correspondence between atomic partial structure and its electron count results. In the conceptual description

of the Wade-type clusters, the relation to the octet-rule is, at first glance, less obvious. For the study of structural implications, a topological implementation of the octet-rule (TORI) within a delocalized bonding scenario is introduced. It builds the bridge between the quantum mechanical bonding analysis by means of delocalization indexes and conceptual electron counts. TORI is based on the average topology of the deltahedral cluster skeletons (Figure 6) as well as on the application of the octet-rule to fractional 2- and 3-center bonds. In this way, two different (hierarchical) types for fulfillment of the octet-rule were identified: the cluster-wise and the local one. The local octet-rule fulfillment also implies the cluster-wise one, but not *vice versa*. The TORI approach opens a way to compare intermetallic compounds containing Wade-type clusters with those containing 8–N type partial structures on the basis of octet-rule implications. The main difference to the 8–N type of partial structures identified by means of TORI is the more flexible way of octet-rule fulfillment in the Wade’s type clusters, where the same cluster topology may be realized with different electron counts, very much in contrast to the ‘classical’ Zintl phases. This opens perspectives to understand the complexity of crystal structures of intermetallic compound [25].

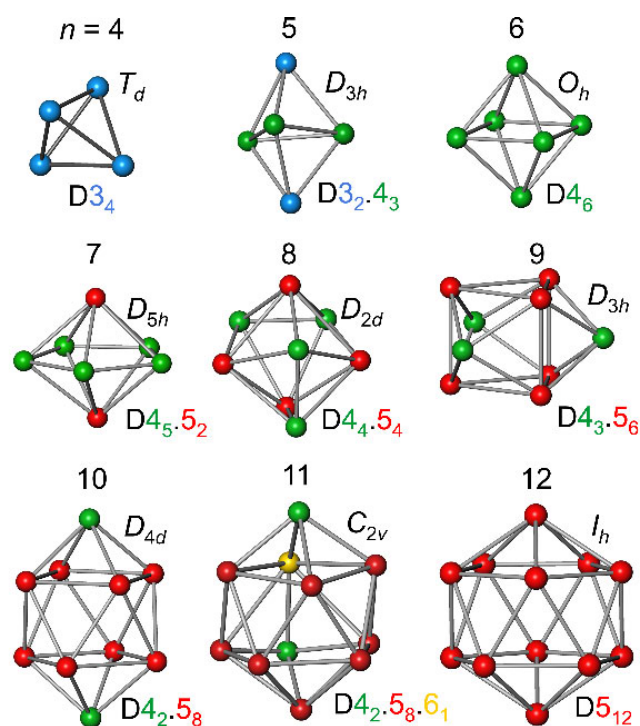


Fig. 6: Deltahedral clusters with 4 – 12 vertices with their symmetry and vertex compositions used for derivation of the TORI approach (after [25]).

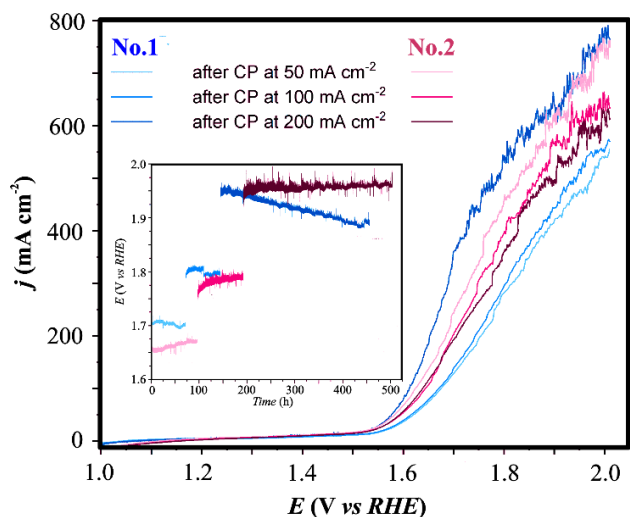


Fig. 7: OER activity and stability (inset) of the new boride catalysts (after [29]).

The issue of chemical bonding in intermetallic compounds proved also successful in exploring the relationships between composition, crystal structure, and properties.

Two types of applications were investigated in detail during the last years – chemical catalysis (see [CMS\\_10\\_Antonyshyn](#), [COLL\\_03\\_Antonyshyn\\_Altendorf](#)) and thermoelectricity (see [CMS\\_08\\_Cardoso-Gil](#)).

The idea to study catalytic properties of intermetallic compounds (cooperation with FHI, Berlin, R. Schlögl group) was already born on the basis of the first investigations of covalent bonding in these materials. The latter was assumed to support the formation of catalytic centers with well-defined chemical environments, which should enhance both the selectivity and the activity (site-isolation concept). At the beginning, the catalysis of the hydrogenation reaction of Pd-containing compounds was at the focus, with the aim to reduce Pd consumption. As a result, the completely new, Pd-free material  $o\text{-Al}_{13}\text{Co}_4$  was discovered [26]. In the following years, these studies transformed into a wider investigation of the chemical properties of intermetallic compounds (cf. also heterophase redox reactions for synthesis of new compounds described above). On the catalytic side, new reactions were investigated, e.g., the ethylene epoxidation (cf. CaAg described above [16]). Currently, water electrolysis with intermetallic compounds is under in-depth investigation because of the demand for materials supporting energy conversion and storage. Besides general studies on the composition and the structure dependence of chemical activity under electrolysis conditions, e.g. of Al–Pt compounds, intermetallic borides are studied with the goal to find new catalysts which prove stable under the harsh conditions in an electrolyzer [27].

The ternary boride  $\text{Hf}_2\text{B}_{2-28}\text{Ir}_{5+8}$  was investigated as a possible step to reduce the amount of iridium in the catalyst as this metal represents the hitherto best performing material for the oxygen-evolution reaction (OER) in water electrolysis. The behavior of this material in the course of the experiments (during which the catalytic activity slightly increased) could only be understood considering bonding features – covalent B–Ir (major) and Ir–Ir (minor, only for non-zero  $\delta$ ) interactions within the anionic boron-iridium framework. In addition, the Ir–B polyanion interacts with the hafnium cations. The cleaving of the crystal structure in the region of the ionic interactions explains the formation of isolated catalytic iridium sites, whereas the breaking of minority Ir–Ir bonds enables the formation of  $\text{IrO}_x(\text{OH})_y(\text{SO}_4)_z$  on the surface, which increases the catalytic activity of the material in the course of the OER experiment [28]. In continuation of this strategy, new Ir-free borides were discovered, which show excellent performance in OER with real (industrial-closed) current densities combined with remarkable stability under such harsh conditions (patent pending, Figure 7 [29]).

Because of the complex interplay of chemical and physical properties of materials in thermoelectric modules, the understanding of the appearance of thermoelectric effects and of the efficiency of thermoelectric materials is difficult without considering atomic interactions [CMS\\_08\\_Cardoso-Gil](#). Systematic analysis of the chemical bonding in thermoelectric materials revealed that the semiconducting or nearly-semiconducting state (necessary condition for a thermoelectric material) appeared based on much more different combinations of bonding types than expected (see Figure 8) [30, 31].

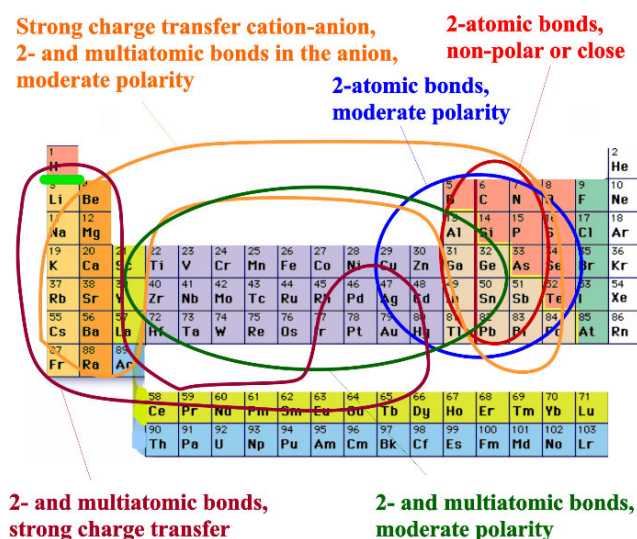


Fig. 8: Combinations of different bonding types in materials showing bandgaps in the electronic DOS (after [31]).

The implementation of the chemical point of view into thermoelectric research was initiated by the finding of additional interactions between guest atoms and the host framework in thermoelectric clathrates, which increases the so-called bonding inhomogeneity (different types of bonding in a material) and, in addition, reduces thermal conductivity. The earlier systematic studies of bonding inhomogeneity and bonding alteration in different crystallographic directions in thermoelectric materials provided insight into the anisotropy of lattice thermal conductivity [32, 33]. Recent research on the relationship between chemical bonding and lattice thermal conductivity was focused on the compound  $Ga_3TM$  with a crystal structure of the  $IrIn_3$  type [34].

Although being considered isostructural, bonding analysis revealed different levels of bonding inhomogeneity, i.e. a different number of atomic interactions (Figure 9).

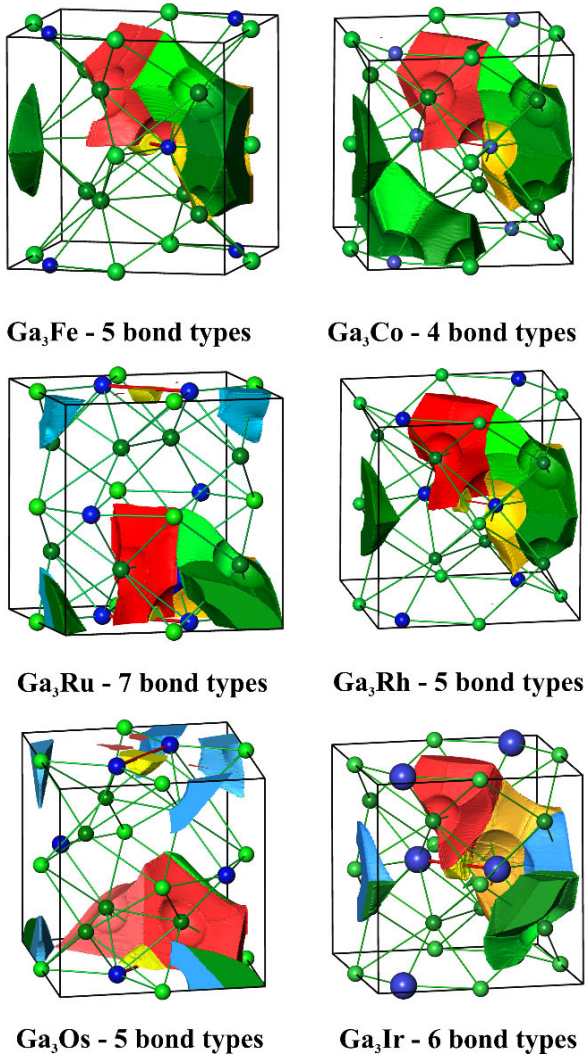


Fig. 9: ELLI-D bond basins in the  $Ga_3TM$  compounds (ideal crystal structure of  $IrIn_3$  type) revealing different bonding inhomogeneity levels.

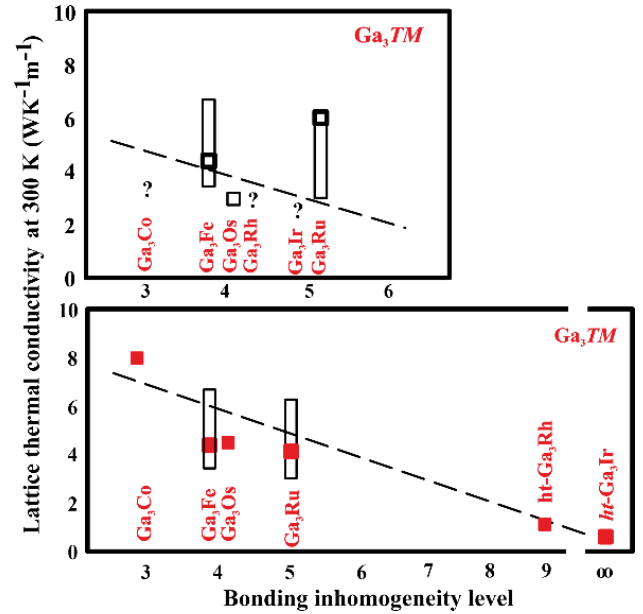


Fig. 10: Lattice thermal conductivity vs bonding inhomogeneity level for  $Ga_3TM$  compounds: (Top) Information obtained from literature in black; (Bottom) Own results in red.

However, the lattice thermal conductivity did not follow the tendency to reduce with increasing inhomogeneity, as it was found in intermetallic clathrates (Figure 10, top). In particular, the behavior of Rh and Ir representatives cannot be understood in this way.

More detailed crystal structure investigations revealed that the crystal structure  $ht-Ga_3Ir$  – due to the thermodynamic metastability at ambient conditions – shows essential violations of translational symmetry on the nm-sized level. This leads to a strong increase of the bonding inhomogeneity in the real material. In addition, the crystal structure of  $ht-Ga_3Rh$  disclosed marked crystallographic disorder of gallium positions. All locally ordered models for describing such a disorder yield pronounced bonding inhomogeneities in comparison with the pristine models of the  $IrIn_3$  type. The crystallographic disorder in both compounds is caused by the increasing importance of the Ga–Ga interactions in these materials, which start to compete with the Ga– $TM$  interactions usually characteristic for materials of the  $IrIn_3$  type. Considering the increased bonding inhomogeneity for  $Ga_3TM$  with rhodium and iridium, the obtained tendency in the reduction of lattice thermal conductivity is close to the expected behavior.

The results summarized in this report clearly demonstrate that the key issue for successful research on the chemistry and physics of intermetallic compounds is a combination of experimental chemical and physical techniques combined with quantum mechanical calculations and chemical bonding analysis.

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## Independent Group Leaders

To better introduce our independent group leaders, their expertise and their careers, we briefly present our independent group leaders in the following.

### Claire Donnelly



Master of Physics (MPhys) at University of Oxford in 2013. PhD thesis “Hard X-ray tomography of three-dimensional magnetic systems” 2017 at the ETH Zurich / Paul Scherrer Institute under the supervision of Prof. Laura Heyderman. After a postdoctoral researcher fellowship at the ETH Zurich (Oct. 2017 – Oct. 2018) a Leverhulme Early Career Research Fellowship at the University of Cambridge, Cavendish Laboratory (Group of Prof. Russell Cowburn) followed. Since 2021 Tenure Track W2 Lise Meitner Group Leader (Spin3D) at the MPI CPfS.

#### Recent Awards, Grants and Fellowships

2024 DFG Heinz Maier-Leibnitz Prize  
2023 ERC Starting Grant: 3DNanoQuant  
2023 IEEE Magnetics Society Early Career Award  
2023 Young Investigator at Technical University of Dresden, Germany

2022 Principal Investigator of WPI-SKCM2: Centre for Sustainability with Knotted Chiral Meta Matter, Hiroshima University, Japan

2020 European Magnetism Association Young Scientist Award

2019 L’Oreal-UNESCO For Women in Science UK & Ireland Fellowship

#### Publications and Invited Oral Presentations

35 peer reviewed journal publications, >90 invited talks

### Uri Vool



Bachelor (B.Sc.) in Mathematics and Physics at Hebrew University, Jerusalem in 2010. PhD thesis in Physics “Engineering Synthetic Quantum Operations” 2017 at Yale University, New Haven under the supervision of Profs. Michel H. Devoret and Steven M. Girvin. John Harvard Distinguished Science Fellow at Harvard University, Cambridge in collaboration with group of Prof. Amir Yacoby (Sep 2017 – Feb 2022). Since Mar 2022 Max Planck Research Group Leader (W2) of the Quantum Information for Quantum Materials Group at the MPI CPfS working on hybrid superconducting resonators and scanning magnetometry with nitrogen-vacancy centers.

#### Recent Awards, Grants and Fellowships

2024 Fraunhofer-Max-Planck Cooperation Grant “OptoQuant”  
2023 ERC Starting Grant: Circuit Quantum Electrodynamics Spectroscopy

2023 Young Investigator at Technical University of Dresden

2020. Harvard Quantum Institute Seed Funding Program

2019 American Physical Society Richard L. Greene dissertation Award

#### Publications and Invited Oral Presentations

29 peer reviewed journal publications, >90 invited talks

## Eteri Svanidze



Bachelor's degree in Physics and Mathematics from the State University of New York (Fredonia, USA) in 2009. Master of Science in Applied Physics from Rice University (Houston, USA) in 2011. PhD thesis, "Itinerant Magnets Composed of Nonmagnetic Elements," completed in 2015 under the supervision of Prof. Emilia Morosan. Postdoctoral fellow at the MPI CPfS from 2016 to 2017. Fulbright Research Chair at McMaster University (Hamilton, Canada) and the Centro Brasileiro de Pesquisas Físicas (Rio de Janeiro, Brazil) in 2018. Leader of the Research of Exotic Actinide- and Lanthanide-based Materials (REALM) independent group at MPI CPfS since 2019. Minerva Fast-Track Fellow from 2019 to 2022, and Boehringer Ingelheim Fellow since 2023.

### Recent Awards, Grants and Fellowships

2024 Early Career Actinides Research Award

2023 European Rare Earth and Actinide Society Junior Award

2023 TU Dresden Young Investigator

2022 Deutsche Physikalische Gesellschaft Physicist of the Week

2022 Plus 3 Perspectives Programme grantee

2022 UNESCO and L'Oreal Women in Science Award

2021 Christiane-Nüsslein Volhard Fellow

### Publications and Invited Oral Presentations

49 peer reviewed journal publications, >60 invited talks

## Berit Godge



Bachelor of Arts in Physics at Carleton College (Northfield, USA) in 2016. Master of Science in Applied Physics in 2019 at Cornell University (Ithaca, USA), following PhD in Applied Physics at the same university in 2022 with the thesis "Advances in scanning transmission electron microscopy for materials discovery and innovation" under the supervision of Prof. Lena F. Kourkoutis. After a short University of California Presidential Postdoctoral Fellowship at UC Berkeley (Group of Prof. D. Kwabena Bediako) in 2022, Schmidt Science Fellow at MPI CPfS (2022 – 2024) and since 2024 independent Minerva Group Leader at MPI CPfS and visiting Assistant Professor at Cornell University (Ithaca, USA).

### Recent Awards, Grants and Fellowships

2023 Elisabeth-Schiemann-Kolleg; Max Planck Society

2022 Schmidt Science Fellowship; Schmidt Futures

2022 University of California President's Postdoctoral Fellowship

2022 Miller Research Fellowship; Miller Institute for Basic Research in Science at UC Berkeley

### Publications and Invited Oral Presentations

46 peer reviewed journal publications, 45 invited talks

## 1.5 Lise Meitner Excellence Group: Spin3D

*Group Leader: Claire Donnelly<sup>#</sup>*

**The aim of my Lise Meitner Excellence Group Spin3D is to *experimentally* investigate nanoscale phenomena in three dimensional magnetic and quantum material systems: both topologically non-trivial configurations that exist in three dimensional space, as well as emergent properties such as chirality, that are induced by three dimensional nanopatterning. We take a combined approach, developing techniques to facilitate the transition from 2D to 3D, that we use to investigate the effect of dimensionality across a variety of materials. In this report, I will present an overview of the main achievements of these last years, which form two main research lines, the study of topological textures, and the local control of emergent properties via 3D nanopatterning. Lastly, I lay out a perspective for the coming years.**

Three-dimensional magnetic systems provide a rich playground for fundamental physics, with higher degrees of freedom, new topologies and geometries combining to produce new effects, that range from emergent chirality, complex energy landscapes, to topological textures that occur on nanometre length scales. By patterning magnetic materials on these length scales, one can tailor their properties via geometrical effects. This is particularly promising when it comes to 3D nanostructures, in which one can achieve exotic properties from curvature-induced magneto-chirality to ultra-high texture velocities. In the first years of this nascent field, the direct imaging of the internal magnetic micro- and nanostructure of 3D magnetic systems, however, was not possible, meaning that the field was generally limited to theoretical predictions. Advances in imaging techniques, and nanofabrication, both of which I have contributed to, provided the capabilities to experimentally address key questions in the field.

Starting my Lise Meitner Group in September 2021, my aim was to take advantage of these recent technical advances to make key steps forward in our understanding of the physics of these complex systems: both concerning topological textures in bulk-like systems, as well as controlling the magnetic properties of 3D nanomagnets, to mimic, and go beyond, phenomena found in the bulk.

Since the start of the group, we have achieved key insights into the physics of 3D nanomagnetic systems – as well as further developments in methodologies – with several high impact publications, and more currently in review in high impact journals. Our contributions have been recognised with over 50 invited talks, including two semi-plenaries, and several awards, most recently the DFG Heinz Maier Leibnitz Prize. I have supervised 13 group members (6 Post-docs, 4 PhD students, and 3 Masters Students) funded via my Lise Meitner Group Resources as well as additional funding (including an ERC Starting Grant,

three von Humboldt Postdoctoral Fellowships and one Marie Skłodowska-Curie Postdoctoral Fellowship). Being embedded in the dynamic environment of the MPI-CPfS and the scientific communities of Dresden and the Max Planck Society has led to new ideas, collaborations, and directions of research. I have extended my group’s focus beyond 3D magnetic systems to investigate the broader topic of 3D Quantum Nanomaterials – for which I was awarded an ERC Starting Grant titled “*3DNanoQuant*”.

### Scientific Achievements

In the following, I will give examples of recent highlights from my Lise Meitner Group, which span textures in extended systems, as well as the tuning of properties with 3D nanogeometries.

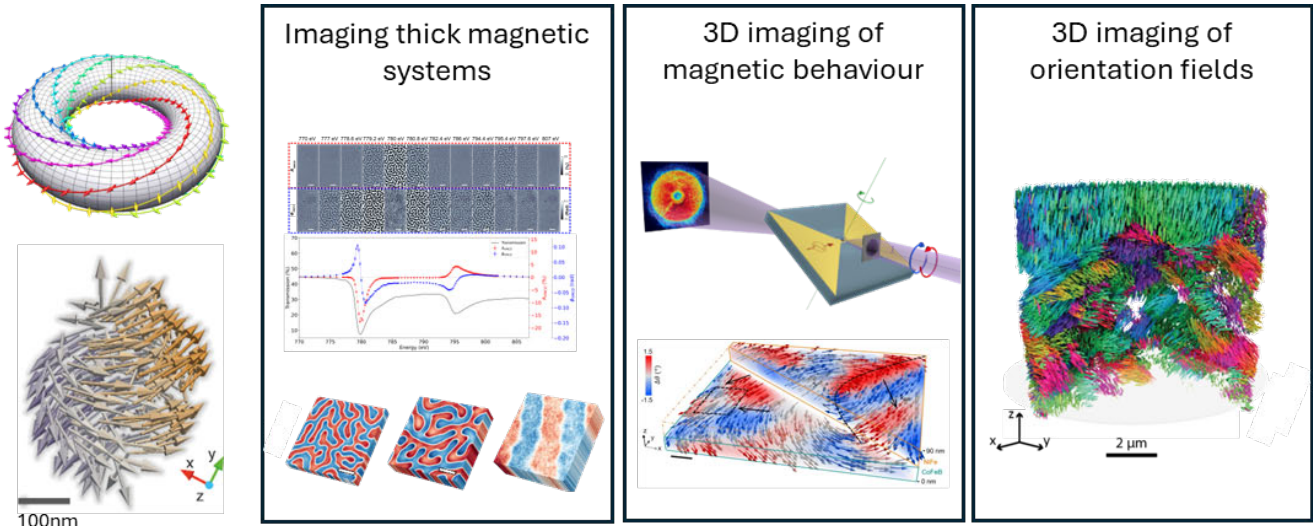
### Topological Magnetic Textures

Topological defects play a key role in the statics and dynamics of material systems. In this part of our research, we map complex 3D configurations, and their dynamics, with an aim to understand and, in the long-term, control them.

#### *Imaging of topologically non-trivial magnetic textures in a wider range of materials*

[Di Pietro Martinez et al., *Phys. Rev. B* **107**, 094425 (2023)],  
[Neethirajan et al., *Phys. Rev. X* **14**, 031028 (2024)]

Although we initially observed our vortex rings in the isotropic ferrimagnet GdCo [1], they were topologically trivial. For topological textures, theory predicted the need for frustration [2] or chirality [3]: and last year hopfion rings were observed in a thin lamella of a chiral magnet [4]. However, the imaging of microsystems, in which such textures would have the freedom to form – and move! – remained limited to rare earth-containing materials [5], and it was not possible to freely explore materials and geometries.



**Fig. 1: Investigating three dimensional topological textures.** Left: our aim is to study – and long-term, control – textures such as magnetic hopfions and Bloch point singularities. To this end we have made progress in three areas: [Left Box]: Through spectroscopic coherent imaging we achieved nanoscale imaging of micrometre thick magnetic systems of arbitrary composition. [Central Box]: By developing new experimental setups, we have imaged the dynamic responses of 3D magnetic textures. [Right Box]: We have extended our 3D imaging capabilities to map 3D orientation fields with linear dichroic orientation tomography, making possible the imaging of local crystal orientations and the identification of grain boundary and topological defects.

We removed this barrier with the development of pre-edge phase imaging [6], a coherent X-ray technique which provides nanoscale imaging of extended magnetic systems of arbitrary composition. With this new capability, we observed first indications of an unconfined magnetic state in a chiral magnet, paving the way to the future study of unconfined 3D magnetic textures. In addition, we demonstrated the broader impact of our technique by applying it to *paleomagnetism* and imaging the configuration of the so-far unexplored giant magnetofossils, whose biogenic origin until now is not known.

Pre-edge phase imaging removes the barrier to studying a wide range of previously inaccessible samples, with potential impact for green energy with non-rare earth permanent magnets, paleomagnetism, and inductive magnets for sensing applications. For further reading please see report [MPRG\\_02\\_Neethirajan](#).

### **Dynamic behaviour of 3D textures in response to external stimuli**

[Finizio et al., *Nano Lett.* **22**, 1971 (2022)],

[Girardi et al., *Nat. Comm.* **15**, 3057 (2023)]

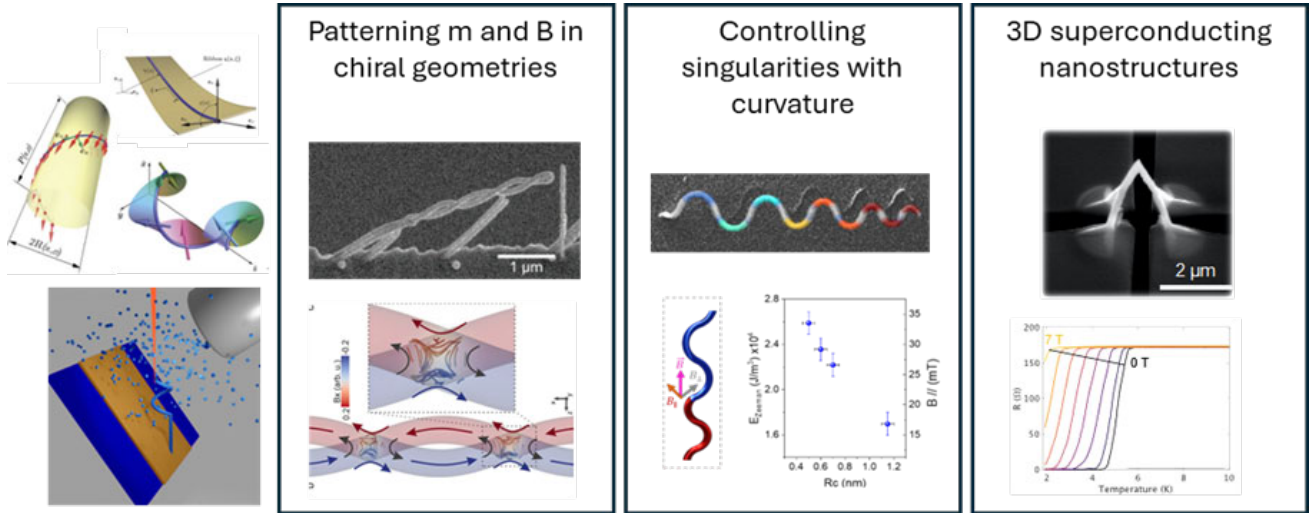
Almost more important than the imaging of complex configurations is gaining insight into their *dynamic* behaviour. For this, one requires 4D mapping, combining 3D magnetic imaging with nanometre spatial and picosecond temporal resolutions. We have developed in situ pump-probe time resolved 3D imaging of the MHz

dynamic response of magnetic configurations [7]. By extending this to arbitrary frequency excitations [8], we have mapped resonant dynamics of magnetic vortices, as well as the 3D distribution and interference of spin waves in a synthetic antiferromagnet [9]. These new capabilities are not only important for 3D textures, but will be key for the growing field of 3D magnonics [10, 11], which promises an efficient solution to conventional computing.

### **3D imaging of systems beyond ferromagnets:**

[Apsenos et al., *Nature (Accepted)*, arXiv.2402.10647]

The imaging of 3D magnetic textures has been highly impactful to the magnetic community. However, mapping 3D configurations is not only relevant for ferromagnets, but a wide variety of materials. We have developed *linear dichroic X-ray orientation tomography*, to directly image 3D orientations with nanoscale spatial resolution. In a first demonstration, we map the local orientation field of a catalyst  $V_2O_5$ , in which we locate and identify nanoscale crystallographic and topological defects [12]. This advance opens the door to the *operando* mapping of a material's nanoscale microstructure, making it possible to determine structure-performance relationships. The natural extension to *other forms of linear dichroism* opens the door to the study of 3D topological textures in antiferromagnets [13] and ferroelectrics [14].



**Fig. 2: Controlling emergent properties with 3D nanopatterning.** The introduction of geometric curvature and chirality (left) leads to local symmetry breaking, and control over a system's properties. In this regard, we have exploited 3D nanoprinting to tune the properties of both magnetic and superconducting nanostructures: [Left Box]: By patterning helical nanostructures, we stabilise bound states in the magnetisation, that lead to topological textures in the magnetic induction. [Central box]: By introducing curved regions into a nanowire, we locally control the symmetry breaking. In this way we gain control of Bloch point singularity-containing domain walls. [Right box]: Through the development of 3D nanoprinting of 3D superconducting nanostructures, we harness geometric anisotropy in the critical field to gain local control of the superconducting state, and realize non-local vortex motion in 3D.

### Tuning emergent properties with 3D nanopatterning

In this area of my research, we harness 3D nanoprinting to explore and tune the properties of materials:

#### **Control of emergent states with geometric chirality**

[Donnelly et al., *Nat. Nano.* 17, 136 (2022)]

Helical nanostructures inherently possess geometric chirality, that combines both curvature and torsion. Previously, we had explored exchange coupled double helices [15] where we observed geometric chirality can be used to induce chiral spin states. We have extended this work to the study of spatially separated double helices, in which the balance of competing energies leads to the formation of a new highly bound state of domain walls [16]. Remarkably, the geometric chirality leads to the imprinting of topological textures in the stray field, proving that we now have the capability of engineering nanotextures in the magnetic induction.

#### **Harnessing curvature to control Bloch point singularities**

[Ruiz Gomez et al., *arXiv:2404.06042 (In Review)*]

Topological defects play a key role in state transformations. However, our understanding of these point defects, and their interplay with chirality, remained limited. In this project, we harnessed curvature-induced chirality to explore the effect of symmetry breaking on the stabilisation of topological defects. By fabricating a model nanowire system with regions of varying curvature, we determined that the resulting local symmetry

breaking leads to an increase in the energy of singularity-containing magnetic domain walls. We exploit this control to pattern asymmetric potential wells and achieve non-reciprocal motion of the defects [17]. This discovery that geometric symmetry breaking can tune the energy landscape of topological defects opens a route to explore the influence of chirality on textures in, for example, antiferromagnets and multiferroics. For further reading see report [MPRG\\_03\\_RuizGomez](#).

#### **Realization of superconducting 3D nanostructures**

[Zhakina et al., *arXiv:2404.12151 (In Review)*]

The same principles of 3D geometrical confinement can be applied to superconductors. We have developed key methodologies: the nanofabrication of 3D superconducting nanostructures with focused electron beam induced deposition, and a framework for 3D finite element time-dependent Ginsburg-Landau simulations with which we can perform experimental and numerical investigations of 3D superconducting nanostructures [18]. Our first demonstration of a 3D superconducting nanostructure, in which we confirm the presence and propagation of superconducting vortices in 3D [18], represents a key step towards 3D fluxonic devices. With these new capabilities, it will now be possible to prototype 3D superconducting nanostructures, to explore emergent anisotropies, and non-trivial transport arising from topological Meissner currents. For further reading see report [MPRG\\_04\\_Zhakina](#).

## Going forward

Three years into my Lise Meitner Group, the field of 3D magnetism is gathering pace. With first experiments having already provided several key insights into the roles of topology, symmetry and complex interactions, we are at an exciting moment in the field, where the move from model systems to the study of more complex configurations and materials promises exciting opportunities for fundamental physics and first applications.

In the next years, we will extend our exploration of three dimensions beyond the materials that we have studied so far, to **explore the wider physics of 3D quantum nanosystems**. For example, we will address chiral magnets (can we tune the properties via a combination of intrinsic and geometric symmetry breaking?), antiferromagnets (can we image 3D Neel vector configurations?), and superconductors (can we influence the order parameter geometrically?). We will continue to work with colleagues at synchrotron facilities to push our experimental capabilities, and explore the opportunities provided by the latest upgrades in synchrotron science (can we exploit increases in coherent flux to probe weak resonant signals previously not accessible?).

Long-term, there are many exciting possibilities. The transition from 2D to 3D, and the principles of topology and symmetry can be applied to various classes of materials beyond what is proposed here: from multiferroics, to unconventional superconductors, and topological materials.

## External Cooperation Partners

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## 1.6 Max Planck Research Group: Quantum Information for Quantum Materials

Group Leader: Uri Vool<sup>#</sup>

**Our group works at the intersection of quantum information and condensed matter physics, and seeks to improve our understanding of quantum phenomena by combining insights from the complex structure quantum materials and the control and coherence available in quantum bits. We utilize coherent quantum systems as sensitive probes to explore the structure of novel materials, and utilize quantum materials to create new hybrid devices for basic science and quantum technology applications. Our group specializes in two experimental techniques: (1) hybrid superconducting circuits in which macroscopic microwave devices are integrated with quantum materials, and (2) local sensing using single spins based on nitrogen-vacancy centers in diamond, and particularly scanning magnetometry measurements. This report will highlight our research capabilities and recent results, and give a perspective on future research directions.**

### Exploring the structure of novel superconductors with microwave quantum circuits

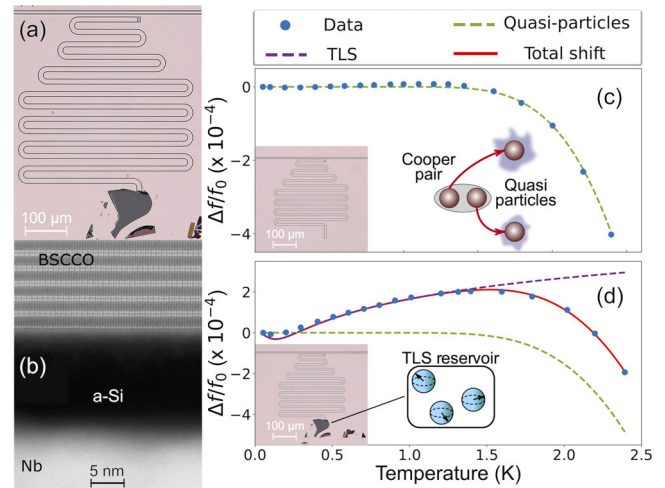
More than a century after its first observation, superconductivity remains a remarkable and puzzling effect. A growing collection of materials is showing a widening selection of different behavior, but their underlying microscopic structure is still a major open question. While most measurements have focused on bulk crystals, there is growing interest in the unique superconductivity of low dimensionality systems such as thin films and van der Waals (vdW) flakes. These systems offer significant advantages such as electrical tunability and the ability to create new materials by stacking different layers into heterostructures, but their small size and delicate nature means that many bulk measurement techniques cannot be applied to these materials, requiring the development of specialized probing techniques.

For example, the London penetration depth is a common probe of the superconducting gap symmetry through its relation to the superfluid density  $n_s$  as  $\lambda_L^{-2} = \mu_0 n_s e^2 / m$ , where  $m$  is the effective electron mass. Deviations of the penetration depth with temperature well below the critical temperature of the superconductor are a strong indicator of lower symmetry and nodes in the superconducting structure [1]. However, it requires large, pure crystal samples placed in a magnetic coil, and is thus inapplicable to nanometer thin and micrometer sized samples.

We overcome this challenge by integrating the samples into superconducting microwave circuits – macroscopic coherent devices which are a leading platform for the implementation of quantum technology [2]. As high-frequency (AC) electrical current passes through the sample, it gives a reactive response that is often described by a kinetic inductance  $L_K = m / n_s e^2 \cdot l / A$ , where  $l$  and  $A$  are the sample length and cross-section, respectively. This inductance is due to the inherent mo-

ment of inertia of the charge-carrying Cooper pairs and is completely separate from magnetic induction, but it affects the microwave circuit in a similar way by shifting its resonance frequency  $\omega_r = 1 / \sqrt{C(L + L_K(n_s))}$ . The geometric term  $l/A$  means that the inductance is actually larger for thin and small samples (as opposed to magnetic induction), making this technique ideal for small samples, thin films, and vdW flakes.

In recent work which started at Harvard University, we used this technique to study a superconductor-ferromagnet bilayer. The ferromagnet can hybridize with



*Fig. 1: Hybrid superconducting resonator with a BSCCO flake. (a) An optical image showing a coplanar niobium resonator made of 50 nm niobium film, with a BSCCO flake exfoliated on top, shorting the center line to the ground plane. (b) Transmission electric microscope image of the BSCCO flake on top of the niobium film, showing an atomically pristine interface. (c-d) Resonance frequency vs. temperature for a niobium resonator without and with a flake, respectively. (c) shows good agreement with the conventional model of thermal quasiparticle generation, while (d) shows a strong upshift in temperature. Images taken from ref. [6].*

the superconducting layer to develop a hybrid superconductor at the interface, where competition with the spin polarization can lead to a reduced symmetry of the superconductor. Even though this system has been studied for many decades, this new measurement technique was able to identify a previously unknown property within it – a two-fold asymmetry in the node structure [3]. Such symmetry is typically associated with so called “p-wave” superconductors, an elusive type of superconductor that is highly sought after for its protected quantum states but has thus far not been identified.

This novel measurement technique is especially useful for exploring new unconventional superconductors in 2D vdW flakes and heterostructures, for which conventional bulk techniques are incompatible. However, the integration of a vdW flake and a thin-film superconducting resonator is nontrivial as the fabrication of both devices has been optimized separately in potentially incompatible ways, and imperfections in the interface can ruin the quality of the resonator as well as the flake. In our group and in collaboration with Dr. Nicola Poccia from IFW Dresden, we have developed a technique to create hybrid resonators by cryogenic exfoliation of the flake in an Argon environment and placing it on top of the resonator in a node of maximal current (see Figure 1a). This technique utilizes developments in cryogenic exfoliation for vdW twisted heterostructures [4].

Our initial devices use a flake of the cuprate superconductor  $\text{Bi}_2\text{Sr}_2\text{CuCa}_2\text{O}_{8+x}$  (BSCCO), which is typically highly sensitive to fabrication imperfections. Transmission electron microscopy measurements done with the SSQM group in our institute show a pristine atomic interface of the BSCCO flake at the interface with the niobium thin film resonator (see Figure 1b). Additionally, the hybrid superconducting resonator maintains a high quality factor of  $3 \times 10^4$ . These experiments show the robustness of our fabrication technique, and its potential for a variety of vdW flakes and heterostructures.

The temperature dependent resonant frequency of the hybrid resonator defers substantially from the conventional niobium resonator. The niobium resonator shows an exponential negative frequency shift due to the generation of thermal quasiparticles within the BCS model and with a gap consistent with thin-film niobium (see Figure 1c). The hybrid resonator, however, shows a significant positive shift of the resonance frequency with temperature before the onset of thermal quasiparticles. Such an effect is often attributed to interaction with a bath of saturable states modelled as two-level systems (TLS) (see Figure 1d). However, such a strong coupling would generally significantly limit the coherence of the resonator, while our observed quality factor remains in-

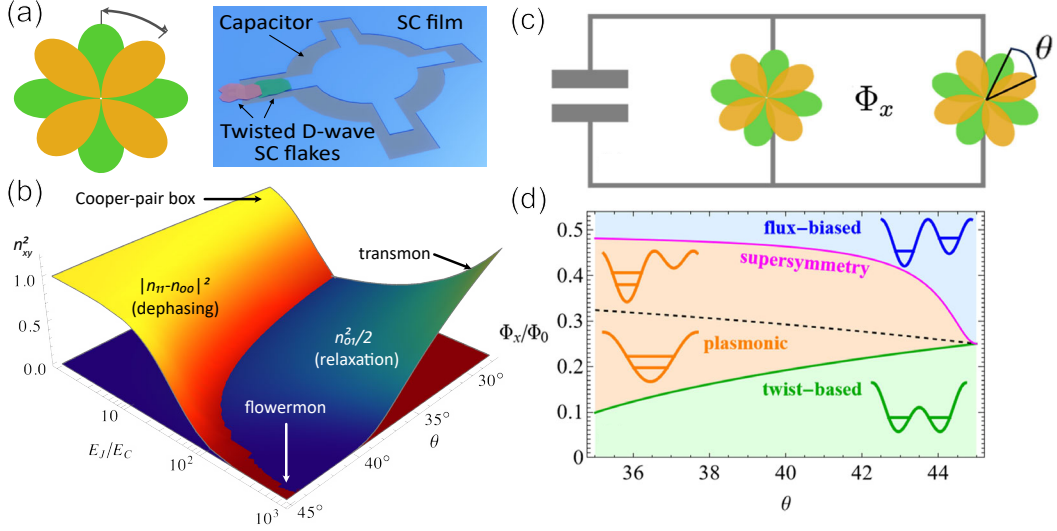
consistently high. This suggests that the bath is mostly made up of low-frequency (sub-GHz) systems within the BSCCO flake, potentially due to weak-pinning pancake vortices which are central to cuprate superconductivity [5]. Additionally, we observe an upshift of the resonance frequency with driving power, indicating a positive non-linearity in the circuit. Thus, our measurements show strong anomalous behavior in the microwave response of the BSCCO flake and further experiments can isolate the microscopic origin of the effect and clarify the rich structure of this unique superconductor. Furthermore, these results show that our hybrid circuits can be used as robust sensors for a wide variety of materials and heterostructures. For more information, see Ref. [6] or the web article [MPRG\\_01\\_Lee](#).

### **Flowermon: A protected qubit based on twisted cuprate heterostructures**

The previous section focused on the use of hybrid superconducting circuits as sensitive probes of unconventional superconductors. However, the unique properties of these materials can also be used to create new devices for quantum technology. Building on our expertise in vdW hybrid superconducting circuits and recent developments in cuprate twisted heterostructures, we design a superconducting quantum bit (qubit) protected from environmental noise by the d-wave symmetry of the cuprate.

Superconducting qubits use the quantized energy levels of an L-C microwave oscillator as the states of an artificial atom for coherent quantum operations. The Josephson junction is a key element of a superconducting circuit as its nonlinear energy potential  $-E_J \cos(\varphi)$ , where  $E_J$  is the Josephson energy and  $\varphi$  is the superconducting phase difference across the junction, breaks the equal energy splitting of the harmonic oscillator levels and allows the qubit states to be addressed individually [2]. The most commonly used qubit, known as the ‘transmon’, is made up of a Josephson junction in parallel with a large capacitor. In this simple design, the qubit is insensitive to drifts in the charge across the junction, significantly improving its coherence time [7]. However, the transmon is still sensitive to electrical fluctuations resonant with its energy splitting, and the large capacitor size couples strongly to fluctuations in its environment. This is currently the key limitation for the scaling of commercial quantum hardware.

In a Josephson junction made of planes of BSCCO flakes, the critical current strongly depends on the twist angle, with a minimum at  $45^\circ$  [4]. This can be attributed to the d-wave order parameter of the cuprate, as a mis-



*Fig. 2: Flowermon qubit. (a) Flowermon design: a twisted d-wave heterostructure Josephson junction shunted by a large capacitor. (b) Matrix elements of the Flowermon for different values of the Josephson energy  $E_J$  and the twisting angle  $\theta$ , showing the protection of the flowermon from both relaxation and dephasing noise. (c) Flux-tunable flowermon made as two twisted d-wave junctions in a flux loop. (d) Phase diagram of the different types of artificial atoms accessible in the flux-tunable flowermon. Images taken from refs. [9, 10].*

match in the momentum of the Cooper pairs on both sides prohibits tunneling. However, the critical current is not completely suppressed at  $45^\circ$ , possibly due to a second order effect where two Cooper pairs tunnel jointly. A Josephson junction dominated by two-Cooper-pair tunneling will have a corresponding energy potential of  $E_J \cos(2\varphi)$ , a double well potential with an inherent degeneracy. This double well structure is related to topology, and a spontaneous symmetry breaking into one of the wells has been described as the emergence of a chiral  $d \pm id$  superconducting order [8].

Our protected qubit, nicknamed 'flowermon' due to the petal shape of the twisted d-wave order, consists simply of such a twisted junction dominated by two-Cooper-pair tunneling and shunted by a large capacitor (see Figure 2a). As the tunneling conserves Cooper pair parity, the two energy states that define the qubit have distinct and opposite charge parities – one consists of only even Cooper pair states and the other only odd. This symmetry prevents any electrical manipulation of the qubit, making it completely insensitive to fluctuations in the electric environment. Together with the protection from charge drifts it inherits from the transmon, the flowermon is strongly decoupled from all noise sources, leading to an exponential improvement in qubit coherence time [9] (see Figure 2b).

In a later manuscript, we explored a slightly more complex system where two d-wave junctions are brought together in a SQUID loop [10] (see Figure 2c). This relatively simple circuit gives rise to a wide phase space of quantum systems by varying the twist angle and the

magnetic flux in the loop (see Figure 2d). These works show that incorporating novel superconductors into circuits can lead to significant improvements for devices in quantum technology, as well as for the exploration of basic effects in quantum physics, both in theory and in practice.

### Scanning magnetometry with a single spin

Atomic defects in a crystal sometimes show remarkable quantum effects. The most notable such defect is the nitrogen-vacancy (NV) center in a diamond lattice, where two neighboring carbon atoms are substituted with a nitrogen and a vacancy. The electron spin of the NV centers maintains high (up to millisecond) coherence at room temperature, and the photoluminescent response of the defect depends on the spin state. These two surprising properties allow for the manipulation and measurement of the spin state – making it a leading implementation of a qubit for quantum technology. The electron spin energy levels are sensitive to the local magnetic field due to the Zeeman effect, and so the NV center can also be used as a highly sensitive magnetometer capable of detecting signal in the nanoTesla range in the atomic resolution of the defect [11].

The NV center can be seen as an artificial atom similar to the superconducting circuit, but while the latter is a macroscopic strongly-coupled system, the former is of truly atomic size. Therefore, it's benefit as a sensor would be best used for local field imaging. The practical limit on the spatial resolution of the NV is set by the

distance of the defect to the material being probed, which is fundamentally limited by the distance of the NV to the edge of the diamond to about 10–15 nm. To utilize this spatial resolution and make the NV a robust center for various samples, we utilize the NV as a scanning probe, where the diamond is etched into a pillar with a single NV center at its apex (see Figure 3a). By scanning the NV defect across a sample and measuring the spin energy state at every point, we can obtain a quantitative map of the local magnetic field with high sensitivity and resolution, across a wide temperature range.

NV scanning magnetometry is most often used to study static magnetic textures in thin films, such as magnetic domains in ferromagnets or anti-ferromagnets, or topological features such as skyrmions (see Figure 3b). However, the magnetic sensitivity of the NV is improved for AC signals, where it can be decoupled from low frequency noise by Hahn-echo sequences and achieve high coherence. Such measurements require syncing the measurement signal with the control pulses of the NV. In previous work, we pioneered the use of this technique for imaging local electrical currents to observe electric hydrodynamic flow [12] and vortices in a Josephson junction [13]. Furthermore, the NV can also be used to image dynamic textures in the GHz range, by manipulating the NV spin states resonantly.

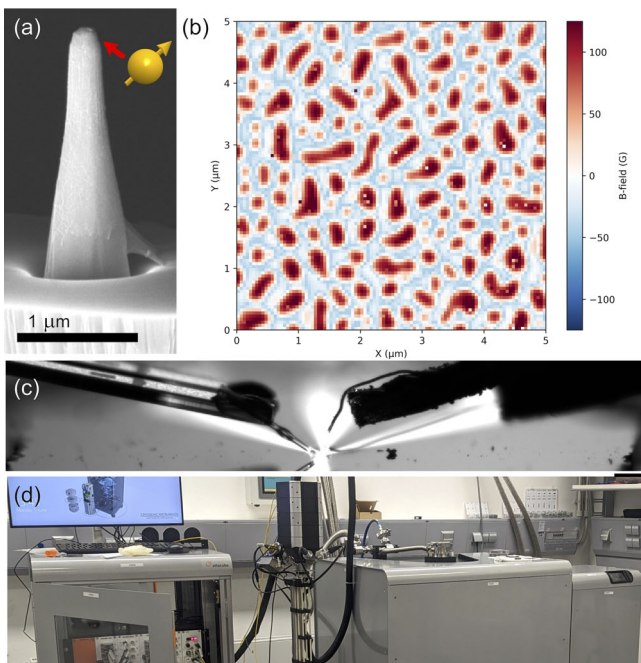


Fig. 3: NV scanning magnetometry (a) Diamond tip with a single NV at its apex (b) Magnetic image of a potential skyrmion lattice in a  $Fe_{3-x}GaTe_2$  flake taken using our ProteusQ setup. (c) Tip and microwave delivery coil in the ProteusQ chamber (d) AttoDry220 cryostat and cryogenic scanning setup.

Our group currently has two NV scanning systems: a room temperature ProteusQ scanning system from Qnami, and a cryogenic scanning system based on the AttoDry 2200 cryostat from Attocube. The ProteusQ system (installed in October 2023) is already operational, and is now being actively used to study various magnetic textures and dynamics, while additional capabilities such as pulsed AC sequences are still being developed. The cryogenic setup allows for scanning at 2–300 Kelvin with a 5-1-1 Tesla vector magnet, and uses custom in-house hardware for microwave qubit manipulation, driving laser and optical measurement, and control of the scanning stages. Cryogenic NV scanning microscopes are at the forefront of the field, with only a few working systems around the world, and offer a significant challenge for their setup and operation. One year after the installation of the cryostat in July 2023, we are now taking the first test images in the cryogenic scanning setup and hope to start using it for scientific exploration soon. For more information, see the web article [COLL\\_01\\_Binger\\_Vool](#).

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## 1.7 Minerva Group: Research of Exotic Actinide and Lanthanide Materials – Exploring old and new mercurides

Group Leader: Eteri Svanidze<sup>#</sup>

Peculiar properties of mercury were realized early on – first records of mercury-based alloys (or amalgams) go back to the Tang dynasty. Initially, the high toxicity of mercury was overlooked, making amalgams popular in dentistry – hence much research was focused on their mechanical behavior. In the end of the 20<sup>th</sup> and beginning of the 21<sup>st</sup> century the interest in low-temperature properties of mercury compounds was spiked by several discoveries, highlighting that this element has a lot more to offer. This report features several mercury-based systems that have been in the focus of the REALM group. We illustrate that by overcoming challenges associated with experimental work on mercury, we can address many open questions in condensed matter physics and solid-state chemistry.

It is well-known that mercury-based compounds (mercurides) show peculiar characteristics, ranging from high superconducting critical temperatures to topologically non-trivial states. It is likely driven by large spin-orbit coupling of mercury, coupled with complex bonding scenarios frequent in mercury-based materials. However, when it comes to mercury compounds containing lanthanide or actinide elements, not much work has been previously carried out. This is particularly surprising, given that by mixing *d* and *f* orbitals, strong correlations are bound to emerge, giving rise to many peculiar quantum phenomena. *The work of the REALM group explores this knowledge gap by using a set of specialized experimental advances in order to successfully target, synthesize and study materials that show unique chemical and physical properties.* The small energy scales of our compounds, coupled with their complex architectures, give us ample opportunities for tuning, which can lead to further exotic fea-

tures. Overall, *by exploring the unexplored parts of the periodic table, we aim to radically change the realm of quantum materials.*

### Experimental advances

The lack of studies on mercurides can be understood from a chemical perspective – besides high toxicity, reactivity, and vapor pressure, these materials exhibit extreme air- and moisture-sensitivity (Figure 1). Moreover, many questions remain regarding the binary phase diagrams – in particular with respect to the solubility ranges as well as phase existence and compositions. Here, the work of chemists supersedes those of physicists, as for most amalgams and mercurides studies of chemical features are far more common compared to work on physical properties. We tackle mercurides in two complementary ways: first, we perform exploratory synthesis in specialized conditions [1] and report

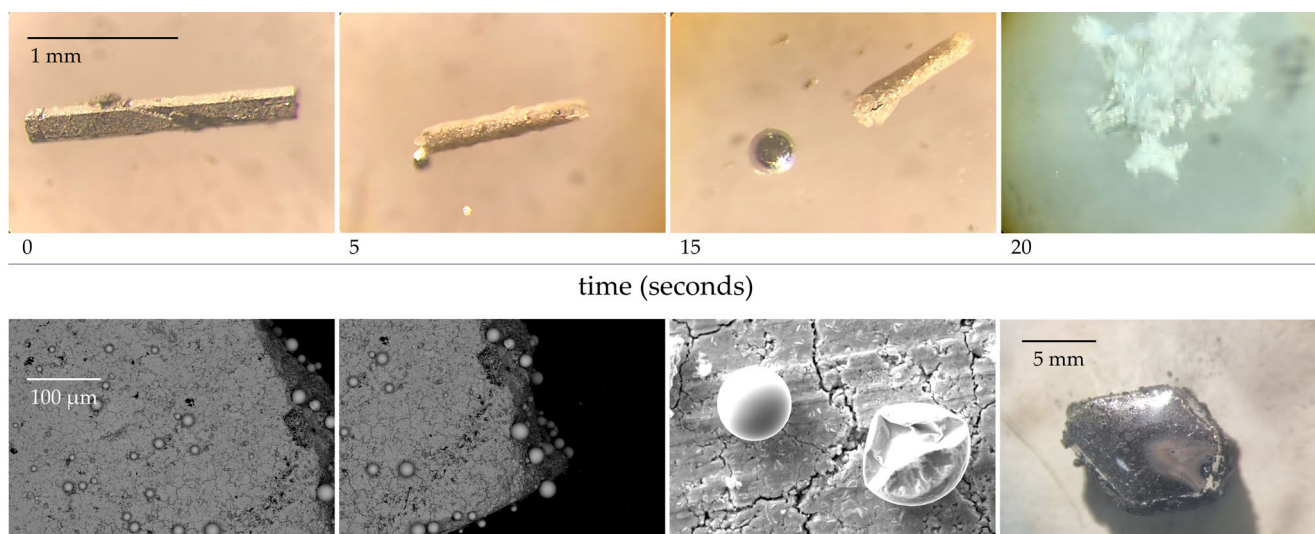


Fig. 1: Decomposition timeline of air-sensitive mercury compounds. Typically, mercurides decompose into oxides/nitrides and elemental mercury. The latter will then dominate the measured physical properties.

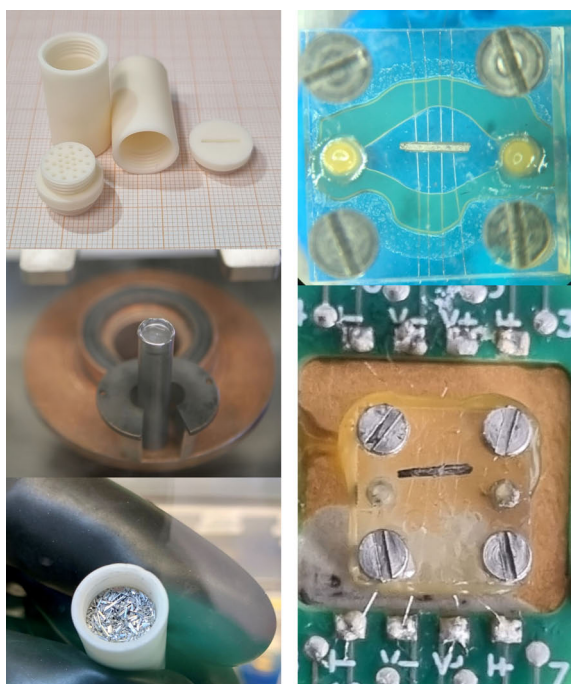


Fig. 2: Custom-made crucibles used to synthesize mercurides are sealed in tantalum and then centrifuged at room temperature (left) [2]. Resistivity cell, designed by our group, which is able to protect air-sensitive samples from decomposition (right) [6].

**CMS\_02\_Leithe-Jasper.** In order to ensure constant stoichiometry and vapor pressure of mercury during synthesis, we have designed custom-made alumina crucibles, which are now available commercially [2], see Figure 2 (left panels). Second, we have been creating new ways to measure electrical resistivity of air-sensitive materials. Typically, electrical resistivity of solid-state materials can be measured by attaching either macro- or micro-scopic leads to the sample surface. These can be secured by welding, applying mechanical pressure, conductive epoxy or a conductive material such as gold by controlled evaporation [3–5]. Neither of these methods work for mercurides, which is why we have designed and manufactured a custom

resistivity cell [6], shown in Figure 2 (right panels). It consists of two sheets of polymethylmethacrylate (PMMA), which are held together by screws. Platinum wires are placed under the sample and then pressed against the sample’s surface. Without contact with the sample itself, the vacuum grease creates a barrier, protecting the sample from the environment. The other end of the wires can be soldered onto a resistivity puck. In mercury-based materials, a surface layer of elemental mercury frequently presents an obstacle when measuring electrical resistivity. As we have shown in our studies [6–8], using our new experimental methodology, we are now able to measure intrinsic electrical resistivity of several mercurides, which remained inaccessible prior to our work. Of course, these advances are not only of relevance to researchers pursuing mercurides, but rather to all those working on air-sensitive materials. This opens up a unique possibility to study electrical properties of previously inaccessible solid-state systems.

### Crystallographic peculiarities

When it comes to crystallographic investigations of mercury-containing compounds and alloys, peculiar bonding scenarios are promoted by mercury, giving rise to varying degrees of complexity. The uranium-mercury binaries are an excellent example of the range that mercurides span – from simple structures with 3 atoms per unit cell (APUC) to exceptionally complex cluster-like materials with 444 APUC – see Figure 3. We have postulated that high coordination observed in these compounds is one of the reasons behind the enhanced electron masses of these compounds [7, 9].

What is particularly challenging, is to determine the intrinsic structure of mercurides in full-detail. As mentioned above, many of these materials decompose within seconds of exposure to air. Given that for single crystal x-ray diffraction studies, a sample on the order

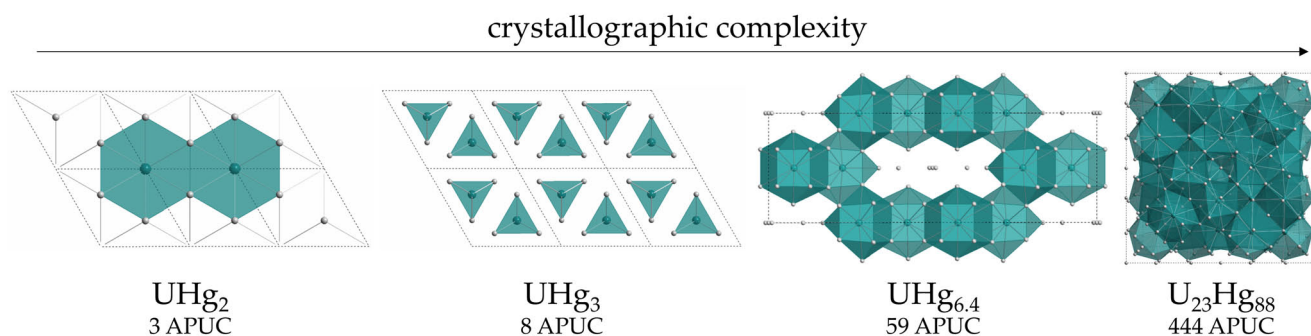


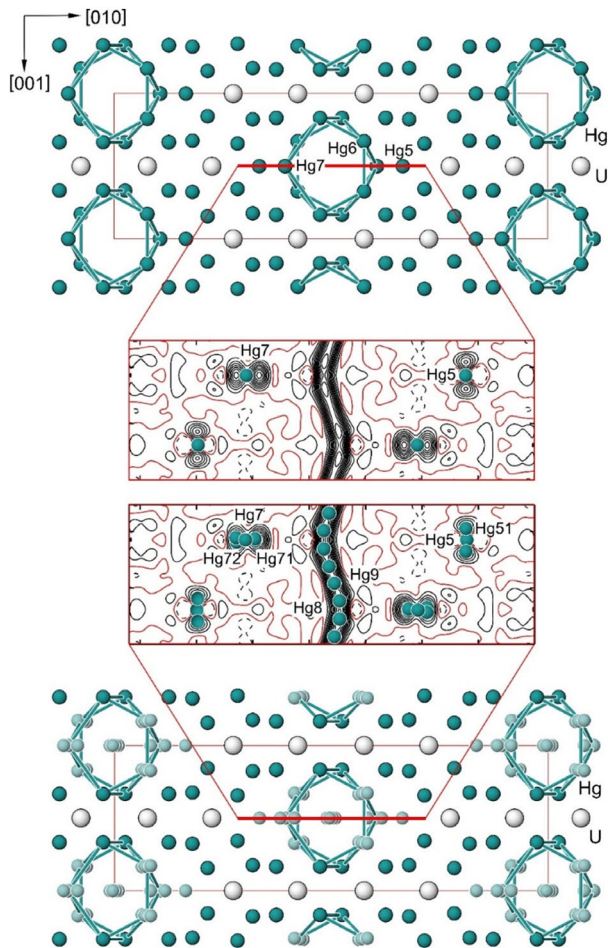
Fig. 3: Structures of mercurides are diverse – from exceptionally simple, as showcased by  $\text{UHg}_2$  (with 3 atoms per unit cell, left) to extraordinary complex, such as  $\text{U}_{23}\text{Hg}_{88}$  (with 444 atoms per unit cell, right) [7,9].

of  $40 \times 40 \times 40 \text{ }\mu\text{m}$  is usually considered – protection of these cuboids, not just from reaction with oxygen/nitrogen, but also from overheating due to the x-ray beam exposure is rather arduous. This is why for many mercurides, only the structures derived from the analysis of the powder diffraction data were available prior to the start of our work. Even for more air-sensitive mercurides, a 20–30-minute scan is possible with the help of some protective membrane (such as Kapton film, for example). The first example of a complex structure that we considered was  $\text{U}_{23}\text{Hg}_{88}$  ( $\text{Sm}_{11}\text{Cd}_{45}$  structure type) [9,10]). While an investigation of its crystal structure was performed back in 1979, powder diffraction data failed to capture one additional crystallographic position. Our single crystal analysis [9] clearly showed that doubling of the unit cell is necessary to account for this. This material is one of the heaviest

uranium-based heavy-fermion compounds and a comprehensive analysis of its structure is the first step in understanding how physical and chemical features of  $\text{U}_{23}\text{Hg}_{88}$  are interrelated [6, 7]. In a newly discovered uranium-mercury binary  $\text{UHg}_{6.4}$  ( $\text{LaHg}_{6.4}$  structure type), we have placed emphasis on structural elucidation of disorder which we knew would likely be present based on our study of isostructural  $\text{LaHg}_{6.4}$  [8] (see also [section 1.4](#)). In the latter, the structural description remained elusive for nearly 50 years, prior to our work which conclusively showed that this quasi-one-dimensional material is crystallographically disordered along the  $c$ -axis. In the  $\text{UHg}_{6.4}$  analogue, the same structural arrangement is seen – with non-integer composition arising due to the extra positions of Hg (for example, around the Hg5 and Hg7 sites, see Figure 4). For both  $\text{LaHg}_{6.4}$  and  $\text{UHg}_{6.4}$ , their disordered structure is rather robust – we did not see any evidence of a homogeneity range in these systems and their physical properties (superconductivity and magnetism) remain unchanged from sample to sample.

### Superconducting properties

Low-temperature properties of mercurides have made significant impact on the world of quantum materials – in many compounds, we are able to observe unconventional superconductivity and unique magnetic configurations. Among superconducting binary mercurides based on lanthanide and actinide elements, we have identified several superconductors. As summarized in Figure 5, superconductivity of  $\text{LaHg}_{6.4}$  [8],  $\text{YHg}_3$  [6] and  $\text{LuHg}_3$  [6] was discovered recently by our group. It is important to note that in all three compounds, various types of crystallographic disorder are present – this already gives a hint regarding conventional superconductivity of these systems. Indeed, all three compounds display low critical temperatures and fields, supporting conventional electron pairing. Given their considerable air-sensitivity, our novel experimental solutions (summarized in Figure 2), were critical in unveiling the properties of these compounds. Interestingly, the limit of superconductivity in binary mercurides seems to be on the order of the superconducting temperature of elemental mercury itself – around 4.2 K. This, of course, poses an important question as to whether or not an intermediate class of mercury-based superconductors can be realized – one that bridges the gap between conventional (low-temperature) superconductors and unconventional (high-temperature) ones. To explore this, we have ventured out to examine mercurides containing alkali- and alkali-earth elements. Here, crystal structures appear to be



*Fig. 4: In the crystal structure of the newly discovered  $\text{UHg}_{6.4}$  the distribution of the difference electron density in the part of the  $(200)$  plane clearly shows that some atoms are missing in the structure (upper panels). By modifying the structure of  $\text{UHg}_{6.4}$  to include split positions around Hg5 and Hg7 sites, the gaps in the density disappear, confirming that the structure model is now complete (bottom panels) [7].*

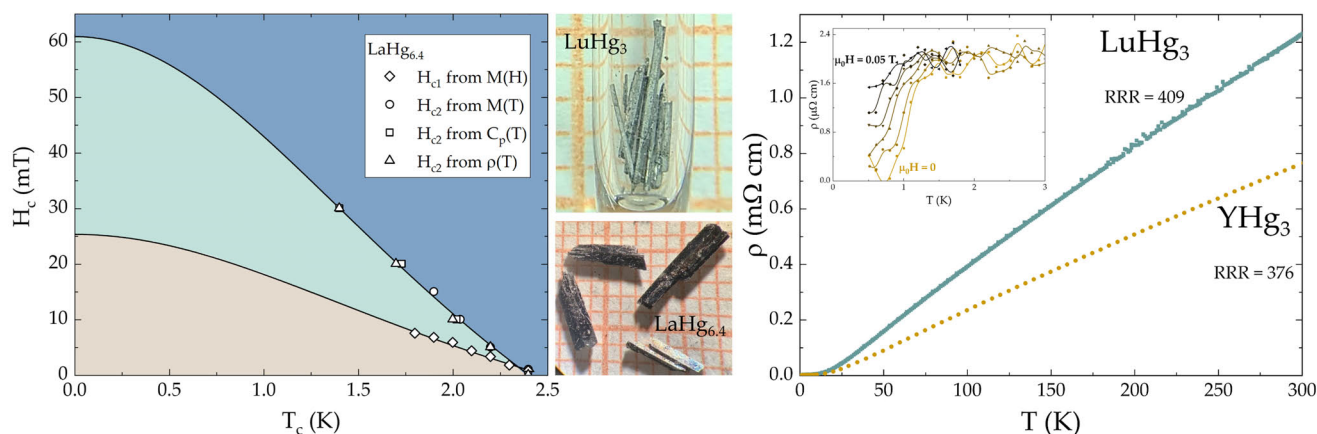


Fig. 5: Understanding of superconducting mercurides is now possible – synthesis of mm-sized, high-quality single crystals coupled with careful examination of their chemical and physical properties is now feasible by utilizing our methodologies. So far, superconductivity of mercurides appears to be conventional, as illustrated by  $\text{LaHg}_{6.4}$  [8],  $\text{LuHg}_3$  [6] and  $\text{YHg}_3$  [6].

even more diverse, with nearly 40 structure types available instead of 8 known for the lanthanides/actinides. Our investigations in the strontium, calcium, and magnesium mercurides have already identified several new superconductors. Most of these are conventional, with critical temperatures below 4.2 K. The next step is to explore the superconductivity of materials where both alkali/alkali earth and lanthanide/actinide elements exist in the same structure. We are currently in the process of designing such hybrid systems.

### Future avenues of interest

The space of mercurides is vast – we have just started to examine binary compounds and here we already have a wide range of chemical and physical properties. Besides superconductivity described above, our focus is on magnetism. Complex magnetic configurations, arising due to intricate crystal structures are frequent in mercurides. Our most recent example is the  $\text{Eu}_{10}\text{Hg}_{55}$  system ( $\text{Gd}_{14}\text{Ag}_{51}$  structure type) where distinct sites host either  $\text{Eu}^{2+}$  or  $\text{Eu}^{3+}$ . The magnetic phase diagram of this material is very rich – with multiple magnetic transitions observed as a function of temperature and field. This likely will give a rare chance to observe non-trivial spin textures – for instance, skyrmions, vortices or domain walls. We also plan to explore frustrated mercury materials in search for spin-liquid candidates – which, in principle, should exist but are yet to be observed in mercury-based systems.

Overall, the group’s work explores novel quantum materials, which have so far remained beyond our reach. Through the targeted discovery of new compounds, we will better understand superconductivity and mag-

netism as well as other phenomena caused by strong correlations. A comprehensive characterization of these systems creates a synergetic loop to bring out remarkable quantum states which have either been stipulated or have already been seen in representatives of the respective families. We use advanced tools – in synthesis, characterization and by collaborating with theory – pushing the global methodology further.

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## 1.8 Minerva Group: Synthesis, Structure and Spectroscopy of Tunable Materials (S3TM)

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**Superconducting square-planar nickelates provide an important and intriguing materials platform for direct comparison to the nominally isostructural and isoelectronic high- $T_C$  cuprates. Due to their complicated synthesis, experimental measurements can be particularly challenging to both perform and interpret. Leveraging the expertise within PQM and other departments, our group probes the fundamental characteristics of these new compounds and seeks new routes to tune their properties.**

The discovery of superconducting copper oxides (cuprates) marked a sea-change in condensed matter physics and materials research, launching the ongoing pursuit of high temperature superconductivity. Spanning a wide range of chemical formulas and crystal structures, the superconducting cuprates all share atomic planes of square-planar  $\text{CuO}_2$  and nominal  $3d^9$  copper ion electron filling. Building upon these common motifs, it was theoretically predicted [1] that compounds containing nickel – neighboring copper on the periodic table – with similar structural and electronic configuration may also host superconductivity. After nearly two decades, superconducting nickelates were finally realized in 2019 [2], expanding to include (to-date)  $R_{1-x}D_x\text{NiO}_2$  ( $R = \text{La, Nd, Pr}$ ;  $D = \text{Sr, Ca, Eu}$ ) and  $\text{Nd}_{n+1}\text{Ni}_n\text{O}_{2n+2}$  ( $n = 4-8$ ) [3].

Due to their thermodynamically metastable configuration, superconducting square-planar nickelates have only been stabilized by two-part synthetic processes, which involve growth of a high-quality crystalline precursor of a more stable Ni oxidation state, e.g.  $d^7$  ( $\text{Ni}^{3+}$ ) followed by a topotactic reduction process to remove oxygen and

thereby reduce the Ni valence to the requisite  $d^9$  ( $\text{Ni}^{1+}$ ) filling. A “dome” of superconductivity is observed upon hole-doping from  $\text{Ni } d^9$ , either by chemical substitution or control of atomic layering order. In the five years since their discovery, the exploration of fundamental similarities – and differences – to the closely related cuprates has remained of great interest as a route to understanding key ingredients for unconventional superconductivity. A survey of the superconducting nickelates and key experimental results were compiled in collaboration with B. Y. Wang (Stanford University) and K. Lee (Massachusetts Institute of Technology) [3].

Since its inception in October 2022, the Synthesis, Structure and Spectroscopy of Tunable Materials (S3TM) Minerva Group has been primarily focussed on experimental investigation of these new materials in collaboration with local and international partners.

**Tunable disorder** A key challenge for many fundamental experimental measurements is the geometry of superconducting samples – to-date limited only to very thin (<15 nm) epitaxial thin films – and the *ex situ* chemical reduction process degrades the specimen surface [4, 5]. Thus, experimental measurements of band structure and superconducting gap symmetry by techniques such as angle-resolved photoemission spectroscopy [6, 7], single-particle tunneling experiments [8], and London penetration depth [9, 10] have so far been challenging. By controllably introducing disorder in superconducting nickelate thin films, we examine the dependence of superconductivity on pair-breaking defects in an effort to distinguish between a nodal and fully-gapped order parameter [11]. To date, our group has been awarded three successful proposals to leverage high-energy electron irradiation at the SIRIUS Facility (R. Grasset, École Polytechnique) for this purpose and completed three experimental runs, led by PhD student A. Ranna who joined the group in February 2023. Measurements across a wide range of samples including all three rare-earth cation species from different synthesis groups around the world (H. Hwang, Stanford University; M. Bibes,

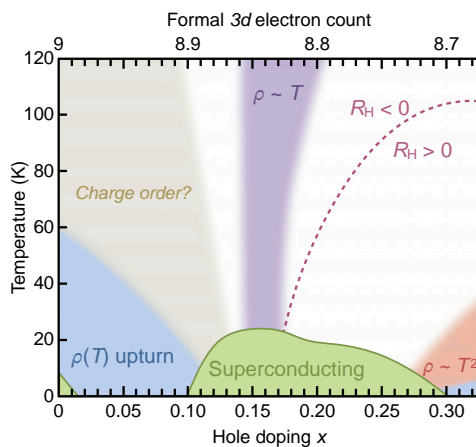


Fig. 1: Emerging phase diagram of superconducting square-planar nickelates, tuned by chemical hole-doping (bottom axis) or, equivalently, formal nickel ion electron count (top axis). From [3].

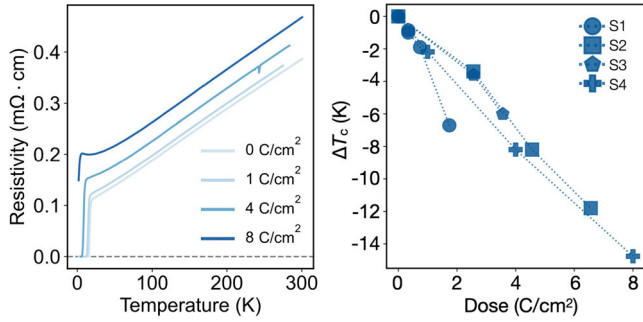


Fig. 2: Pair-breaking disorder controllably introduced into high-quality optimally hole-doped  $\text{Nd}_{1-x}\text{Sr}_x\text{NiO}_2$  thin films systematically raises electrical resistivity and lowers superconducting transition temperature  $T_C$ .

L. Bernardo Iglesias, Laboratoire Albert Fert; Y. Nie, Nanjing University) yield consistent results (Figure 2), namely a systematic suppression of superconducting transition temperature  $T_C$  and increase of residual resistivity with increasing dose, consistent with a sign-changing superconducting order parameter. First results are in preparation for a scientific manuscript; additional experiments scheduled for fall 2024 will provide data for future publications concerning details of specific chemical (e.g., cation or doping) dependence.

**Bulk spectroscopies** Despite nominal structural and electronic similarities, several studies have demonstrated that nickelate electronic structure differs significantly from cuprates, particularly in relation to metal hybridization [12, 13]. Many spectroscopic techniques, however, are limited by the accessible sample geometry, complicating precise measurements of orbital configuration. Led by postdoc E. Abarca Morales (joined April 2023, collaborative support from PQM/PCM), we adapted the non-resonant inelastic x-ray scattering (sNIXS) [14] technique pioneered in the PCM department for orbital imaging to directly probe the hole charge density around the Ni-site in bulk crystals of  $\text{LaNiO}_2$  (P. Pupal, MPI-FKF) at the DESY Petra III beamline (Hamburg). Accounting for the highly twinned nanostructure of the bulk crystals, our measurements are quantitatively consistent with a dominantly  $\text{Ni } d_{x^2-y^2}$  orbital character. More generally, these results provide an important demonstration of the capability for this technique beyond model systems.

We have also conducted a suite of spectroscopic measurements at the TPS 45A NSRRC beamline (Taiwan) on a series of multilayered square planar nickelate thin films (J. Mundy, Harvard University) [15], including resonant photoemission (resPES), valence spectroscopy, x-ray photoelectron spectroscopy (XPS), and hard x-ray photoelectron spectroscopy (HAXPES), which will be supported by current efforts to model our results in collaboration with dynamical mean field theory (DMFT)

experts (D. Takegami, Waseda University; A. Hariki, Osaka Metropolitan University).

**Tunable properties** In addition to chemical and structural tunability, our group is pursuing mechanical means to access or manipulate superconductivity in nickelates. In collaboration with the PQM Strain Group (E. Gati, H. Noad), we have begun efforts to investigate nickelate compounds under uniaxial pressure.

Beyond superconducting nickelates, our group is further engaged in several collaborative efforts within CPfS and the broader MPG to investigate the nanoscale structure and properties of quantum materials, including work with E. Svanidze, U. Vool, C. Felser (MPI-CPfS); P. Moll (MPI-MPSD, Hamburg); P. Pupal, M. Hepting, B. Keimer (MPI-FKF, Stuttgart).

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## 1.9 Emeritus Research Group: Solid State Physics

*Director Emeritus: Frank Steglich<sup>#</sup>*

A historical overview was given of the research on Strongly Correlated Electron Systems (SCES) from its very beginning all the way up to the current status [1]. Central to this was the discovery of the first unconventional (heavy-fermion, HF) superconductor  $\text{CeCu}_2\text{Si}_2$  [2], the enigmatic properties of which had led to various, partly conflicting explanations [3]. Recent ARPES measurements [4] have confirmed that  $\text{CeCu}_2\text{Si}_2$  is a two-band  $d$ -wave superconductor with a fully open energy gap [3,5], despite a sign-changing superconducting order parameter. The latter is mainly concluded from the existence of a “spin resonance” in the inelastic neutron-scattering (INS) spectra inside the superconducting gap [6], exactly at the propagation wave vector of the spin-density-wave order that forms nearby in the phase diagram [7]. In a recent article [8], all of the “spin resonances” found in **HF superconductors** could be ascribed to antiferromagnetic (AF) paramagnons – hinting at  $d$ -wave superconductivity (SC) [9]. This is in contrast to the cuprate high- $T_c$  superconductors, where the spin resonance is considered a triplet excitation of a  $d$ -wave condensate [10].

In the Fritz London Memorial Prize lecture at LT 29 [5], the unusual properties of the AF HF metal  $\text{YbRh}_2\text{Si}_2$  ( $T_N=70$  mK [11]) are discussed. Here, AF nuclear order develops at  $T_A \approx 2$  mK [12, 13] among the two (randomly distributed) isotopes carrying a nuclear spin, i.e.,  $^{171}\text{Yb}$  and  $^{173}\text{Yb}$ . At  $T_c \approx 2$  mK, bulk HFSC sets in, while granular SC is found already near 10 mK [12, 14]. According to [12], HFSC at ultra-low  $T$  emerges once the primary  $4f$ -electronic spin order, which is detrimental to SC [11], has become sufficiently weakened by the competing nuclear order. The latter is the dominant part of a *hybrid* type of order which includes a minor phase with  $4f$ -electronic spin order, different from the primary one. This is explained by a three-component Ginzburg-Landau treatment, which reveals that *two* magnetic phase transitions to take place successively (at  $T_N$  and  $T_A$ , respectively) require *three* different magnetic order parameters to begin with (starting with two order parameters, only one phase transition is obtained) [12]. The spin susceptibility  $\chi(\mathbf{q})$  of  $\text{YbRh}_2\text{Si}_2$  is highly anisotropic and thus responsible for both AF [11] and ferromagnetic (FM) [15] quantum critical fluctuations. It therefore exhibits maxima at the wave vectors  $\mathbf{q} = \mathbf{q}_{\text{AF}}$  and  $\mathbf{q} = 0$ , respectively. Another maximum in  $\chi(\mathbf{q})$  appears to exist at a finite  $\mathbf{q} = \mathbf{q}_1$ , different from  $\mathbf{q}_{\text{AF}}$  [12], see below. Knapp *et al.* [13] believe that no such second

$4f$ -electronic order forms and, instead, the primary order persists in the whole low- $T$  range. From the results of ref. [12] as well as ref. [13], the ordered low- $T$   $4f$ -moment  $m_1$  is estimated to exceed the tiny moment of the primary AF phase above  $T_A$ ,  $m_{\text{AF}} \approx 0.002 \mu_B$  [16], by a factor of order ten. In a scenario like the one chosen in [13] this implies that, concurring with the onset of SC,  $m_{\text{AF}}(T)$  has to strongly *increase* upon cooling. However, the primary order appears to become *weaker* below 10–20 mK [12], which was attributed to its competition with the nuclear short-range order [17], as evidenced by a large nuclear spin entropy in the same  $T$ -window [12, 13]. Also, the superconducting phase transition was found to be of first order [12], implying the absence of the primary AF phase at sufficiently low  $T$ . Here, the  $4f$ -derived spins are aligned antiferromagnetically by an RKKY polarization along a propagation wave vector different from  $\mathbf{q}_{\text{AF}}$ . This confirms the existence of a third maximum of  $\chi(\mathbf{q})$  at  $\mathbf{q} = \mathbf{q}_1$ .

For the first time, *direct spectroscopic evidence* for the competition between local Kondo screening and long-range AF order could be provided through high-resolution photoemission measurements on the Kondo-lattice system  $\text{CeCoGe}_3$  exhibiting a high Néel temperature,  $T_N = 21$  K [18]. These measurements reveal a weakly dispersive  $4f$ -band at the Fermi energy near the Z-point. Its intensity shows a logarithmic increase upon cooling and starts to deviate from this Kondo-type behavior slightly above  $T_N$ . Eventually it ceases to grow further below  $T \approx 12$  K.

For a long time, FM quantum critical points (QCPs) were assumed to be prohibited in clean systems, yet such a phenomenon was recently revealed [19] under a moderate hydrostatic pressure in  $\text{CeRh}_6\text{Ge}_4$ , with local-moment-type of FM order [20]. The  $4f$ -derived magnetic moments in  $\text{CeRh}_6\text{Ge}_4$ , like the ones in  $\text{YbNi}_4\text{P}_2$  [21], reside along chains with a large interchain distance. ARPES measurements have proven that the strength of the  $4f$ -conduction electron hybridization is anisotropic in momentum space and is much stronger along the Ce-chain direction as compared to that within the perpendicular basal plane [22]. This highly anisotropic hybridization was corroborated by neutron-powder-diffraction experiments as well as zero-field  $\mu\text{SR}$  measurements, which revealed coherent oscillations below the Curie temperature  $T_C = 2.5$  K [23]. These results indicate in-plane FM ordering consisting of reduced Ce-moments. By analyzing the magnetic susceptibility and INS

results, a crystal- field (CF) level scheme was derived which accounts for the easy-plane magnetocrystalline anisotropy. Here, the low-lying first excited CF state exhibits a significantly stronger hybridization than the ground state and results in a lowest-lying quasi-quartet [23] – in agreement with a ‘Kadowaki-Woods’ analysis which indicates that the effective  $Ce^{3+}$  ground state is four-fold degenerate [19]. A study of a partial isoelectronic chemical substitution of Ge by Si in  $CeRh_6Ge_4$  showed that  $T_C$  of  $CeRh_6(Ge_{1-x}Si_x)_4$  is smoothly suppressed at the critical concentration  $x_c \approx 0.125$ , where non-Fermi-liquid behavior with  $C(T)/T \propto \ln(T^*/T)$  is observed [24]. In ref. [25] it was found for the **LaRh<sub>6</sub>Ge<sub>4</sub>** homologue that the normal Hall resistivity is electron-like for magnetic fields along the *c*-axis but hole-like in the basal plane. According to first-principle calculations, this direction-dependent switching of the carrier type arises within a single band with a special geometry leading to carriers on the same Fermi surface orbiting as electrons along some directions, but holes along others. Measurements of the electrical resistivity of  $EuCd_2As_2$  under pressure have revealed an intriguing insulating dome at pressures  $p_{c1} \approx 1 \text{ GPa} < p < p_{c2} \approx 2 \text{ GPa}$ , which is situated between two regimes with metallic transport [26]. The insulating state can be fully suppressed by a small magnetic field, leading to a colossal negative magnetoresistance on the order of more than 100%, accessible via a modest field of  $\approx 0.2 \text{ T}$ . This could be attributed to consecutive phase transitions of  $EuCd_2As_2$  from a magnetic topological insulator to a trivial insulator, and further to a Weyl semimetal, with the latter resulting from a pressure-induced change in the magnetic ground state. The colossal magnetoresistance is caused by a field-induced polarization of the Eu-derived *4f* magnetic moments, which transforms  $EuCd_2As_2$  from a trivial insulator to a Weyl semimetal. These findings underscore weak exchange couplings and weak magnetic anisotropy as ingredients for discovering tunable magnetic topological materials with desirable functionalities.

### Cooperation Partners

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## 1.10 Max Planck Fellow Group: Hassinger Group – Unconventional Magnets, Metals and Superconductors

Group Leader: Elena Hassinger<sup>#</sup>

Odd-parity superconductivity is a rare state of matter in which the superconducting wave function is odd under inversion symmetry. Since the total wave function of electronic states needs to be antisymmetric with respect to electron exchange, this directly implies a symmetric spin-wave function, i.e. a spin-triplet state. Until recently, it was believed that this requires ferromagnetic interactions as in superfluid  $^3\text{He}$ . In 2021, a collaboration between my group and the groups of S. Khim and M. Brando reported two-phase superconductivity in the heavy-fermion material  $\text{CeRh}_2\text{As}_2$ . Based on the anisotropic experimental phase diagram in magnetic field and its angle dependence in combination with theory, we were able to show that a magnetic field induces a phase transition from an even-parity to an odd-parity superconducting state. Interestingly, the odd-parity state is stabilized by locally broken inversion symmetry at the Ce site in a centrosymmetric crystal structure. Boosted by our discovery, this mechanism to stabilize odd-parity superconductivity – not relying on ferromagnetic interactions – is now gaining attention in the field of unconventional superconductivity. Our group has been exploring the properties of this extraordinary superconducting state and its competition with other unconventional orders in  $\text{CeRh}_2\text{As}_2$  with the aim to find other potential candidates for odd-parity superconductivity in the future.

Our fruitful research on  $\text{CeRh}_2\text{As}_2$  during the past three years has revealed several fundamentally new states of matter that can be summarized in the schematic phase diagrams in Figure 1, (see also [PQM\\_05\\_Brando](#), [PQM\\_06\\_Khim](#)). First, we reported the discovery of the remarkable and unique two-phase superconductivity with  $T_c = 0.3$  K and its explanation based on the locally non-centrosymmetric crystal structure in a scenario in which an even-parity superconducting state switches to an odd-parity state with  $c$ -axis field [1]. This

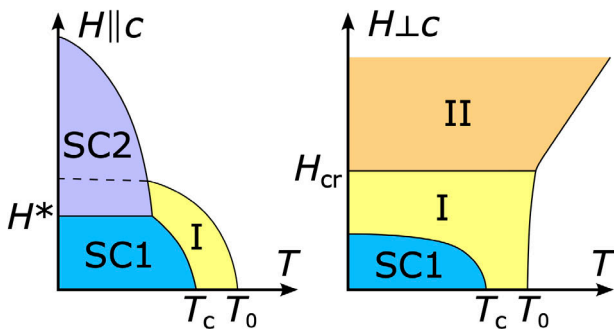


Fig. 1: Schematic phase diagram of  $\text{CeRh}_2\text{As}_2$  for fields along ( $H \parallel c$ ) and perpendicular ( $H \perp c$ ) to the tetragonal  $c$  axis resulting from [1,4,11]. Two-phase superconductivity is observed for  $H \parallel c$ , but not for  $H \perp c$ . The state SC1 is identified as an even-parity state, the state SC2 as an odd-parity state which can explain both phase diagrams. Two anisotropic normal state orders are also observed. Phase I is suppressed for  $H \parallel c$ , whereas for  $H \perp c$ , it remains roughly constant and then changes to Phase II via a first-order phase transition.

publication in *Science* was highlighted by an accompanying Perspective Article [2] and a publication in *Physics Today* [3].

Since the transition temperatures are low ( $T_c = 0.3$  K and  $T_0 = 0.5$  K) and critical fields are high ( $H_{c2} \parallel c = 16$  T), the experiments on this material require extreme experimental conditions. Our group has the technical expertise required since we focus on bulk measurements of ac susceptibility, electric and thermal transport in a wide range of very low temperatures down to 30 mK, high magnetic fields up to 17 T, and pressures up to 3 GPa.

Before going into the stunning physics of  $\text{CeRh}_2\text{As}_2$  in more detail, I would like to highlight that local inversion symmetry breaking at the relevant atomic sites is in fact rather common among unconventional superconductors such as the multiphase superconductors  $\text{Upt}_3$  and  $\text{UTe}_2$  as well as iron pnictides, cuprates and some transition metal dichalcogenides. However,  $\text{CeRh}_2\text{As}_2$  is so far the only compound showing an even to odd-parity transition. It is therefore of crucial importance to understand the relevant mechanisms in this compound compared to others.

As a test of the parity-switching scenario, we determined the angle dependence of the superconducting upper critical fields which agrees perfectly with predictions within the scenario [8]. However, this scenario doesn't consider the normal state order "Phase I" (setting in at  $T_0 = 0.5$  K in zero field) out of which superconductivity evolves. Such an order might alter the symmetry considerations for superconductivity significantly. Based on thermodynamic properties and mag-

netic probes we established the phase diagram of this phase for both field directions as also depicted in Figure 1 [4, 11]. The strong and unexpected increase of  $T_0$  with inplane fields gives a strong hint that Phase I is not a simple antiferromagnetic state as in other heavy-fermion superconductors. Instead, the field dependence of  $T_0$  reveals a mixing of the two lowest lying crystal-electric-field doublets leading to the possibility of an order with quadrupolar degrees of freedom [4], and report [PQM\\_05\\_Brando](#). The relevance of such an original state is reinforced by the fact that  $\text{CeRh}_2\text{As}_2$  is close to a quantum critical point of this order (the point where it is suppressed to  $T = 0$  by pressure). Evidence for quantum criticality in zero pressure comes from non-Fermi liquid behavior observed in the specific heat and resistivity [4], but the Wiedemann-Franz law seems to be held [7]. This points to the unusual situation in which fluctuations of the unconventional Phase I order parameter are involved in the pairing mechanism of the unconventional superconducting state.

A comparison with the sister compound  $\text{LaRh}_2\text{As}_2$  provides evidence for the relevance of strong correlations. This compound has the same crystal structure and a superconducting state at a similar  $T_c$ , but its superconducting state has low critical fields [9]. The difference originates in the absence of strong correlations associated with the presence of  $f$  electrons in Ce compounds.

In  $\text{CeRh}_2\text{As}_2$ , nuclear magnetic resonance measurements by our collaborators K. Ishida and his group from Kyoto give some first microscopic insight into the normal state order. At one of the As sites they find a broadening of the spectral line interpreted as the onset of local fields due to antiferromagnetic order below  $T_c$  [5]. Furthermore, they find evidence for two-dimensional fluctuations above the order [6] and for spin-singlet pairing in both superconducting states [10]. Intriguingly, the antiferromagnetic order seems to be constricted in their measurements to SC1. Such a behavior would allow for alternative scenarios for the transition from SC1 to SC2 and would require some kind of coupling of superconductivity with antiferromagnetism. However, our  $c$ -axis phase diagram suggests that Phase I couples only very weakly to superconductivity since no significant kink is present in the  $T_c$  vs  $H$  curve where  $T_0$  crosses  $T_c$  at around 6 T as presented in Figure 1 [11].

## Outlook

Our pressure work [13, 14] gives further insight into many of the open questions in this material. It reveals a pressure-induced quantum critical point of Phase I around which superconductivity forms a dome. Furthermore, the two superconducting phases survive up

to a pressure far above the critical pressure. This implies that the parity transition does not depend on the presence of Phase I. Structural information on both Phase I and the superconducting states and our ongoing work on the angle dependence of Phase I will be crucial for our understanding of the physics in  $\text{CeRh}_2\text{As}_2$  and how it compares to other locally non-centrosymmetric superconductors in the future.

## Cooperation Partners

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## 1.11 Max Planck Fellow Group: Ruck Group

Group Leader: Michael Ruck<sup>#</sup>

Crystals of weak 3D topological insulators (TIs) of the  $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ -type can be seen as nano-periodic multilayer heterostructures of 2D TIs spaced by topologically trivial insulators. The newest member,  $\text{Bi}_{12}\text{Rh}_3\text{Ag}_6\text{I}_9$ , exhibits 2D cationic conductivity, which allows to adjust the Fermi level electrochemically. Magnetoresistance measurements reveal Landau quantization and chirality, coinciding with a drastic drop in resistivity across the layers. In accordance with theoretical predictions, this is strong evidence for the formation of a collective [1+1]-dimensional “sheath state” arising from coherent tunneling between protected edge states. This first observation of a macroscopic system of some  $10^5$  coupled, chiral, quantum-mechanically identical spin channels with protected spin orientation is promising for use in spintronics.

Topological insulators (TIs) are characterized by a bulk energy gap, but host gapless, spin–momentum locked states at their boundary. These surface states are protected by time-reversal symmetry and are robust against various perturbations and defects, spatial inhomogeneities and nonmagnetic impurities [1]. This robustness renders TIs as promising materials for the development of devices with low power consumption as well as for spintronics and quantum computing. In a weak TI (WTI), spin–momentum-locked states appear on selected surfaces and can be helical or chiral. WTIs can appear in the form of electronically decoupled stacked 2D TIs. As they are 3D objects, no substrate is required, but their edge states are exactly like in 2D TIs, making them suitable for device applications.

The first experimentally verified WTI was the crystalline bulk compound  $\text{Bi}_{14}\text{Rh}_3\text{I}_9$  [2]. Its protected edge states were revealed by scanning tunneling microscopy (STM) in artificial channels created by atomic force microscopy [3]. In the crystal structure, 2D TI layers  $[(\text{Bi}_4\text{Rh})_3\text{I}]^{2+}$  are spatially separated and electronically isolated by  $[\text{Bi}_2\text{I}_8]^{2-}$  spacers. As the

termination of stacking at the crystal faces necessitates a local change in composition, the sample is always n-doped, which creates an undesirable alternative transport channel.

A new WTI of the  $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ -type,  $\text{Bi}_{12}\text{Rh}_3\text{Ag}_6\text{I}_9$ , has spacer layers  $[\text{Ag}_6\text{I}_8]^{2-}$  (Figure 1). Angle-resolved photoelectron spectroscopy in combination with DFT calculations showed a wide topological bandgap of 286 meV, created by strong spin–orbit coupling, and topological invariants  $\mathbb{Z}_2 = (0;0,0,1)$ . Single-crystal X-ray diffraction and impedance measurements revealed 2D cation conductivity in the spacer layers (Figure 2). This for the first time allowed eliminating electronic doping by electrochemically adjusting the Ag content [4]. Transport measurements on such an electron-precise bulk semiconductor crystal led to the discovery of a previously predicted but never observed emergent low-temperature quantum phenomenon [4]. The first remarkable fact is a drop of the electrical resistivity perpendicular(!) to the layers below 3.2 K, following a  $T^3$  law. This hints at coherent tunneling between the 2D TI layers [5], which are separated by less than 1 nm. The tunneling connects the 1D edge

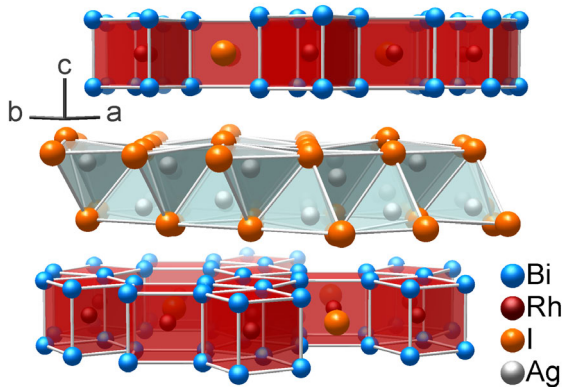


Fig. 1: Section of the crystal structure of  $\text{Bi}_{12}\text{Rh}_3\text{Ag}_6\text{I}_9$ . Kagome nets of edge-sharing Rh-centered Bi-cubes (red) with  $\text{I}^-$  ions in their hexagonal voids constitute the 2D TI layer  $[(\text{Bi}_4\text{Rh})_3\text{I}]^{2+}$ . Edge-sharing tetrahedra (light blue) form the  $[\text{Ag}_6\text{I}_8]^{2-}$  spacer.

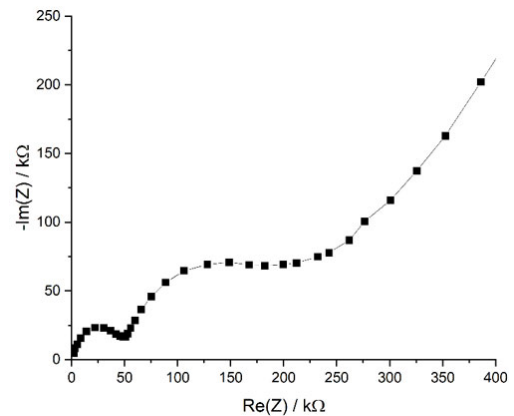


Fig. 2: Impedance spectrum of  $\text{Bi}_{12}\text{Rh}_3\text{Ag}_6\text{I}_9$  at room temperature. Semicircles indicate ionic conductivity of about  $10^{-6} \Omega^{-1} \text{cm}^{-1}$ .

states of all 2D TI layers in the crystal, creates a kind of 2D surface state and thereby improves the conductivity across the stack.

The new “sheath” state is responsible for a pronounced dip of the (positive) magnetoresistance in small fields below 5.18 K (Figure 3a). A striking feature of the magnetoresistance is the incipient asymmetry at very low magnetic fields evident below about 2 K (Figure 3a). The asymmetry is inverted as the starting magnetic field of the experiment is reversed. This is consistent with the assumption of a chiral transport system formed by the edge states of the 2D TI states. It is also in line with the smooth transition to the sheath state, in which the topology should not change. As the chirality persists, the sheath state should be regarded [1+1]-dimensional, which makes it fundamentally different from the 2D surface states of a strong TI.

Moreover, oscillations of the resistance are observed (Figure 3b), which can be described using the Lifshitz-Kosevich expression:

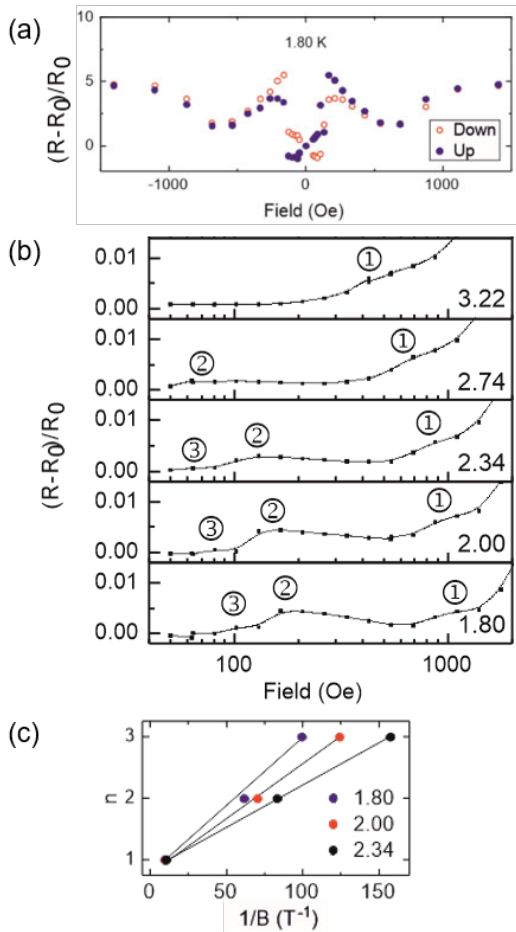


Fig. 3: (a) Magnetoresistance of  $Bi_{12}Rh_3Ag_6I_9$ . (b) Temperature dependence of the magnetoresistance. The temperature (in K) is given in the corners, circled numbers mark resistance maxima. (c) Linear fits of the maxima index vs. inverse magnetic field according to the Lifshitz-Kosevich formula.

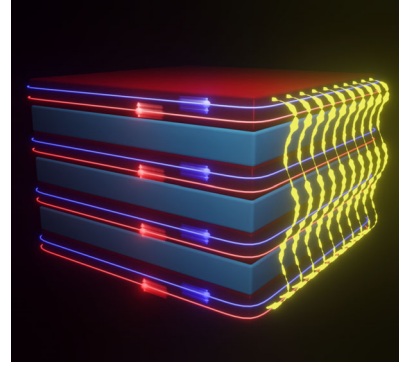


Fig. 4: Emergent sheath surface state by coherent tunneling between quantum mechanically identical edge states in a crystalline stack of 2D TIs.

$$\frac{\Delta R}{R_0} \sim \cos \left[ 2\pi \left( \frac{E_F}{\hbar\omega_c} + \frac{1}{2} + \beta - \delta \right) \right]$$

Local maxima appear whenever the argument of the cosine is a multiple of  $2\pi$ . Linear fits of the Landau index  $n$  vs. the inverse magnetic field (Figure 3c) give total phase shifts  $(\beta - \delta)$  of 0.30 to 0.36, indicating a non-zero Berry phase and the presence of Dirac fermions [6]. It has to be stressed that this orbit quantization was observed on a bulk crystal of  $Bi_{12}Rh_3Ag_6I_9$  and not on a 2D object or an artificial few-layer heterostructure.

In a weak magnetic field, the emergent sheath surface state (Figure 4) is a chiral macroscopic system of some  $10^5$  layers with only one protected spin channel and one spin orientation. Thus,  $Bi_{12}Rh_3Ag_6I_9$  is a seemingly perfect material for faultless spin transport.

### External Cooperation Partners

Nicolás Pérez (IFW Dresden); Friedrich Reinert and Giorgio Sangiovanni (Universität Würzburg).

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## 1.12 Max Planck Fellow Group: Molenkamp Group

Group Leader: Laurens Molenkamp<sup>#</sup>

We report the current status of projects from the Molenkamp group done in collaboration with groups in MPI Dresden. These projects combine the expertise of the Molenkamp group in low temperature transport, thermoelectric transport, and Molecular Beam Epitaxy (MBE) with the wide expertise of the various groups in MPI Dresden to study the properties of HgTe based topological materials, Delafossites, and Heusler materials.

### Thermoelectric Transport in HgTe Weyl Semimetals

Dirac and Weyl semimetals have garnered significant attention recently due to their unique linear band dispersion in three dimensions, allowing for the exploration of Weyl and Dirac quasiparticles. In this study, we investigate the thermoelectric transport properties of Weyl semimetals realized in compressively strained HgTe films and their correlation to the predicted gravitational anomaly.

An electrostatic gate fabricated on the sample allows to precisely tune the Fermi level close to the Weyl point, facilitating the study of intrinsic Weyl transport in HgTe. The low device temperature (1.33 K) suppresses electron-phonon heat relaxation and minimizes phonon drag effects. This ensures that the observed phenomena are primarily driven by intrinsic carriers. In addition, we employ fully electronic methods for thermal conductance measurements, utilizing Johnson-Nyquist noise to determine the electron temperature and current heating techniques to alter the temperature of the electronic subsystem.

Our device features an H-bar structure consisting of two long channels ( $40 \times 4 \mu\text{m}$ ) and an interconnecting island ( $4.5 \times 6 \mu\text{m}$ ), each equipped with independent

top gates. The two channels, with their Fermi levels tuned to the n-type conducting regime, act as the heater and detector, while the island's Fermi level is tuned near the Weyl point. By applying a DC current to the heater, electrons are raised to a higher temperature than the bath, inducing heat flow through the Weyl material to the detector. Careful measurements and analysis allow us to extract the thermal conductance of the HgTe Weyl semimetal.

Under an in-plane magnetic field aligned with the electric field or temperature gradient, we observe a positive thermal and electrical conductance (negative electrical resistance), respectively (Figure 1). Although the positive magneto thermal conductance hints at a possible connection to the gravitational anomaly, the thermal conductance is directly linked to the electrical conductance via Wiedemann-Franz law (Figure 2). This suggests that the mechanisms involved in both heat transport and electrical transport are the same with no additional or anomalous mechanisms of heat transport involved. Additionally, thermopower measurements of HgTe from the same device conform to Mott's relation, further supporting these conclusions.

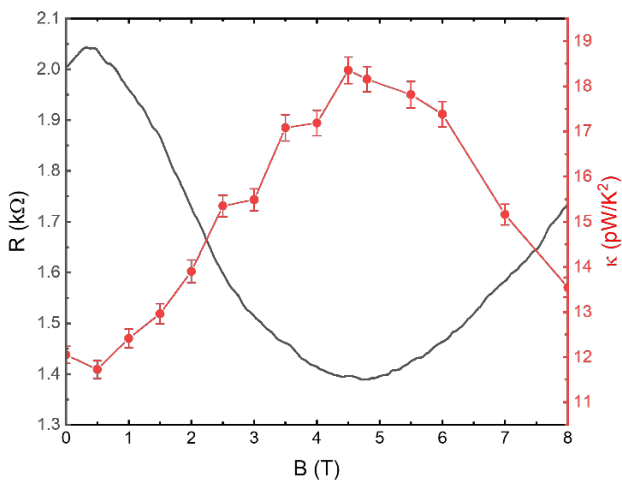


Fig. 1: In-plane magneto resistance,  $R$  and thermal conductance,  $\kappa$  of the island. Island fermi level is tuned close to the Weyl point.

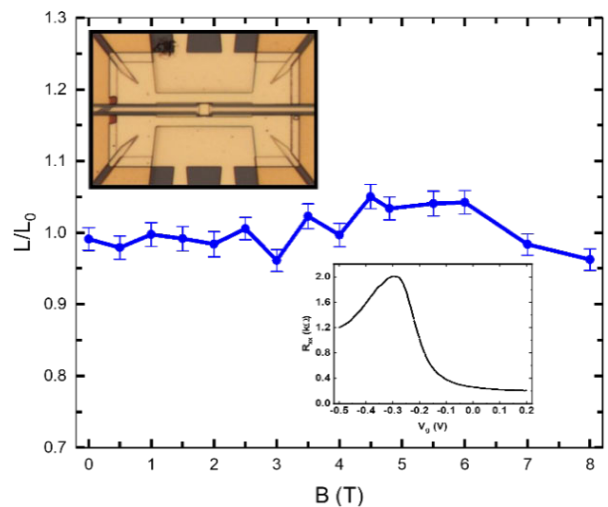


Fig. 2: Lorenz ratio derived from  $R$  and  $\kappa$  of the island. The insets display the device and a gate scan of the island resistance, with the peak corresponding to the Weyl point.

## Current Heating and Electron collimation experiments in PdCoO<sub>2</sub> Delafossite

We concentrate in this study on PdCoO<sub>2</sub>, which is a quasi-two-dimensional delafossite metal with a hexagonal fermi surface, and shows interesting electrical properties combining high in-plane conductance, unconventional magnetoresistance, and evidence of electron hydrodynamic flow [2]. Here our aim is to further investigate the existence of electron hydrodynamic flow in this material, utilizing the current heating technique discussed in [3]. This project is carried out in collaboration with the Mackenzie group, providing assistance to device fabrication using their focused ion beam (FIB) facility (Figure 3).

The main challenge in applying current heating technique arises from the use of traditional meanders in the contacts used for mitigating the issues of current inhomogeneity in PdCoO<sub>2</sub>. These meander shaped contact dissipate the majority of the heat within itself without allowing the heat to propagate into the channels, and thus reducing the overall electron heating efficiency. We solved this problem by developing a novel lithographic approach to establish side contacting for PdCoO<sub>2</sub> channels. However, our current heating experiments in PdCoO<sub>2</sub> channels (5×30 μm) showed no significant changes in the differential resistance measurements. This is possibly due to the overall high density in PdCoO<sub>2</sub> and the rapid redistribution of dissipated energy among the vast number of electrons in the Fermi sea, hence preventing substantial electron heating. This indicates that probing electron hydrodynamic flow using current heating methods may not be viable for PdCoO<sub>2</sub>.

Additionally, we conducted electron collimation experiments in PdCoO<sub>2</sub> channels. We observed the

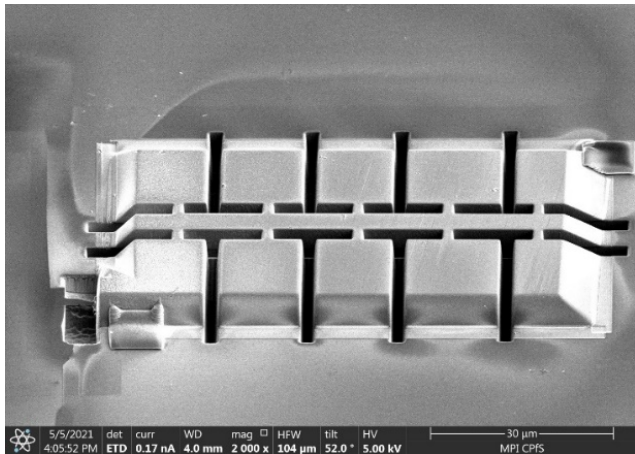


Fig. 3: SEM image of PdCoO<sub>2</sub> channel after FIB patterning.

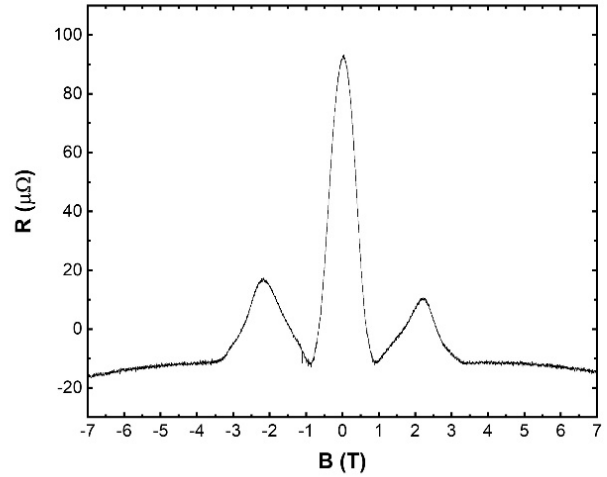


Fig. 4: Collimation signal from PdCoO<sub>2</sub> channel under the influence of magnetic field.

appearance of secondary peaks along with negative signals at high magnetic fields along with the expected zero field collimation signal (Figure 4). A Monte Carlo simulation of the device indicates that the negative signal at high field can be attributed to the possibility of electrons detaching from the boundary due to electron-phonon or electron-impurity scattering. The detached electrons can diffuse through the bulk material reaching a distant detector and results in a negative signal. We are currently investigating the origin of the secondary peaks by performing the collimation experiments on PdCoO<sub>2</sub> channels with various fermi surface orientation. We are also planning to do a width dependent studies of these devices which may provide more understanding to the underlying mechanisms.

## Linear and Nonlinear Planar Magneto-transport of HgTe-based topological materials

The surface states of three-dimensional topological insulators (3DTIs) exhibit strong in-plane magneto-transport effects, such as anisotropic magnetoresistance [4] and the planar Hall effect [5]. A band-structure-related origin for these effects, suggested only recently, involves the anisotropic backscattering of surface state electrons due to the in-plane field-induced tilt of the Dirac cone, caused by nonlinear terms in the band dispersion [6]. However, the studies so far failed to account for experimental reality implied by the (irregular) fluctuations of the effects' amplitude as a function of the applied in-plane magnetic field. This is evident from the longitudinal magnetoresistance of the topological surface states of a compressively strained 3D HgTe device shown in the first panel of Figure 5. Understanding these fluctuations is crucial,

as they also appear in the nonlinear planar magnetoresistance, as illustrated in the second and third panels of Figure 5, seriously complicating the observation of various nonlinear magnetotransport phenomena that have been recently proposed.

To address the physical origin of these field-dependent fluctuations, we invoke the presence of density inhomogeneities in our structures. We model the effect of these charge puddles on the transport properties using a network model (see Figure 6), where low density regions are represented as a chain of independent potential barriers, with each barrier modeled as a two-terminal resistor [7]. The fundamental idea of our simulations is that each puddle by itself exhibits pronounced fluctuations in the magneto-conductance due to lateral super-resonant tunneling to its neighbors, facilitated by the tilted Dirac dispersion [8]. The combined network of puddles is then responsible for the overall magneto-transport behavior.

The tunneling transport of charge carriers through these puddles is inherently nonlinear, influenced by the applied excitation as well as the width and depth of the potential barriers created by the puddles. This tunneling results in harmonic distortion of the applied signal, leading to subtle nonlinearities in the overall I-V characteristics. While these nonlinearities may be difficult to detect in DC measurements, they become apparent through lock-in techniques, allowing for the measurement of second (and higher) harmonic signals.

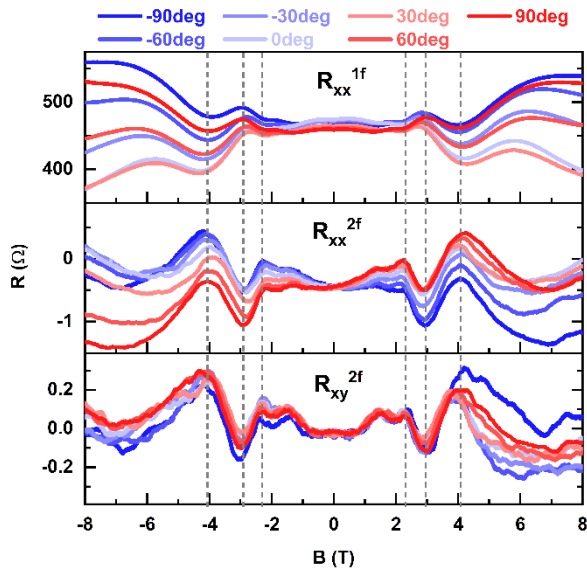


Fig. 5: First and second harmonic resistances of a 94 nm thick compressively strained HgTe sample, gated to the topological surface state regime, measured as a function of the in-plane magnetic field at varying angles between the electric and magnetic fields.

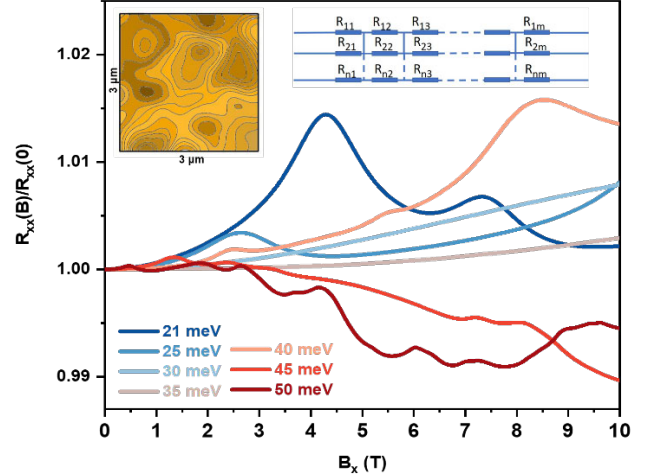


Fig. 6: Resistance fluctuations as a function of the in-plane magnetic field for different Fermi levels, simulated using the puddle-network model. Schematic of the potential landscape in our samples and a resistor network representing the coupled puddles in the inset.

This finding underscores the need for careful interpretation of experimental results, as even a simple charge puddle network can produce nonlinear responses that might be mistaken for more complex mechanisms. Moreover, given that charge puddles are an inevitable outcome of thin film growth of narrow gap materials, these effects are not exclusive to topological materials; they are expected to occur very generally in materials with Dirac dispersion and sizable spin-orbit coupling, such as transition metal dichalcogenides.

### Effects of Uniaxial strain on HgTe based topological materials

Previously we have demonstrated that HgTe films can be grown to exhibit different topological states depending on the strain imposed by the substrate. Specifically, 3DTI and Weyl semimetal phases are induced by either tensile or compressive strain, respectively. In this project, we are exploring the possibility of inducing a topological phase transition by applying external uniaxial strain using a pressure cell (shown in the inset of Figure 7), developed at MPI-CPFS.

At Würzburg, the pressure cell, equipped with piezoelectric actuators [9], is mounted in a flow cryostat that can reach a base temperature of 3 K. This setup allows us to perform low temperature transport experiments while continuously adjusting the applied strain. Simultaneously, we employ Raman spectroscopy to directly monitor the strain in real-time, as depicted in Figure 7.

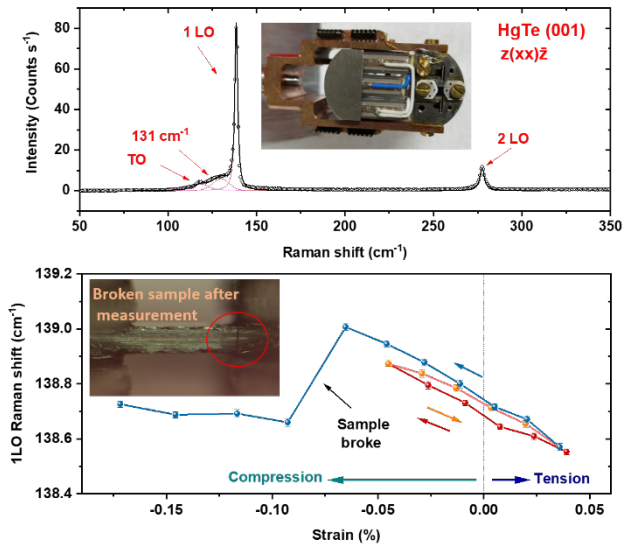


Fig. 7: (top) Raman spectrum of a bulk HgTe (001) sample at 5.6 K using Ar<sup>+</sup> (2.41 eV) laser. Photograph of the pressure cell used to apply uniaxial strain in the inset. (bottom) Raman shift as a function of the applied uniaxial strain. Image of the broken sample after measurement in the inset.

However, it turned out that the application of this method is very limited for the use of crystalline materials like HgTe or CdTe, because tetrahedrally bonded semiconductors are prone to cleavage, under relatively small amounts of mechanical strain, especially along their natural crystallographic planes of cleavage, such as the {110} plane [10]. This structural fragility imposes a limit on the amount of pressure that can be applied before the samples cleave during measurement, as shown in Figure 7 (bottom).

## Cooperation Partners

This project is a collaboration with the Department for Physics of Quantum Materials (A. P. Mackenzie).

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## 1.13 Max Planck Fellow Group: Davis Group

Group Leader: J.C. Seamus Davis<sup>#</sup>

In this report we present the status of the projects from the Davis Group at MPI-CPfS.

### Discovery of an Electron-Pair Density Wave State in Transition-Metal Dichalcogenides

Cooper-pair density wave (PDW) states occur when electron-pairs are formed with finite momentum and then condense into a static periodic crystalline state. To explore whether TMD sustain PDW, we developed high-speed atomic-resolution milliKelvin scanned Josephson-tunnelling microscopy (SJTM). We discovered a PDW state in NbSe<sub>2</sub> with commensurate domains with discommensuration phase-slips at the boundaries, conforming to those of the lattice-locked commensurate CDW. Most importantly, because many TMDs sustain both CDW and superconducting states, an abundant new arena for PDW physics emerges [1].

### QPI Signature of a Pair Density Wave State in the Cuprate Pseudogap Phase

An unidentified quantum fluid designated the pseudogap (PG) phase is produced by electron-density depletion in the CuO<sub>2</sub> antiferromagnetic insulator. Current theories suggest that the PG phase may be a pair density wave (PDW) state. By visualizing the temperature dependence of the electronic structure from the superconducting into the pseudogap phase, we demonstrated QPI signatures as predicted specifically for the temperature dependence of an 8a0-periodic PDW, indicating that a pure PDW state occurs in the pseudogap phase [2].

### Atomic-scale Visualization of Electronic Fluid Flow

Atomic scale visualization of electronic fluid flow has no precedent. Pursuing that objective, we generalized our recent innovations in superconducting-tip scanning tunnelling microscopy, to image electron-pair velocity  $v_s(\mathbf{r})$  of the flowing electronic superfluid in superconducting NbSe<sub>2</sub>. We demonstrated atomic-scale visualization of the flow patterns in an electronic fluid, with speeds ranging from stationary up to 10,000 km/h = MACH 10 [3].

### Electron pairing mechanism of copper-oxide high-T<sub>c</sub> superconductivity

In cuprates, virtual transitions of electrons between adjacent planar Cu and O atoms, occurring at a rate  $t/\hbar$  and across the charge-transfer energy gap  $\mathcal{E}$ , generate ‘superexchange’ spin–spin interactions of energy

$J \approx 4t^4/\mathcal{E}^3$  in an antiferromagnetic state. However, hole doping this CuO<sub>2</sub> plane converts this into a very high temperature superconducting state whose electron-pairing is exceptional. Anderson’s proposal for the mechanism of this intense electron-pairing is that, while hole doping destroys magnetic order it preserves pair-forming superexchange interactions governed by the charge-transfer energy scale  $\mathcal{E}$ . To explore this hypothesis for the first time directly at atomic-scale, we combine single-electron and electron-pair (Josephson) scanning tunneling microscopy to visualize the interplay of  $\mathcal{E}$  and the electron-pair density  $n_P$  in Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+x</sub> where variations of both  $\mathcal{E}$  and  $n_P$  occur due to alterations in unit cell geometry. The data reveal directly the response of the electron-pair condensate to varying the charge transfer energy. Concurrence of predictions from theory for hole-doped charge-transfer insulators with these observations, then indicates that charge-transfer superexchange is the electron-pairing mechanism of cuprate superconductivity [4].

### Visualizing the atomic-scale origin of metallic behavior in Kondo insulators

A Kondo insulator is, by definition, electrically insulating in bulk at low temperatures. However, several recent experiments have detected signatures of metallicity within this Kondo insulating phase. To explore this mystery, we visualized the real-space charge landscape within a Kondo lattice and discovered nanometer-scale puddles of metallic conduction electrons centered around uranium-site substitutions in the heavy-fermion compound uranium ruthenium silicide (URu<sub>2</sub>Si<sub>2</sub>) and around samarium-site defects in the topological Kondo insulator samarium hexaboride (SmB<sub>6</sub>). These defects disturbed the Kondo screening cloud, leaving behind a fingerprint of the metallic parent state. Our results suggest that the three-dimensional quantum oscillations measured in SmB<sub>6</sub> arise from these Kondo-lattice defects [5].

### Discovery of Pair Density Wave State in UTe<sub>2</sub>

Spin-triplet topological superconductors should exhibit many unprecedented electronic properties. The newly discovered CDW state in UTe<sub>2</sub> motivated the prospect that a PDW state may exist in this material. To search for it, we visualize the pairing energy-gap with  $\mu\text{eV}$ -scale energy-resolution using superconductive

STM tips. We detect three PDWs, each with peak-peak gap modulations circa 10  $\mu\text{eV}$  and at incommensurate wavevectors  $P_{i=1,2,3}$  that are indistinguishable from the wavevectors  $Q_{i=1,2,3}$  of the prevalent CDW. From these data and given  $\text{UTe}_2$  as a spin-triplet superconductor, this is the first spin-triplet pair density wave state [6].

### Discovery of Orbital Ordering in Cuprate $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$

Theories for cuprates usually concentrate on the intra-atom Coulombic interactions dominating the  $3d^9$  and  $3d^{10}$  configurations of each copper ion within the  $\text{CuO}_2$  unit cell. However, if Coulombic interactions also occur between electrons of the  $2p^6$  orbitals of each planar oxygen atom, spontaneous orbital ordering may split their energy levels with the charge-transfer energy  $\mathcal{E}$  separating the  $2p^6$  and  $3d^{10}$  orbitals becoming distinct for the two oxygen atoms. We introduced sublattice resolved  $\mathcal{E}(r)$  imaging to  $\text{CuO}_2$  studies and discovered intra-unit-cell rotational symmetry breaking of  $\mathcal{E}(r)$ . Overall, the data reveal a  $Q=0$  orbitally ordered state that splits the oxygen energy levels by  $\sim 50$  meV [7].

### Dichotomous Dynamics of Magnetic Monopole Fluids

A recent advance in the study of emergent magnetic monopoles was the discovery that monopole motion is restricted to dynamical fractal trajectories [8], thus explaining the characteristics of magnetic monopole noise spectra [9]. We applied this new theory to explore the dynamics of field-driven monopole currents, finding them comprised of two quite distinct transport processes: initially swift fractal rearrangements of local monopole configurations followed by conventional monopole diffusion. To explore these novel perspectives on monopole transport, we introduced simultaneous monopole current control and measurement techniques using SQUID-based monopole current sensors. For the canonical material  $\text{Dy}_2\text{Ti}_2\text{O}_7$ , we measure net monopole current  $J(t) = \dot{\Phi}(t)/\mu_0$  generated by applying an external magnetic field  $B_0(t)$ , where  $\Phi(t)$  is the time-dependence of magnetic flux threading the sample. These experiments find a sharp dichotomy of monopole currents, separated by their distinct relaxation time-constants before and after  $t \sim 600$   $\mu\text{s}$  from monopole current initiation and a loss angle  $\theta(f)$  exhibiting a characteristic transition at frequency  $f \approx 1.8$  kHz over the same temperature range. Finally, the magnetic noise power is also dichotomic, diminishing sharply after  $t \sim 600$   $\mu\text{s}$ . This complex phenomenology represents a new form of heterogeneous dynamics generated by the interplay of fractionalization and local spin configurational symmetry [10].

### Pair Wavefunction Symmetry in $\text{UTe}_2$ from Zero-Energy Surface State Visualization

If  $\text{UTe}_2$  is a topological spin-triplet superconductor, it should have odd parity so that  $\Delta_{-k} = -\Delta_k$  and, in addition, may break time-reversal symmetry. A distinctive identifier of all such nodal spin-triplet superconductors is the appearance of an Andreev bound state (ABS) on surfaces parallel to a nodal axis, in the form of a topological surface band (TSB). Moreover, theory shows that specific TSB characteristics observable in tunneling to an  $s$ -wave superconductor distinguish between chiral and non-chiral  $\Delta_k$ . To search for such phenomena in  $\text{UTe}_2$ , we employ  $s$ -wave superconductive scan-tip imaging and discover a distinct TSB signature, an intense zero-energy Andreev conductance maximum at the (0–11) crystal termination. Its imaging yields quasiparticle scattering interference evidence for two  $\Delta_k$  nodes aligned with the crystal  $a$ -axis. Most critically, the zero-energy Andreev conductance peak splits into two finite-energy particle-hole symmetric conductance maxima as the tunnel barrier is reduced. Overall, this combination of a zero-energy Andreev conductance maximum at the  $\text{UTe}_2$  (0–11) surface, internodal scattering along the  $a$ -axis, and splitting of Andreev conductance maximum due to  $s$ -wave proximity, categorizes the superconductive  $\Delta_k$  of a  $\text{D}_{2h}$ -symmetry crystal as the odd-parity non-chiral  $\text{B}_{3u}$  state [11].

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## 1.14 Collaborative (Inter-departmental/group) Research Activities

Although most of our projects are collaborative to some degree because the combination of physics and chemistry expertise is core to our mission and operation, a few projects are so fundamentally based on joint work that it is more appropriate to report them in this special section of the report than in the contributions from the individual departments or our independent research groups, i.e., Lise Meitner, Minerva and Max Planck Research Groups.

**Nitrogen vacancy magnetometry (H. Binger<sup>#</sup>, Lise Meitner Group Spin3D; U. Vool<sup>#</sup>, Max Planck Research Group IQM) [COLL\\_01\\_Binger\\_Vool](#)**

Nitrogen vacancy (NV) centers are atomic defects in the diamond lattice that couple to various local phenomena such as magnetic field. Their long coherence, ease of manipulation, and operation across a wide temperature range have garnered significant interest for quantum computing and sensing applications. Recently, the NV has been incorporated into a scanning probe microscope by carving bulk diamond into a pillar with the NV at its apex, allowing for imaging magnetic textures on the nanometer scale. While it has mostly been used to image static magnetization, there is a growing interest in measuring dynamic effects such as local currents and magnetic excitation due to the improved NV sensitivity at high frequencies. Through shared expertise in quantum information and condensed matter physics, two NV scanning setups have been developed and optimized: a room-temperature scanning probe microscope and a variable-temperature cryogenic scanning probe microscope. After an overview of quantum sensing and NV magnetometry the challenges and capabilities of the unique setup and ongoing measurements are discussed.

**Magnetic properties of high-pressure phases  $RESi_3$  (U. Schwarz<sup>#</sup>, Chemical Metal Science; S. Wirth<sup>#</sup>, Physics of Correlated Matter) [COLL\\_02\\_Schwarz\\_Wirth](#)**

Rare-earth metal silicides  $RESi_3$  ( $RE = Tb, Dy, Er,$  and  $Tm$ ) with  $YbSi_3$ -type crystal structure exhibit Curie-Weiss paramagnetic behavior above their respective Néel temperatures  $T_N$  and antiferromagnetic ordering below  $T_N$ . The values of  $T_N$  follow a de Gennes scaling and hence, the coupling of the magnetic moments is likely mediated by the so-called RKKY interaction, i.e., via the conduction electrons. Isotypic  $SmSi_3$  exhibits van Vleck paramagnetic behavior evidencing partially filled electronic states.

**Spectroscopic view onto the catalyst's states (I. Antonyshyn<sup>#</sup>, Chemical Metal Science; S. G. Altendorf<sup>#</sup>, Physics of Correlated Matter) [COLL\\_03\\_Antonyshyn\\_Altendorf](#)**

Catalysis studies require an exhaustive analysis of the catalyst material in the pristine state as well as after (electro)catalysis to be able to track the possible changes of the material and to interpret the catalytic data correctly. An extension of the library of systematically studied catalysts allows to elucidate the nature of catalytically active sites or specific steps of the reaction mechanisms. Powerful X-ray diffraction and metallography methods shed light on the phase and composition changes, morphological alterations, segregation effects, etc. In addition, spectroscopic studies provide insight into the electronic state of the elements on the surface of the catalyst, where the actual catalytic reaction takes place. The collaboration illustrates the power of combined catalytic studies, spectroscopy, and quantum chemical calculations.

**Orbital selective commensurate modulations of the local density of states in  $ScV_6Sn_6$  probed by nuclear spins (R. Guehne<sup>#</sup>, Topological Quantum Chemistry; M. Baenitz<sup>#</sup>, Physics of Quantum Materials) [COLL\\_04\\_Guehne\\_Baenitz](#)**

The two-dimensional kagome network has emerged as a key structural motif in modern solid-state physics, because these networks host special electronic states related to Dirac cones, van Hove singularities, and flat bands, providing a rich playground for the study of critical phenomena. The V-based kagome metal  $ScV_6Sn_6$  exhibits an unconventional charge density wave below  $\sim 96$  K. To illuminate the interesting phenomena as well as the structural and electronic properties of  $ScV_6Sn_6$  from a microscopic perspective,  $^{51}V$  nuclear magnetic resonance and density functional theory have been employed. The dynamics of the local magnetic field reflect the changes in the density of states of V, while the static local magnetic field reveals a substructure of Fermi level states, suggesting an orbital-selective modulation of the local DOS.

<sup>#</sup>Main collaborators from the respective departments/groups



## 2. Structure and Organization of the Institute

### 2.1 Governance and Compliance

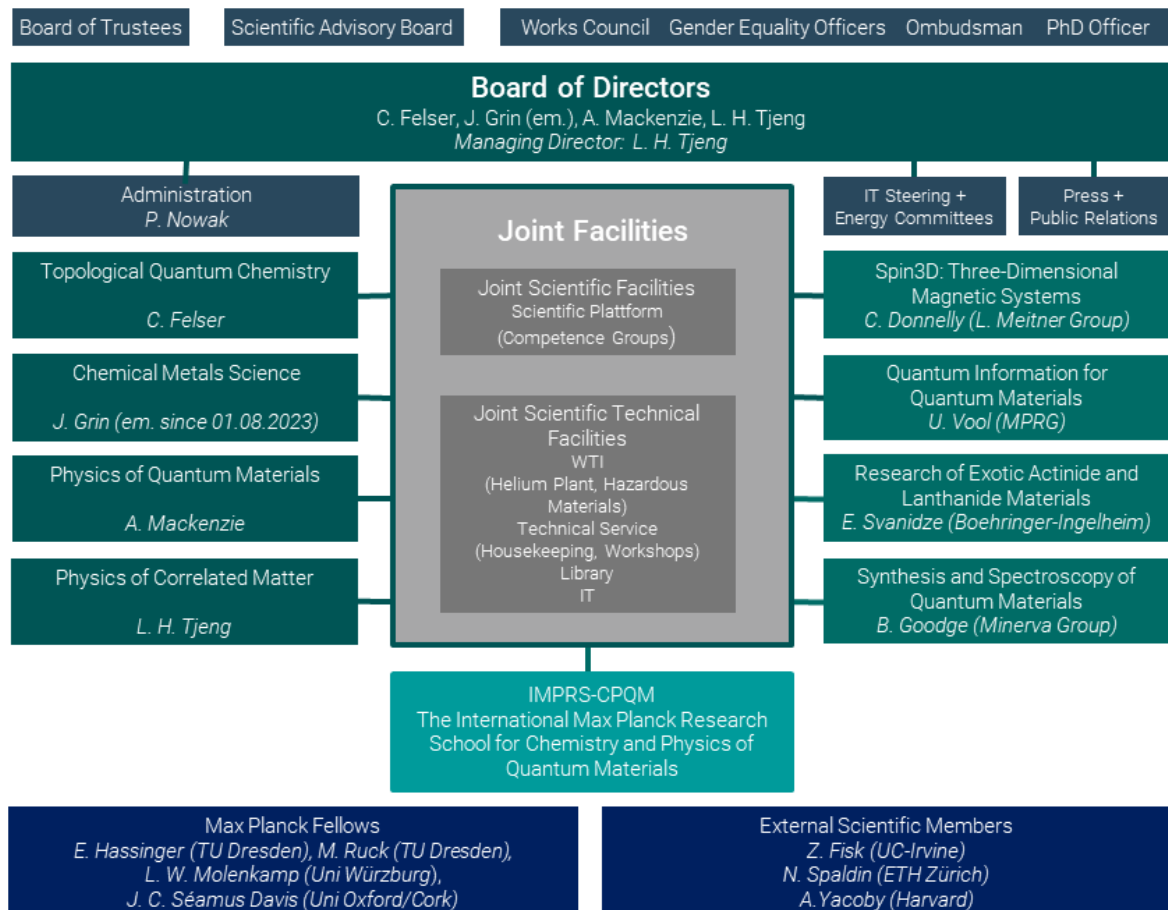
The organisational structure of our Institute has remained largely unchanged. A Works Council as well as an IT Steering Committee and Energy Committee have been added. The chart below provides an overview.

The scientific activities of the Institute are led by the Departments for „Topological Quantum Chemistry” (TQC; Claudia Felser; former Solid State Chemistry), „Physics of Quantum Materials” (PQM; Andy Mackenzie), „Physics of Correlated Matter” (PCM; Liu Hao Tjeng), and „Chemical Metal Science” (CMS; Juri Grin), as well as the Lise Meitner Excellence Group „Spin3D: Three-Dimensional Magnetic Systems” (Claire Donnelly), the Max Planck Research Group (MPRG) „Quantum Information for Quantum Materials” (Uri Vool), the Minerva Fast Track Programs „REALM” (Eteri Svanidze, from Sep. 2023 funded by the Boehringer Ingelheim Foundation) and

„Synthesis and Spectroscopy of Quantum Materials” (Berit Goodge, Schmidt Fellow until Sep. 2024).

The MPRG groups „Physics of Unconventional Metals and Superconductors” (Elena Hassinger) and „Nanostructured Quantum Matter” (Johannes Gooth) ended in 2022 and 2023, respectively.

Close scientific collaboration with the Technical University Dresden is anchored by the Max Planck Fellowship of Michael Ruck from the Chemistry Department and Elena Hassinger (since 2022). Our scientific collaboration with the German university sector is further enhanced by the Max Planck Fellowship of Laurens Molenkamp of the Julius-Maximilians-Universität Würzburg, with an added international dimension provided by the Max Planck Fellowship of J.C. Séamus Davis of the University of Oxford and University College Cork. Impulses for new scientific projects are provided by the External Scientific Member Zacharias Fisk of UC-Irvine, Amir Yacoby of Harvard and Nicola Spaldin of ETH Zurich.



The Board of Directors receives advice and recommendations from the Scientific Advisory Board, the Board of Trustees, the Works Council (nine members with Helge Rosner as chair), the Gender Equality Officers (Gudrun Auffermann - until 08/2023, Renate Hempel-Weber - until 11/2023, Elena Gati - since 09/2023, Vicky Hasse and Ramona Schrodtt - since 04/2024), the Ombudsman (Peter Höhn), and the PhD Officer (Burkhard Schmidt).

The Board of Directors receives assistance in its decision-making from the Head of the Administration (Petra Nowak) and Institute Committees on finances, technical services, computer services, library, safety issues. The Board of Directors also maintains close contact with the representative of the scientific staff for the CPT Section of the MPS: Steffen Wirth (until 9/2023) and Ulrich Schwarz (since 10/2023).

As a temporary measure during the pandemic (2020-2023), a crisis team was established comprising the Managing Director and his Deputy plus the Safety Officer, Gender Equality Officer and heads of key technical facilities. Marcus Schmidt's role as Safety Officer was considerably expanded to include occupational health issues and Oliver Stockert was serving as Home Office Advisor.

After the IT breach in November 2022, a recovery team was established consisting of the Managing Director and his Deputy plus the head of the IT department Jens Gerlach and representatives of the four departments. In addition, Burkhard Schmidt was appointed as Information Security Officer. In mid-2023 the crisis team was converted into an IT Steering Committee chaired by Burkhard Schmidt and Jens Gerlach.

The tremendous surge in energy and helium prices in Germany in 2022 associated with the Ukrainian war formed the motivation to set up an Energy Committee, comprising the Managing Director, the head of the technical services Andreas Schwoboda, the safety officer Marcus Schmidt, and representatives of the four departments and the administration.

Our MPI participates in the MPG's risk management system. We have established a team of scientists and administrators to manage issues in the area of „Export Control“. Printed copies of the „Rule of good science“ are available in our library and can be viewed digitally via the MAX website. From there, our employees can also access other important rules of the MPG, along with other documents on the „routing slip“ that every new employee receives. We have appointed a trained conflict mediator (Renate Hempel-Weber).

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## 2.2 Pandemic Response

The goal of our pandemic response was to maintain core operations as far as possible, while giving ultimate priority to the safety of our staff. In March 2020 a crisis team was established to develop appropriate rules of operation, in close cooperation with the central crisis team of the MPG. Unlike many scientific institutions world-wide, we never had to enforce a shut-down. Considerable credit for this has to go to our staff, who exercised care both in their personal lives and, especially, in the work-place.

The measures that we took include: mobile working to reduce simultaneous office occupancy and thus maintain the recommended safety distance, providing free coronavirus test kits (until spring 2023), offering vaccinations by the company doctor from BAD (2021 and 2022).

Mental health became an urgent issue. While the PhD students and postdocs expressed their wish to have a professional psychologist or psychotherapist to be available at a regular basis inside the Institute, we were not able to fulfill this on legal grounds. What we were able to do is: (a) to offer exercises from the Employee and Manager Assistance Program (EMAP) of the Max Planck Society organized by the Fürstenberg Institute, (b) to compile and offer a list of foreign language psychologists and psycho-therapists in the Dresden area as well as the services available at the TU Dresden and University of St. Andrews, (c) to offer courses on „Mental Health First Aid” and „stress management” on a regular basis in the Institute so that each new cohort students and postdocs has access to them.

14 mental health first aiders were trained and certified according to the mental health first aid principle by Zentralinstitut für Seelische Gesundheit Mannheim. Their job is not to diagnose or treat those affected. But they are there to listen, offer uncomplicated first aid and refer people to professional organisations or people who can provide professional help. Confidentiality is of course the top priority.

## 2.3 Response to IT Breach

On 11 November 2022, a massive amount of data was deleted or encrypted in the computer system of our Institute. This concerned not only the central storage system but also laboratory PCs for data taking.

A recovery team was set up consisting of the Managing Director and his Deputy plus the head of the IT

department and representatives of the four departments and administration. The task of the team was (1) to assess the damage, (2) to determine the cause of actions to get back to normal operation, and (3) to coordinate the efforts to possibly retrieve the deleted or encrypted data.

The recovery team found that the breach became wide-spread due to flaws in the architecture of the IT system and that data was irretrievably lost due to the improper implementation of the central back-up concept.

Two weeks after the breach, we were able to have a rudimentary email system in place, and two months later, our regular email system. All laptops and laboratory PCs were scanned for malware, and if clean, backups were made. The time needed to resume office and laboratory operations depended strongly on individual cases. Newer computers not requiring specialized software were back online within two weeks. The administration needed about two months before it regained full connection with the central administrative system. Most strongly disrupted were operations with older instruments which run with software that turned out to be obsolete: many months or longer of efforts were needed.

While data on the central storage system and laboratory PCs was irretrievably lost, not all the associated information was lost. Many scientists have their personal backup, others have the information in the form of hard copies or processed data such as files containing figures, tables, presentations, and manuscripts. Nevertheless, several PhD students have suffered serious setbacks costing them several months to recover (for which we have extended their contracts accordingly). In one particular case, for example, one student had to repeat three months' worth of measurements.

The MPG's Information Security Officer and colleague IT managers from other MPIs visited us in Jan. 2023. This ad-hoc MPG-IT security team assessed the situation and our recovery actions, and provided us with recommendations how to rebuild the IT infrastructure: how to improve the security and robustness of the network, and how to set up a reliable backup system. We have followed and are following the recommendations closely. We wished that such a team would have been readily available at the Max Planck wide level for checking each MPI for the technical fitness of the IT system.

On the organizational level we have also made adaptations. We have appointed an Information Security Officer: Burkhard Schmidt. In mid-2023 the

IT recovery team was converted into an IT Steering Committee co-chaired by the Information Security Officer and the head of the IT department.

More information concerning the IT breach and the implementation of the recommendations of the ad-hoc MPG-IT security team will be provided by Burkhard Schmidt upon request (bs@cpfs.mpg.de).

## 2.4 Response to Energy Crisis

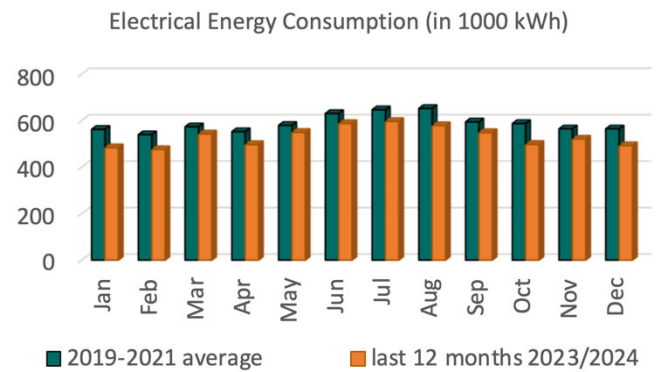
The tremendous surge in energy and helium prices in Germany in 2022 associated with the Ukrainian war formed a serious threat for our ability to carry out our in-house research activities. An Energy Committee was set up to identify measures for savings while at the same time minimising the disturbance to productive science.

By far the largest financial burden is for electricity consumption, followed by the costs for heating of the building and purchase of new helium.

A detailed look at the time profile and other characteristics of electricity usage reveals that most of the electricity is used for engines: cooling machines for laboratory air and temperature control, for water cooling of instruments, for the central helium liquefier, and for various pumps and engines in the laboratories. One of the measures we took was to reduce the air flow of the laboratories by 50 percent during off-office hours, requiring that activities with potentially high risk can be carried out only during office hours. We also practiced systematically the use of liquid nitrogen precooling for the liquefaction of helium. We increased the cooling temperature of the server rooms, and we installed sun protection foils on windows and accelerated the conversion of the lighting to LED.

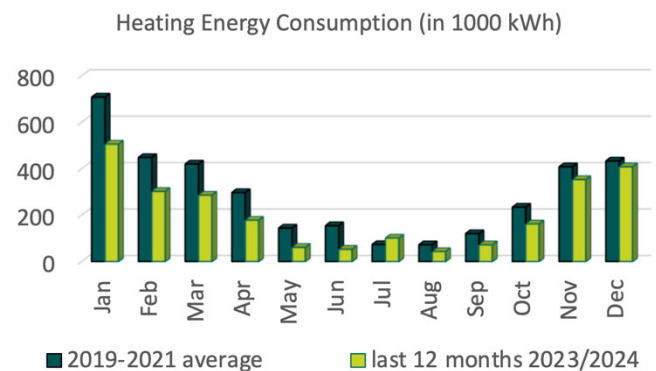
These measures resulted in an overall reduction of the electricity consumption by about 10 percent as can be seen from the chart below which compares the situation in the last 12 months with that of the average of 2019 – 2021 period. Perhaps we could have hoped for more but here we would like to note that our Institute has now more research activities than in the quiet 2020 – 2021 Covid years, during which we did not take any energy saving actions.

Our Institute is one of the first Max Planck facilities to apply for and receive approval to install a photovoltaic system as part of the „Max Planck Solar” program. Once planning has been completed, installation is scheduled to begin in 2025. We then expect to generate about 5 percent of our annual electricity consumption



ourselves. Other measures such as the implementation of natural air flow cooling of the „Wintergarten” during summer as well as the increase of the temperature of the cooling water are also planned.

Reducing the energy consumption for the building was a straightforward exercise. During off-office hours, we lowered centrally the heating temperature and during the Christmas break we even kept it at an absolute minimum. An overall energy reduction of about 25 percent was achieved, please see the chart below which compares the situation in the last 12 months with that of the average of 2019 – 2021 period.



Liquid helium is essential for daily research work. We use about 140,000 to 170,000 liters of liquid helium annually. The price of new helium has more than doubled since 2021, from ca. 15 EUR/liter to 35 EUR/liter now. A key challenge here was to reduce the overall losses as much as possible. We now have managed to keep the losses to around 5-8 percent. This was achieved through both technical and organizational measures. The tightness of the recovery system was regularly checked, and the plant was technically maintained and modernized (installation of a new control system, installation of new high-pressure valves and optimization of the gas supply system). Obviously, reducing helium losses was not only motivated by financial constraints, but also necessary for reasons of sustainability, as helium is a finite resource.

## 2.5 Promotion of Junior and Guest Scientists and Career Development

At any one time we host around 100 graduate students and post-docs, and have devoted considerable time over the past years to providing them with a good environment in which to work.

### Graduate student education and supervision

The main program for graduate students at the MPI CPfS, the International Max Planck Research School for Chemistry and Physics of Quantum Materials (IMPRS-CPQM, <https://imprs-cpqm.mpg.de>), has entered its second six-year funding period at the beginning of 2022. In the IMPRS-CPQM, the Institute collaborates with the TU Dresden and the University of St. Andrews, Scotland as its partner universities. The extension of the central funding through the end of the year 2027 enables us to continue the well-established procedures for recruiting and training of our students. In a more general view, the framework offered by the IMPRS-CPQM, e.g. regarding coursework and supervision of the doctoral students, has fully matured since its inception, and has benefitted from occasional fine-tuning of various aspects, the latter in particular thanks to helpful suggestions by the review board of IMPRS-CPQM and also by the students themselves.

In addition, we also have successfully recruited several excellent students through the Max Planck Graduate Center for Quantum Materials (MPGC-QM, <https://www.quantummaterials.mpg.de/>), a doctoral program jointly offered by seven Max Planck Institutes including MPI CPfS, working in the field of quantum materials. Our students in MPGC-QM are by default also members of IMPRS-CPQM, and additionally have access to dedicated courses and events offered by the MPGC, which are specifically tailored for its elite students across all participating institutes.

The vast majority of our students are members of IMPRS-CPQM, either through direct recruitment for IMPRS-CPQM or on account of their recruitment through the MPGC. As other avenues for recruitment are also available for PIs at the Institute, e.g. relying solely on departmental funds or external grants, we aim to keep the distinction between the different classes of students as small as possible: IMPRS-CPQM courses and events are open to all graduate students, and – likely even more importantly – the same guidelines for supervision and monitoring apply for all students

across the institute. In particular, the Thesis Advisory Committees, which are individually set up for each student at the MPI CPfS, are working well overall. More details about the supervision of our PhD students can be found at the IMPRS website <https://imprs-cpqm.mpg.de/45308/supervision>.

In the Supervision Agreement, which each student enters with their supervisor(s), both parties commit to following the principles of Good Scientific Practice. This commitment implicitly includes training and guidance of junior researchers with respect to this important matter.

For the mentoring of the doctoral students, in particular at the early stages of their stay at the MPI CPfS, the doctoral students have established and organize a „buddy program”, in which incoming students pair up with a more senior student who serves as a guide to navigate the life of a doctoral student. Obviously, the Thesis Advisory Committee also plays an important role in mentoring the students regarding all aspects of developing a successful career.

The Institute and, in particular, the student community itself organise and offer a variety of events related to the development of careers inside and outside academia. These events include, but are not limited to, workshops for the acquisition and improvement of transferable skills, seminars targeted at exploring career opportunities, and talks – often by former graduate students – highlighting individual career paths and how those benefitted from having acquired a doctoral degree in chemistry or physics. More information on those activities can be found in the Addendum.

The position of the PhD Officer at the Institute, which is held by Dr. Burkhard Schmidt, is set up outside the framework of IMPRS-CPQM to ensure its independence. The PhD Officer acts as a contact person for PhD students in all matters, with a focus on the students' well-being, both on a personal and professional level. The latter in particular covers conflicts of students with their supervisors and mediation in such cases. The students also can raise concerns about compliance with the framework for the work and supervision of junior researchers, as it is established at the Institute or within the Max Planck Society in general.

The PhD Officer also proactively holds regular meetings with students as individuals and also the student representatives in order to get an overview of issues affecting the student community at the institute.

## **Community-building among post-docs**

Similar to the PhD representatives, the post-doc community, which is much more diverse than the PhD community, has since a few years established post-doc representatives offering help for this group of scientists. The pandemic was likely particularly difficult for our post-doc because of career pressures.

## **Graduate employability**

We believe that the employability of our graduates is excellent: Of the 30 PhD students graduating from the groups of the Institute staff in the assessment period 21 found employment in academic research science, 7 in industry, and from 2 we have no information.

A list of PhD students (past and current), their supervisors and their whereabouts (as far as known) can be found in the Addendum.

In addition, all PhD students (including students who are only completing part of their doctorate at the Institute) are listed in the supplement 'Data, Facts, and Figures' (available at the SAB meeting) with their period of employment and funding.

## **Academic career advancement, professorships offered**

The Institute encourages post-docs, group leaders and senior scientists to participate in career development courses, e.g., leadership courses about time management, self-organization and mental stress or the Schiemann-Kolleg workshops. In addition, the Curiositas Lectures, organized by the PhD students, provide insight into the work of former scientists no longer working in academia.

The assessment period has seen strong performance from research staff wishing to further advance their academic careers. Those moving on to established positions elsewhere include:

Elena Hassinger (MPRG „Physics of Unconventional Metals and Superconductors“) was appointed as a professor at the TU Dresden and become a Max Planck Fellow of our institute in September 2022.

Johannes Gooth (MPRG „Nanostructured Quantum Matter“) was appointed to the chair of experimental solid-state physics at the Rheinische Friedrich-Wilhelms-Universität in Bonn in February 2022.

Qingge Mu has left our institute in December 2021. She has taken up an associate professor position at the

Institute of Physical Science and Information Technology at the Anhui University, Hefei, China.

Yan Sun has taken up an associate professor position at the Institute of Metal Research, Chinese Academy of Science, Shenyang in October 2021.

Elena Gati was appointed a W2 position at MPI-CPfS combined with an Honorary Professorship at TU Dresden.

You-Sheng Li has taken up an assistant professorship at the National Taiwan University in Taipei.

Berit Goodge accepted the offer for an assistant professorship at Cornell University, United States.

Alexander Steppke became a Permanent Staff Scientist at the Paul Scherrer Institute, Villigen, Switzerland.

Veronika Sunko accepted the offer for an assistant professorship at IST Austria.

Igor Markovic has taken up an assistant professorship at University of Birmingham, UK.

## **Recruitment procedures**

For the recruitment of PhD students, the IMPRS places regular calls for applications (on its webpage) and holds recruitment workshops once per year. It uses a central electronic data base to administer all applications. In contrast, for post-doc positions, candidates often send unsolicited applications or applications after having a personal contact. Also, advertisements are posted on the MPG website and increasingly on science-oriented job exchanges.

Concerning the science-supporting area, the Institute has also noticed a shortage of specialists when recruiting suitable people. e.g., in the IT department or the different workshops. The traditional channels via the MPG/MPI website, advertisements in local newspapers and the job center/employment office no longer seem to be effective in finding suitable people. The problem is also known to the general Max Planck administration in Munich, as the topic was hotly debated during an online meeting of the communications department in June 2024, which was attended by many public relations and press officers from various MPIs.

## **Helpline Dresden**

The MPI CPfS has been supporting the helpline in Saxony since 2017. The Helpline is a multilingual support service for emergency communication. It works closely with the regional offices of the fire and rescue services and the situation centres of the police emergency services.

## 2.6 Diversity and Equal Opportunities

### Personnel data

The Institute strives to maintain a healthy gender mix among its scientists. Over the past assessment period the gender balance has been approximately 50-50 female-male among our graduate students. At each of the post-doctoral and group leader levels, approximately 33% of our staff are female, rising to 50% at W2 (Associate Professor) level and, since Prof. Grin's retirement, 33% at Director level. A recent focus of the institute's management has been to improve the imbalance at group leader level, appointing and promoting 5 female scientists to group leadership and W2 positions during the assessment period. We are particularly pleased to note that over 20 prizes and awards went to female staff and graduate students during the same period.

A remaining area of concern is among the non-group leading staff scientists with permanent contracts, among whom the female-male ratio is less than 10%. While we would be keen to see this improved, it is a historical problem that can be tackled by purely internal means only as a reaction to retirements, many of which will occur in the medium- rather than the short-term.

### Child care facilities

To assist its members with young families, the institute has 20 places in three group nurseries in the immediate vicinity of the institute. So far, the demand from (new) employees for these places has been met immediately or within a very short time.

### Establishing a gender-equitable work-place

Another of the institute's top priorities is to promote equal opportunities and establish gender-equitable working conditions. In collaboration with the Board of Directors, the Gender Equality team—comprising Gudrun Auffermann and Renate Hempel-Weber (until 2023), and Elena Gati (since 2023), Vicky Hasse, and Ramona Schrodtr (since 2024)—has been actively implementing our equal opportunity initiatives, as outlined in our gender equality plan. The team provides guidance to employees on balancing work and family life, offers information on career development measures, and serves as a key contact for resolving conflicts. They also organize various training sessions aimed at conflict prevention.

The Gender Equality Officer Team regularly participates in workshops organized by the Central Gender Equality Officer of the MPG, is embedded in several gender equality networks and takes care of gender-fair language in the institute. It also works with the local and central administration and the PhD and post-doc representatives to provide a suite of training courses, most of which are available to all genders. Activities in the assessment period include:

#### 2021:

24<sup>th</sup> – 25<sup>th</sup> August: Workshop „Developing your research brand” for group leaders and advanced postdocs. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

#### 2022:

23<sup>th</sup> – 24<sup>th</sup> August: Workshop „Developing your research brand” for group leaders and advanced postdocs. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

8th December: Visit of the Central Gender Equality Officer Dr. Ulla Weber at our MPI. Discussion with Gender Equality Team, the Head of Administration and the Managing Director about local gender-related subjects.

#### 2023:

11<sup>th</sup> February: International Day of Women in Science activity: The PhD Students organized a streaming of the movie „Picture a Scientist“.

8<sup>th</sup> March: International Women's Day activity: The PhD Students organized discussion rounds, led by Elena Hassinger and Claire Donnelly, on the impact of unconscious bias on career in science.

June-December: Redesign of the gender equality plan of the institute (2024-2026) by mutual consent of the Board of Directors, the Head of Administration and the Gender Equality Officer Team.

24<sup>th</sup> – 25<sup>th</sup> August: Workshop „Developing your research brand” for group leaders and advanced postdocs. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

October: Mental Health First Aid Training for volunteers in the Institute.

27<sup>th</sup> November: Curiositas Seminar, organized by the PhD Students, on „Gender, identity and culture in physics“ (Speaker: Prof. Anna Danielsson, Stockholm) (see also in Addendum).

## 2024:

13<sup>th</sup> – 14<sup>th</sup> May: Elisabeth Schiemann Kolleg Workshop hosted at our MPI-CPfS and organized by Claire Donnelly and Berit Goodge, the Schiemann Fellows at our Institute, and our Schiemann Kolleg mentor, Andy Mackenzie.

12<sup>th</sup> June: Election of the Gender Equality Officer Team (07/2024-11/2028).

21<sup>th</sup> – 22<sup>th</sup> August: Workshop „Developing your research brand” for group leaders and advanced postdocs. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

Petra Nowak is the contact person of our institute in the framework of the Career Steps Network of the MPG and continuously provides our scientists with information to support them at different steps of their career. In addition to these local activities, Gudrun Auffermann has served as Gender Equality Officer of the CPT Section from 2019 to 2023.

## 2.7 Works Council\*

(\*text supplied by Works Council)

The first works council at the MPI CPfS was constituted after the election in November 2023 on 14.12.2023 and began its diverse work. The Works Council was elected with a high voter turnout of 64% and consists of 9 members from 4 lists with a large number of potential substitutes.

The Works Council has a balanced composition in terms of employee structure (non-scientists, scientists, post-docs and doctoral students) and gender (5 women, 4 men).

The works council sees itself as a body that represents the interests of the employees of the MPI CPfS in constructive dialog with the institute management. We attach great importance to being available to all employees effectively and confidentially. To this end, the works council has been provided with a works council room by the institute management, where its regular office hours are also offered.

Committees have been elected to ensure the effective organisation of the works council's tasks. Among other things, a works committee is responsible for the prompt processing and approval of personnel matters, such as new appointments or contract amendments. A working time committee deals with all issues relating to working time. In particular, we develop models - in consultation with the management of the MPI CPfS -

on how working time can be recorded and organised within the framework of legal requirements.

Communication with the institute's management is maintained through regular monthly meetings. Works meetings for all CPfS employees are held once a quarter in German and English.

## 2.8 Achievements: Scientific Awards, Fellowships and Memberships

During the assessment period members of our institute have received various scientific awards, not only Directors and Emeritus Directors, but also our junior research staff and graduate students.

Concerning our Directors, Claudia Felser won in 2022 the Max-Born-Preis and Medaille, jointly awarded by the German Physical Society and the British Institute of Physics. In the same year she also received the Wilhelm Ostwald Medaille of the Saxon Academy of Science and the Liebig Medaille by the Society of German Chemists. In 2023 she was awarded the EPS Europhysics Prize and elected to the Hall of Fame of German Research. Juri Grin was appointed as honorary professor at the Institute of Low Temperature and Structural Research of the Polish Academy of Sciences in Wroclaw in 2022. In 2024 he received the Carl Hermann Medaille of the German Society for Crystallography. Max Planck Fellow Séamus Davis won the Buckley Prize in 2022. Christoph Geibel was awarded a Wilhelm Heraeus Visiting Professorship at the Goethe University Frankfurt in 2022 and Joshua Goldberger received a Friedrich Wilhelm Bessel fellowship to stay at our institute in the same year.

Major mid-career prizes also went to Max Planck Research Group leaders, staff and postdocs. Elena Gati was appointed as Honorary Professor at TU Dresden in 2024. Claire Donnelly was awarded the IEEE Magnetics Society Early Career Award in 2023 and the Heinz-Maier-Leibnitz Preis in 2024. Eteri Svanidze received the „For Women in Science” award in 2022, the Junior award from the European Rare Earth and Actinide Society in 2023 and the Actinides Medal at the Journées des Actinides in 2024. Maia G. Vergniory was appointed as APS Fellow by the American Physical Society in 2022. Kazuki Imasato was awarded a Young Leader International Scholarship from the Minerals, Metals & Materials Society and Yu Pan received the ITS Postdoctoral Scholar in Thermoelectrics Award, both in 2023.

Our graduate students picked up a large number of well-deserved awards and prizes, demonstrating that the future of the field is in good hands. Qun Yang received for her thesis the Otto Hahn Medaille and the Otto Hahn Award of the Max Planck Society in 2023. For her thesis Philippa Helen McGuinness was also awarded an Otto Hahn Medaille in 2023. Conference talk and poster prizes were won, e.g., by Büşra Mete, Chia-Chi Yu, Natalia Glorizova, and Paul Simon.

The detailed list of awards can be found in the Addendum.

## 2.9 Statistical Summary of Publications and Invited Talks

In this section we provide a brief statistical analysis of our primary forms of disseminating our results, namely our publications and the talks that we give at conferences and at other institutes. We mention talks in this section because they are important both for increasing

the visibility of our Institute and of our non-Directorial staff. All departments have the default policy that any junior scientist or PhD student attending a conference should present either a contributed talk or a poster on their research.

### Publication statistics

In section 1 of this Status Report and the related web-based research summaries we discussed research highlights and associated publications. In Table 1 below, we provide statistics on our volume of publication from May 2021 to June 2024, in a format that shows the extent of inter-departmental publication. The institute's total numbers of publications for the period are shown in bold. The total outputs of the individual departments, the independent research groups and the collaborative work within the institute are specified in detail.

Roughly half of the publications are in open access journals (see table I), number of OA publications in general strongly increasing since 2020.

<i>Year</i>	<b>2021</b>	<b>2022</b>	<b>2023</b>	<b>2024</b>	
<i>Months</i>	05-12	01-12	01-12	01-06	
					<i>Sum</i>
Publications total	<b>185</b>	<b>318</b>	<b>275</b>	<b>182</b>	<b>960</b>
Chemical Metal Science – Grin	35	47	51	19	152
Physics of Correlated Matter – Tjeng	50	83	90	70	293
Physics of Quantum Materials – Mackenzie	50	75	66	37	228
Topological Quantum Chemistry – Felser	61	93	69	46	269
Lise Meitner Group Donnelly	-	12	10	8	30
Max Planck Research Group Vool	-	-	-	1	1
Minerva Group/Boehringer Fellow Svanidze	2	7	4	3	16
Minerva/Schmidt Group Goodge	-	-	2	3	5
Max Planck Fellow Hassinger	2	6	1	0	9
Max Planck Fellow Ruck	9	17	12	7	45
Max Planck Fellow Molenkamp	1	0	1	0	2
Max Planck Fellow Davis	3	2	3	2	10
Interdepart. Collaborations	26	17	22	17	82
Open Access	91	162	131	93	477

*Table 1: The first row of the table (bold) provides the total number of publications per year for the institute. In the following, this is subdivided into contributions (authored or co-authored by an author) from the departments, the independent research groups and the Max Planck Fellows. In addition, the joint publications from two or more departments are given. The last row indicates the open access publications per year.*

The complete list of publications - separated into publications in scientific journals and in university theses (dissertations) - can be found in the Addendum.

### **Open access**

Materials physics and parts of materials chemistry have for a long time operated a major open access vehicle not available to many other fields – the preprint archive ArXiv, to which the Max Planck Society makes a financial contribution. Almost all journals now allow posting of a late-stage manuscript on this site, containing both all the information in the final published version and a reference to that publication. We already make extensive use of this facility, and our policy is to make it a systematic requirement for all submissions on topics covered by it. In physics, it has become a far more widely-used vehicle for the dissemination of results than open access journals, and has the advantage of not being subject to the large paper-by-paper fees charged for Open Access by many journals. In some cases, it is still appropriate to opt for journal-based Open Access and in those cases our staff are encouraged to do so. For all publications, we make systematic use of the publication repository of the Max Planck Society.

### **Invited talks**

During the assessment period, Institute members gave more than 400 invited talks at international conferences, workshops and individual institutions. 169 plenary, keynote and invited talks were given by the directors. The independent group leaders gave approximately 103 (24%) such talks, and non-directorial staff (staff scientists, post-docs and PhD students) a further 126 (29%). Due to the pandemic, 66 of these talks were given virtually. Details can be found in the Addendum.

## **2.10 Cooperation and Networks: Cooperation with National and International Research Institutes and Companies**

In keeping with the nature of our field, a large proportion of our work is in collaboration with partners outside our Institute. We prefer to keep these collaborations informal and therefore administratively light-touch wherever possible, but we also run a number of formalized collaborations where the links are stronger

and long-term, and involve regular travel of personnel. Here, we provide a brief summary; extensive details are provided in the Addendum.

### **Major international collaborations involving formal agreements**

The Physics of Correlated Matter department led by Hao Tjeng has strong links with the scientific communities of Taiwan and Korea. These have been formalized in Memoranda of Understanding with the NSRRC, NCTU and NHTU in Taiwan, and via the Max Planck Center of Complex Phase Materials with POSTECH (Korea) and NSRRC-NCTU-NHTU (Taiwan). Our Institute continues to be an active partner within the Max Planck -UBC-UTokyo Center for Quantum Material, a collaborative venture between the Max Planck Society, the University of British Columbia (Canada) and the University of Tokyo (Japan). Juri Grin leads a collaboration with the National University of Lviv in Ukraine and Claudia Felser two further collaborations, with the Czech Academy of Sciences and the Weizmann Institute respectively. A formal agreement also exists regarding the participation of TU Dresden and the University of St Andrews in IMPRS-CPQM, along with a broader agreement with St Andrews regarding shared doctorates. Our Institute and the University of St Andrews are also partners in the Max Planck Graduate Centre for Quantum Materials.

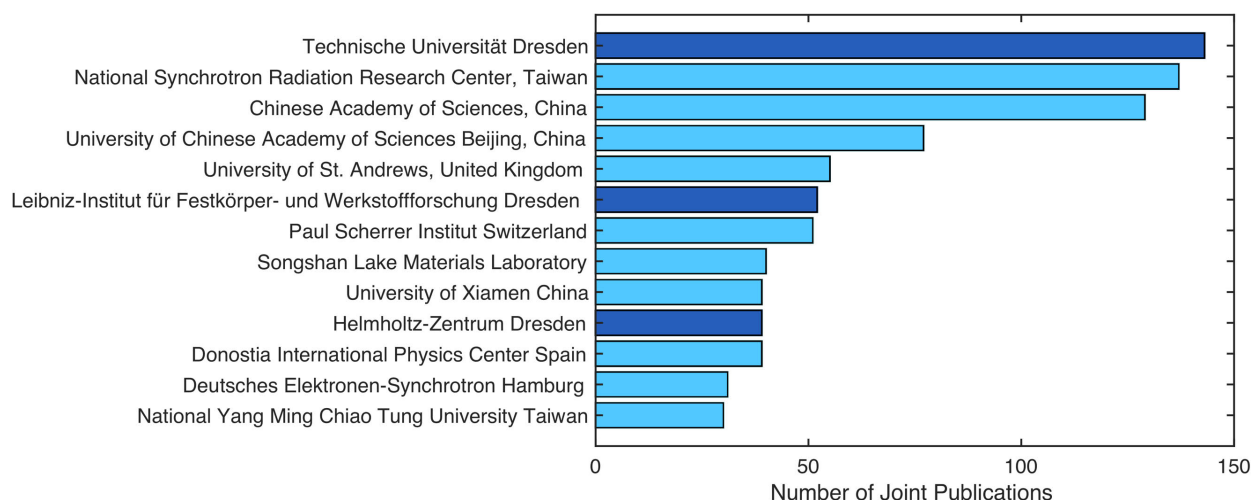
### **Scientific partners (from publications)**

The most direct evidence of our collaborative science comes from an analysis of our publications. During the assessment period, we jointly authored papers with more than 150 institutions elsewhere in Germany and beyond. As seen below in the diagram of joint publications with external partners, our Institute has quite strong links to the local research institutes in Dresden, but also collaborates significantly with international institutes. A detailed list with the most important external institutions can be found in the Addendum.

### **Industrial partners and patents**

Currently, we have mainly collaborations with smaller companies spawned from research by Institute members such as Razorbill (cryogenic strain cells) and Innovative Measurement Technology (dilatometers).

## Scientific Partners from Publications



In the census period we have submitted several invention disclosures and applied for patents. The inventors and the working titles are:

- Claudia Felser, Liang Fu, Yang Zhang: *Moiré metal for catalysis*
- Iryna Antonyshyn, Juri Grin, Peter Höhn, Marcus Schmidt: *Method of Forming a Catalytically Active Material for Electrochemical Energy Conversion*
- Iryna Antonyshyn, Ulrich Burkhardt, Juri Grin, Fatma Aras, Robert Schlögl: *Exceptionally robust and active  $TMCo_3B_2$  ( $TM = Zr, Hf$ ) catalyst precursors for oxygen evolution reaction*
- Claudia Felser, Bin He, Yu Pan: *Bi-Sb alloys as Thermoelectric Material*
- Manuel Brando, Peter Bogatikov, Ludwig Holleis: *Magnetpulsgenerator*
- Claudia Felser, Xia Wang, Chandra Shekhar: *Topological homochiral crystals with intrinsic chiral active sites for improved water electrolysis and fuel cells energy efficiency*

### Research grants and national collaborations

Our members are partners in one Deutsche Forschungsgemeinschaft (DFG) Collaborative Research Center (SFB) with TU Dresden, one DFG Collaborative Research Center (SFB Transregio) with the Goethe-Universität Frankfurt a.M., Karlsruhe Institute of Technology and Johannes-Gutenberg-Universität Mainz, one DFG Cluster of Excellence, ct.qmat, with TU Dresden and Julius-Maximilians-Universität Würzburg, one DFG Research Unit, three DFG Priority Programs, ten DFG Individual Grants and five Individual Grants by different non-governmental driven foundations. In addition, we are partners in

several EU and international grants including one ERC Advanced Grant, one ERC Starting Grant, three EU Grants under the HORIZON 2020 Framework Programme and we host two EU Marie Skłodowska-Curie Individual Fellowships and one Horizon MSCA 2021 Postdoctoral Fellowship. Finally, as mentioned above, we are funded members of the Max Planck Graduate Center for Quantum Materials.

## 2.11 Service: Committee Work and Teaching

We are conscious of the privileged position that we hold as a well-funded research-intensive Institute, and therefore encourage our staff to retain strong links with the rest of the community through appropriate service on external committees and university teaching.

### Committee work

The Directors and several senior scientists of the Institute are members of numerous national and international committees and panels.

In particular, staff members are actively involved in review panels for beam time allocation at large scale facilities. A list is included in the Addendum.

### Teaching

Members of our Institute carry out teaching activities on a regular basis. This is not only service to the partner University (TU Dresden) but forms also an excellent opportunity for our non-director scientists to improve and demonstrate their capabilities in teaching and educating students, which is of utmost importance for the advancement of their careers in academia.

Obviously, our teaching is also an opportunity for students to get acquainted to our research field and our Institute, which may motivate them to do a Bachelor, Master or PhD project with us.

In the period April 2021 – June 2024 period (semesters at TU Dresden start in April and October), Institute members have given more than 27 lecture courses and 27 teaching seminars with a total teaching load of more than 60 SWS (Semester Wochen Stunde = hours per week per semester). This corresponds to approximately five different lecture courses per semester with 2 SWS per course on average.

The lectures range from basic courses to courses on specialized topics, and are given not only to Physics and Chemistry students, but also to students from the Engineering, Business-Engineering, Materials Science, Geography and Teaching departments of TU Dresden.

A detailed list of our teaching activities is included in the Addendum.

## 2.12 Conferences, Workshops and Seminars

Using a combination of our own venue and, for physics, collaboration with our colleagues in the neighboring Physics of Complex Systems Institute, we believe that we have established Dresden as a known global focal point of our field. We strive to maintain this position by organizing large numbers of conferences and workshops for up to 100 each (consistent with our capacity), as well as occasional larger meetings held elsewhere in the city. We also participate actively in the Program and Advisory Committees of the majority of the large international conferences in our field. This aspect of our activities was hit at the beginning of the assessment period particularly hard by the pandemic, but we still hosted 13 workshops and meetings, and 77 seminars and colloquia from external scientists in the assessment period, making use of virtual events as appropriate. A list can be found in the Addendum.

## 2.13 Knowledge Transfer and Public Relations

Our scientific relations team tries to reach out to the community and keep them informed about our work in a vivid and eye-catching way. This is particularly successful during the Long Night of Science in Dresden (LNDWDD), which has been taking place

on a Friday evening shortly before the summer vacation for 20 years now. In 2021 and 2022, we took part in the events held virtually, but this was no comparison to the nights with face-to-face encounters and exchanges. Since our institute was one of the initiators of this event in 2004 – at that time as part of the „Highlights of Physics”, all employees of the institute were looking forward to the twentieth and thus anniversary edition on 30.06.2023. We were able to welcome more than 3600 curious guests to the institute and inform them about our research with guided tours, experiments, children's laboratory and get into conversation with the guests.

The MPG and the six Max Planck Institutes in Saxony pursued the same goal – to talk to interested citizens and present our science – in the event series „30 years of MPIs in Saxony”. In cooperation with the GV, the MPIs put together an extensive program in the Kulturpalast in the middle of Dresden's city center in addition to the festive and closing event in the rooms of the Herkuleskeule: from lectures for students (Elena Gati and Eteri Svanidze), to the Science Café (Uri Vool) to the well-attended reading „Planck oder Als das Licht seine Leichtigkeit verlor” by Steffen Schroeder in the Central Library to their own formats at the institutes. Another crowd-puller was the MPG's (accompanied) traveling exhibition „Pioneers of Knowledge” in the Kulturpalast. It attracted not only visitors who had become aware of it through advertising via various channels, but also the odd chance visitor.



“30 years of MPIs in Saxony” – Schüler Campus: Elena Gati after her lecture for pupils on the stage of the “Herkuleskeule”.



*“30 years of MPIs in Saxony” - Science Cafè: Uri Vool in discussion with interested Dresden citizens.*

Every year we welcome a lot of international scientists to enhance scientific exchange and also to carry out their own projects. In addition, we host several events mainly aimed at internal communication. The first to be mentioned are the „Curiositas Lectures”, which are organized by the PhD-representatives. Also worth mentioning are the events for National and International Women's Day, which were organized in 2022 and 2023 by dedicated female PhD students and scientists. The film „Picture a Scientist” was shown on 10.02.2023 followed by a discussion. Furthermore, on International Women's Day (08.03.2023) a very well attended event – containing lectures and discussions – took place and was also attended by many of our male colleagues.

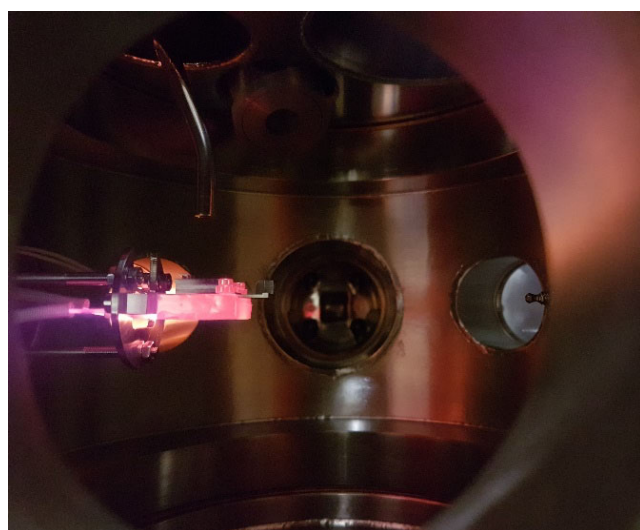
Another noteworthy initiative from the scientific community is the following: Our scientists read an article about a call for help from a grammar school in the countryside about no longer being able to offer physics lessons. Several of them – especially from the physics research groups – got together and last year invited a group of school students to visit the Institute. The supporting program consisted of visits to laboratories and experiments, some of which could be carried out by the students themselves, and was attended with great interest. We received a very positive response from the students, teachers and the school management.

Pictures sometimes say more than words and often serve as an introduction to further communication. This is another reason why the MPG has created a virtual Advent calendar in recent years. On St. Nicholas Day 2023, visitors were able to take a look inside a UHV heating station after opening the little door. The picture comes from Prof. Tjeng's group and was taken at the beamline TPS45A1.



*What's happening right now? - Interested students and their teachers from Lommatzsch experimenting during their visit to the Institute in December 2023.*

The „Graphic design students meet scientists” project, which was initiated in 2016 and resumed in 2023, is also to be understood under the same motto. In the first sub-project, TQC group leaders met with students from the „Hochschule RheinMain” under the direction of Christina Pouss, who has been designing special graphics for and with the TQC department for some time. Using the information from these discussions, the students developed proposals for the design of websites, which were presented during a visit to the institute in November. A second group of 15 students continued the project with the topic „Posters for the LNDWDD” in the first half of 2024 and presented their work at the institute in early July. The proposals developed are to be used as eye-catchers at the LNDWDD 2025.



*This was hidden behind door number 6 of the MPG 2023 virtual advent calendar.*

The public relations team supports the press officer Helge Rosner by posting press releases on the Institute's website and, if necessary, on national and international information platforms for journalists. The team also maintains the general and some group pages on the Institute's website. In spring 2021, the public relations team was also in charge of migrating the content of the old Institute intranet to the MPG-internet MAX, and is still responsible for the subsequent maintenance and administration of MAX. Further training and networking in dealing with both management content systems is therefore a matter of course.

The public relations team sees cooperation with the MPG-GV and, above all, networking with local

institutions as an important task. A representative example of this is „Dresden Concept“, under whose leadership a small image brochure with brief descriptions of all Dresden's scientific institutions is planned for fall 2024. On February 3, 2024, the „Brandmauer-Aktion“ demonstration - organized by Dresden Concept - took place in Dresden's city center. Around 4,000 academics including institute employees took part to send a signal for democracy.

Ingrid Rothe was Head of Public Relations until August 2023, assisted by Liane Schröder with technical tasks. From September 2023, she took over from I. Rothe and, like Ms. Rothe before her, is supported by two student assistants.