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 2015 – April 2018

Institute Philosophy and Strategy

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; maximising the level of control in material synthesis, for example to minimize defect levels; the identification and study of giant response functions at phase boundaries in materials at the borderline of standard metallic behavior; understanding the chemical nature of intermetallic compounds and related materials through experimental, theoretical and computational investigation of their chemical bonding; and high resolution measurement of chemical bonding related physical properties. Physicists and chemists are also encouraged to work together on 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.

The cover displays an image of the clathrate-I compound $K_7B_7Si_{39}$, recorded with the new, double-corrected atomic-resolution electron microscope JEM-ARM300F ("Dresden Grand ARM"). This transmission electron microscopy image displays atoms in black. The rosette-like features correspond to columns of polyhedral cages along the cubic [100] direction. The resolution of the microscope makes it possible not only to resolve the positions of all atoms in projection along [100], but also to distinguish between the boron and silicon atoms which statistically occupy crystallographic positions. Investigations by Transmission Electron Microscopy and Scanning Transmission Electron Microscopy with atomic resolution allow for a deeper understanding of the real structure of intermetallic compounds, e.g. site occupancy and point defects in the clathrate framework, which have a strong impact on the physical properties.

IMPRESSUM

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Executive Summary

The period May 2015 – April 2018 has been seen ongoing development of our Institute. In the following section, we summarize the most important changes, and provide some overall performance statistics.

New senior staff and independent research groups
We have recruited one new Max Planck Research Group leader (Johannes Gooth), extended the Max Planck Fellowship of Michael Ruck (TU Dresden) and appointed a new Fellow, Laurens Molenkamp (U. Würzburg). In addition, we have appointed three new group leaders (Simone Altendorf, Alexander Komarek and Chandra Shekhar) to permanent contracts.

Summary of overall publication statistics
Over the three-year period covered by this report, Institute members have published 844 papers in Web of Science (2015-2017) recognized journals. Many of our papers were published too recently for citation statistics to be a particularly useful guide, but by the end of June 2018 they had received nearly 6320 citations, with 140 papers cited 10 or more times and an *h*-index of 33. Many of our papers appeared in leading journals, e.g. 30 in Physical Review Letters, 70 in Science or Nature group journals, 14 in Applied Physics Letters, 10 in the Angewandte Chemie, 5 in Proceedings of the US National Academy of Sciences and 3 in the Journal of the American Chemical Society. Further details of these statistics and the breakdown between departments are given in Section 2.7.

Invited talks
During the census period, Institute members gave approximately 550 talks at international conferences, workshops and individual institutions. About 60% of these were given by group leaders and more junior staff.

Prizes and awards
Over the census period we are pleased to say that scientists at all levels of our activities have seen their achievements receive external recognition. PhD graduates Mark Barber, Stephen Edkins, Heike Pfau and Alexander Steppke received, between them, three Otto Hahn Medals, two Springer Thesis Awards and the Richard L. Greene Dissertation Award of the American Physical Society. APS Fellowships were awarded to Frank Steglich and group leader Steffen Wirth, the IUPAP Young Scientist in Low Temperature Physics Prize to Clifford Hicks, and the Nicolas Kurti European Science Prize to Philip Moll, while Claudia Felser was elected to the Leopoldina and the IEEE and Andy Mackenzie to the Royal Society, and Juri Grin was awarded an honorary doctorate by the Ukrainian Academy of Sciences.

Summary of institute scientific staff
We comprise four departments of approximately equal size in which, in addition to the Directors, are 33 staff scientists with permanent posts, 13 of whom are responsible for our Scientific Platform. We have approximately 60 Postdocs and 50 PhD students at any given time. The technical and administrative services are shared between the departments and provided by 88 staff members. A breakdown between the departments of the numbers for the scientific staff and Postdocs plus PhD students are given in Section 2.2.

PhD training
A major focus of our activity over the assessment period has been to structure the PhD training that we offer. Since its establishment in 2016, 22 PhD students have begun work at our International Max Planck Research School for Chemistry and Physics of Quantum Materials (IMPRS-CPQM), with 6 more recruited for an autumn 2018 start. The training framework of IMPRS-CPQM has been set as the standard for all our graduate students, whether or not they are directly funded by it. Our PhD officer, Dr. Burkhard Schmidt, monitors the effectiveness of these changes in close contact with the PhD students.

Gender balance
We actively seek leading female scientists to build the base that our field needs for the future. We now have females in leadership positions at all levels of our Scientific and Administrative staff, and over half of IMPRS-CPQM students are women. In 2017 the Gender Equality Plan and equal opportunities website were created.

Career development
One of our targets is to provide a good platform for the scientific careers of our junior staff. In the assessment period twelve of them (Ricardo Dos Reis, Di-

ego Franco, Elena Hassinger, Maurits Haverkort, Julie Karel, Pallavi Kushwaha, Zhiwei Li, Wei Liu, Philip Moll, Ajaya Nayak, Sanjay Singh and Binghai Yan) have accepted senior and junior Professorships or Lectureships at universities in Germany, China, India, Australia, Brazil, Argentina, Switzerland and Israel. Details are given in Section 2.4 and in the Addendum.

TU Dresden
The collaboration with our 'local' university is structural and long term. We have had a formal agreement with the TU Dresden since 1999. The scientific activities are presently anchored by the Max Planck Fellowship of Michael Ruck of the Institute of Inorganic Chemistry of the TU Dresden, by our participation in the DFG Collaborative Research Center and Research Training Group of the Physics Department, by several common projects funded by DFG, and by our new IMPRS. Members of our institute contribute substantially to teaching at the TU Dresden and we are also part of the 'Dresden-Concept' research alliance that helped the TU Dresden with their successful bid to the Excellence Initiative.

Civic contribution
We co-led, with support from the President, the establishment of Helpline Dresden, designed to provide English language support for scientists in difficulty. We are delighted to say that the Saxony Integration Ministry has taken over as the main sponsor of the Helpline, which is now available to all.

Building extension
In February 2018, an office extension with 50 work places and a seminar room was completed. The coordination of these activities was organized by Dr. Marcus Schmidt and the architecture office Wendt-Klemm.

Structure and Content of this Status Report

In the opening section of the Report we provide an overview of central theme of our work: our research activities and achievements. Each of the four departments (A. Mackenzie, L.H. Tjeng, C. Felser, and J. Grin), the MPRGs of E. Hassinger and P. Moll, the work of the emeritus directors F. Steglich and R. Kniep, and the Max Planck Fellowship group of M. Ruck as well as the plans of L. Molenkamp (who joined the Institute on 1 January 2018, only) are described in separate sections. Collaborative (inter-departmental/group) research is strongly encouraged in our Institute, so we highlight selected joint ventures in section 1.11.

Section 2 describes the administrative, financial 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 Science Advisory Board site visit in January 2016. We cover all the points raised in the 'Rules for Scientific Advisory Boards' document of the Max Planck Society, but have altered the order from the one given there.

We have designed our style of reporting somewhat differently to the one that we see used by other Max Planck Institutes. 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 brief 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.

The report is organized as follows:

Chemical Metals Science

Director: Yuri Grin

Group leaders: Iryna Antonyshyn, Michael Baitinger, Horst Borrmann, Ulrich Burkhardt, Peter Höhn, Miroslav Kohout, Andreas Leithe-Jasper, Reiner Ramlau, Marcus Schmidt, Ulrich Schwarz, Igor Veremchuk, Frank Wagner

Intermetallic compounds contain elements located left of the Zintl line in the Periodic Table. They are formed and exist under conditions of electron deficiency. As a consequence, on the one hand, the classical concepts of chemical bonding in inorganic materials, namely valence scales and electron counting rules, do not work for these substances because of the low number of available valence electrons. On the other hand, the development of new concepts based e.g. on quantum chemical calculations is hindered by the complexity of the crystal and electronic structure of these compounds. Balancing these considerations is at heart of the research at the Department of Chemical Metals Science.

Due to the boundary conditions above, the general strategy of research on intermetallic compounds at the Chemical Metals Science department is based on the interplay of experimental and theoretical techniques and is performed in four main directions: i) synthesis of new substances and development of the new preparation routes, ii) characterization of chemical composition, thermodynamic stability, crystal structure and microstructure of materials, iii) analysis of chemical bonding, and iv) studies on chemical and physical properties and their relationship to chemical bonding and crystal structure of new substances and materials.

Systematic analysis of the chemical bonding in intermetallic compounds reveals a special role of polyatomic and multi-center interactions. The assumption of similar energy gains for different kinds of such interactions makes understandable the existence of several compounds even with close compositions in a two- or multi-component systems. Concerning the preparation, many of these phases are not directly accessible from the melt. Thus, the development and study of new preparation ways for intermetallic compounds is an important theme of the department research in the reporting period. Heterophase redox reactions particularly offer new possibilities in the preparation of intermetallic phases. The interaction of boron trihalides with elemental transition metals using the developed crucible-free hot-wire technique (Figure 1) leads to the formation of binary borides. Contrary to the traditional techniques, the products comprise – if any – much less usual impurities containing oxygen and/or carbon[1]. In this way, single-phase hafnium diboride was obtained by a reaction of solid hafnium with gaseous boron

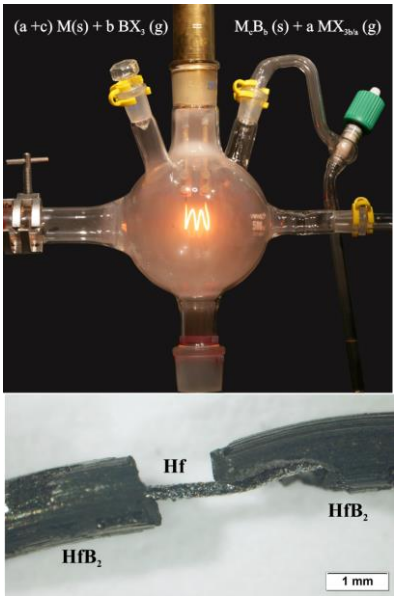

Fig. 1: Crucible-free synthesis of borides: (top) experimental setup; (bottom) reaction products with M = Hf and X = Br.

tribromide at temperatures between 800 °C and 1200 °C according to

$5\ Hf(s) + 4\ BBr_3(g) \rightarrow 2\ HfB_2(s) + 3\ HfBr_4(g)$

and contains only 0.05 mass% of oxygen despite the high affinity of hafnium to oxygen[2].

The redox preparation in ionic liquids was previously used for the synthesis of intermetallic clathrates. The oxidation of Li_2C_2 by SnI_4 in toluene at a moderately low temperature of 80 °C led to an amorphous but nano-patterned foam of elemental carbon which is structurally related to the precursor phase. Recently this technique was applied for the preparation of transition metals compounds[3]. An amorphous phase with the bulk composition Zn_2Si_5(:H,OH) was obtained by oxidation of the precursor phase Li_2ZnSi

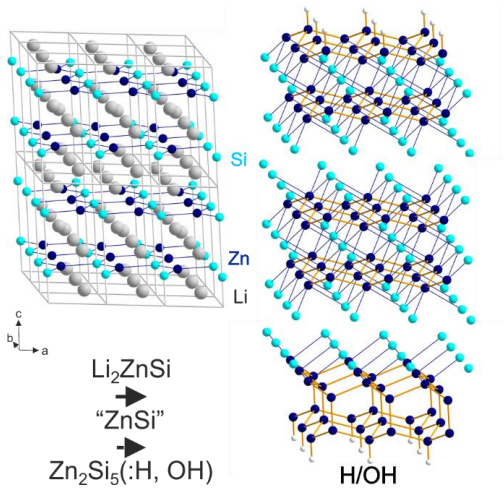

Fig. 2: Reaction scheme for the oxidative conversion of Li_2ZnSi to Zn_2Si_5(:H, OH) and structural concept for the new amorphous metastable intermetallic phase.

at the remarkably low temperature of 80 °C in the ionic liquid of n-dodecyltrimethylammonium chloride (DTAC) and $AlCl_3$. After removal of elemental Zn segregations by dilute aqueous HCl, the product was structurally amorphous according to HRTEM, which is consistent with the absence of Bragg reflections in the XRPD pattern and the features of the Raman spectrum. Zn_2Si_5(:H,OH) forms layers embedded in a matrix of a silica by-product. The amorphous phase segregates into crystalline Zn and α-Si on annealing at 150 °C. The bulk composition Zn_2Si_5 of the amorphous phase was derived from the XRPD pattern of the decomposition product by refinement of the Zn-to-Si ratio. Bulk Zn_2Si_5 is surface-terminated by Si-H and Si-OH groups (Figure 2)[4].

A particular route of redox preparation is opened by electrochemical reactions. In cooperation with the former MPG partner group at Moscow State University, electrochemical intercalation of Li-ions into tetragonal $Fe_{1+\delta}Se$ was realized. Electrochemical treatments were performed in a two electrode setup with metallic Li as the counter and (pseudo) reference electrode. The obtained product $Li_xFe_{1+\delta}Se$ (x = 0.07, δ is close to zero) is stable only in the electrical field and decomposes spontaneously after turning off the electrochemical cell. Although the amount of intercalated lithium is rather small, its incorporation results in a remarkable rise of the superconducting transition temperature up to 44 K. Quantum-mechanical calculations show that Li occupies the octahedrally coordinated position, while the $[Fe_2Se_2]$ layers remain basically unmodified[5].

An important state parameter for chemical preparation is pressure. Continuing our development of high-pressure high-temperature preparation protocols, synthesis of new intermetallic compounds from different families was performed[6]. Synthesis in systems with components which differ only slightly in electronegativity, and where no phase formation is observed at ambient pressure, turned out to be particularly interesting. In addition to the previously reported $CoBi_3$, recently the preparation of *hp*-CuBi has succeeded by direct reaction between copper and

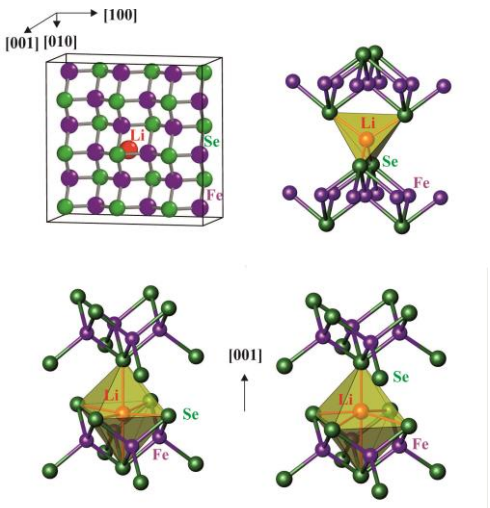

Fig. 3: The optimized tetragonal model structure of Li_xFeSe (x = 1/18, top left) is essentially preserved by relaxation. Li fills tetrahedral (top right) and octahedral voids (ideal – bottom left, optimized -bottom right) [5].

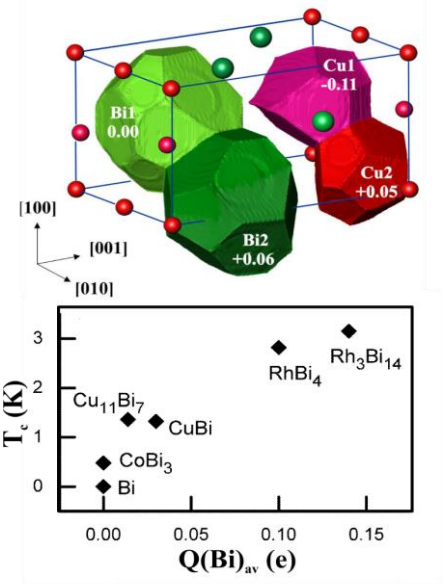

Fig. 4: Low QTAIM atomic charges in hp-CuBi (top) and critical superconducting temperature T_c for the bismuth-containing substances vs. the average charge transfer $Q(Bi)_{av}$ per Bi atom.

bismuth at a pressure of 5 GPa and a temperature of 720 K. The crystal structure contains slabs of puckered Cu layers sandwiched between Bi planes. The analysis of the chemical bonding with position-space techniques reveals a very low charge transfer between Bi and Cu (0.1 *e* and below). The Bi-Cu-Bi slabs are characterized by four-center Bi-Cu-Cu-Cu bonds. These entities are interconnected in bulk by van-der-Waals interactions of the bismuth lone-pairs (Figure 4). *hp*-CuBi represents the hitherto missed example of spatial lone-pair separation of two-dimensional structural entities among the intermetallic compounds of bismuth. The critical superconducting temperatures of the stable compounds comprising the heavier 4d metal rhodium are significantly higher than those of the (metastable) high-pressure compounds with the lighter 3d metals copper and cobalt. On the other hand – even if the number of the superconducting compounds investigated is not very large - the substances with lower average charge transfer (per atom) reveal noticeably lower critical transition temperatures (Figure 4). The non-polar character of atomic interactions in *hp*-CuBi is in empirical accordance with the appearance of superconductivity at low temperature[7].

Systematic application of the recently developed and optimized traditional techniques makes accessible preparation of new families of intermetallic compounds, in particular with elements, which – for different reasons – do not allow straightforward synthesis.

A series of new compounds was manufactured in binary and ternary systems of beryllium[8]. Beside the interesting physical behavior of BeAu and $CeBe_xPd_3$, remarkable bonding features are revealed in $Be_{21}Pt_5$ – a rare γ-brass-type phase formed by main-group elements. Its crystal structure with 416 atoms per unit cell is - from the crystallographic point of view – characteristic of a special family of intermetallic compounds called complex metallic alloys (CMA). Because of the large difference in the scattering power of the components and the mimicked wrong symmetry, the crystal structure had to be solved by a combination of synchrotron and neutron powder diffraction data. The structural pattern of $Be_{21}Pt_5$ is described as a 2×2×2 superstructure of the γ-brass structure or 6×6×6 superstructure to the simple bcc structure with a distinct distribution of defects. The main building blocks of the crystal structure are four types of polyhedral nested units (clusters) with compositions $Be_{22}Pt_4$ and $Be_{20}Pt_6$. Analysis of chemical bonding applying the electron localizability approach revealed strongly polar polyatomic and multi-center bonding, in accordance with the low valence electron count per atom in $Be_{21}Pt_5$. A new type of atomic interaction in intermetallic compounds – cluster bonds involving 8 or even 14 atoms – is found in this compound (Figure 5). Polyatomic interactions within the polyhedral nested units and three-center polar inter-cluster bonds result in a three-dimensional framework resembling the structural arrangement of NaCl[9].

Crystallographic complexity of intermetallic compounds is – at least partially – caused by (sometimes tiny) bonding fluctuations between different parts of the structure. While in $Be_{21}Pt_5$ it originates from tiny bonding and compositional differences between the zero-dimensional entities (polyhedral nested units, clusters), the complexity of the crystal structures of new Mn-containing ternary nitridometallates[10] can be understood as originating from the intergrowth of one-dimensional structural units with special bonding features in the plane perpendicular to the common trigonal axis (Figure 6). The compounds $Ca_{12}[Mn_{19}N_{23}]$ and $Ca_{133}[Mn_{216}N_{260}]$ were obtained by a (gas-solid) reaction of Ca_3N_2 and Mn with nitrogen. Both structures are characterized by

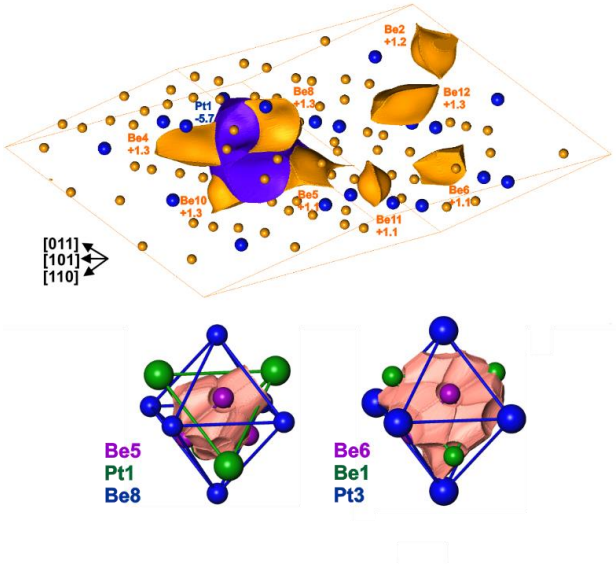

Fig. 5: Chemical bonding in $Be_{21}Pt_5$: (top) high QTAIM atomic charges reveal strong polarity of Be-Pt interactions; (bottom) the ELI-D basins of the 8c (eight-atomic, left) and 14c (14-atomic, right) interactions in the polyhedral nested units reflect the electron-deficient situation in the compound [9].

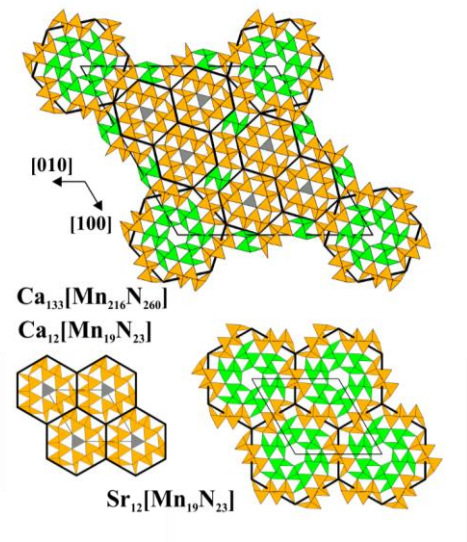

Fig. 6: Structural complexity in ternary nitrido-manganates by two-dimensional intergrowth of one-dimensional structural units with different bonding features (grey triangles bare Mn atoms forming only Mn-N bonds, all other Mn atoms participate in the Mn-Mn interactions).

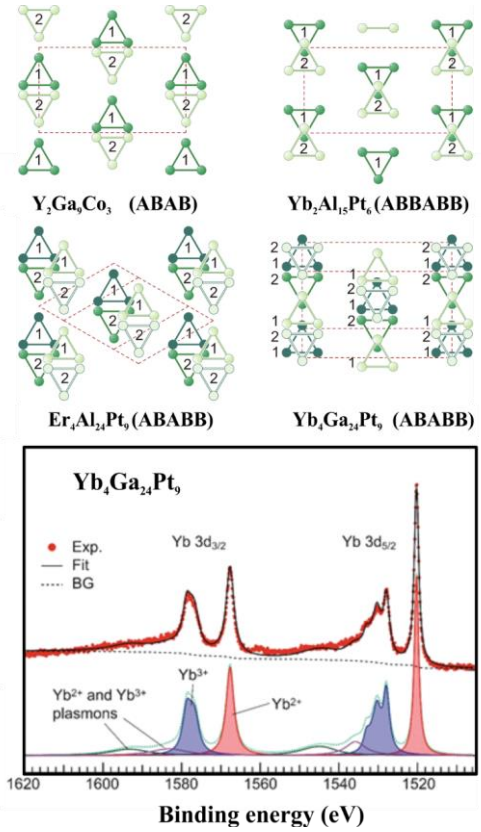

Fig. 7: (top) Stacking sequences of the slabs R_4E_6 (A) and $E_{12}T_6$ (B) in the crystal structures of the $Y_2Ga_9Co_3$ family (R - rare-earth metal, E – triel element, T – transition metal). (bottom) Valence band spectrum of $Yb_4Ga_{24}Pt_9$ evidencing the intermediate valence state of Yb.

2D nitridomanganate layers containing building blocks of different structural complexity caused by different bonding of manganese atoms. For both compounds, magnetic susceptibility, electron spin resonance measurements and analysis of chemical bonding revealed that only a fraction of the Mn atoms in both structures carries a localized magnetic moment, while for most Mn species the magnetism is suppressed by formation of multicenter metal-metal bonds[11].

A further level of complexity is achieved by one-dimensional intergrowth of two-dimensional structural units with different bonding and composition[12]. The crystal structure of the ternary compound $Yb_4Ga_{24}Pt_9$ is formed by stacking pseudo-trigonal slabs of the compositions Yb_4Ga_6 (A, mostly ionic bonding) and $Ga_{12}Pt_6$ (B, polar covalent interactions). Due to the relatively weak inter-slab interactions, the basic stacking sequence ABABB is often broken. Stacking faults in the structure of $Yb_4Ga_{24}Pt_9$ are caused by the existence of three equivalent possibilities for the stacking of neighboring slabs A. The structure of $Yb_4Ga_{24}Pt_9$ belongs to the large series of intermetallic compounds derived from orthorhombic $Y_2Ga_9Co_3$. The variety of crystal structures and symmetries (from

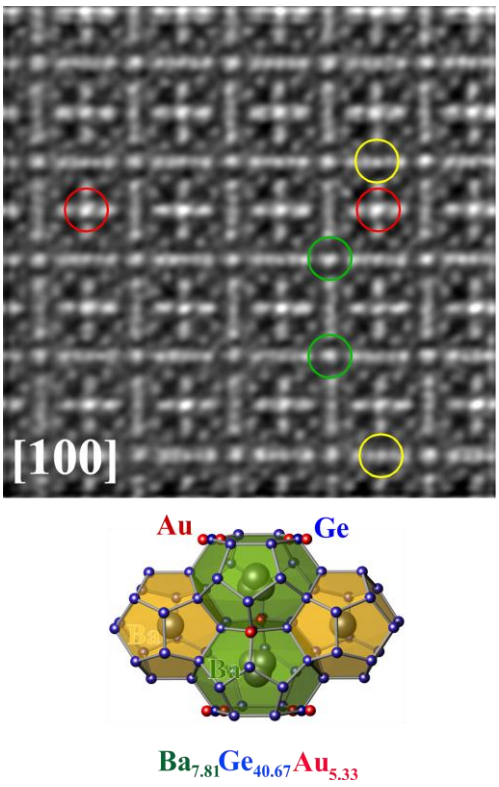

Fig. 8: Real structure of the single crystal of the clathrate $Ba_{7.81}Ge_{40.67}Au_{5.33}$: (bottom) Crystallographic disorder in the framework and its cavities from single-crystal X-ray diffraction data. (top) STEM image of the same crystal along the [100] direction reveals breaking of translational symmetry.

triclinic to hexagonal) represented in this series is caused by the different sequences of the building slabs A and B and by different relative arrangements of the slabs A. Magnetic susceptibility measurements and hard X-ray photoelectron spectra reveal an intermediate valence of ~2.5 for the ytterbium species, in agreement with the results of the low-temperature powder X-ray diffraction[13].

The highest level of structural complexity was recently found in intermetallic clathrates which were systematically studied with respect to their promising thermoelectric properties. Due to the detailed investigation of phase equilibria in the ternary system Ba-Ge-Au, the optimal conditions were found for the crystal growth of the clathrate-I phase[14] resulting in the manufacturing of cm-sized single crystals. These crystals revealed very low mosaicity and were suitable for high-resolution inelastic neutron scattering measurements (Figure 8). In cooperation with partners within the European Integrated Centre for the Development of New Metallic Alloys and Compounds, we succeeded in performing a combined experimental and theoretical study of the phonon lifetime, the determination of which is still at the limits of instrumental capabilities. The first direct and quantitative measurement of phonon lifetimes in a single crystal of the clathrate-I phase $Ba_{7.81}Ge_{40.67}Au_{5.33}$ revealed thermal transport being dominated by acoustic phonons with long lifetimes, travelling over distances from ten to a hundred nanometers[15]. HRTEM[16] and single-crystal X-ray diffraction[17] investigations show that this is connected with the non-periodic breaking of translational symmetry due to the formation of Ba-Au bonds[16].

The systematic use of the characterization techniques established in the department bodes well for in-depth studies on the different families of intermetallic compounds. Beside further progress in the use of HRTEM[16] and X-ray diffraction[17], dedicated developments were made in metallographic analysis, particularly in special applications of electron backscatter diffraction (EBSD)[18]. The EBSD characterization is becoming an important powerful tool for studies on non-centrosymmetric compounds. The absence of an inversion center in the crystal structure is considered as mandatory for models of unconventional magnetic and electronic states like skyrmions or surface conductivity in topological insulators. It is also a precondition for enantioselective catalytic behavior. A combined EBSD and single-crystal X-ray diffraction study on CoSi crystals (structure of the B20 (FeSi) type) shows that the EBSD complete pattern matching approach allows distinguishing enantiomorphic crystal structures already in the microstructure without performing the complete high-resolution single-crystal X-ray diffraction structure determination (Figure 9). This method allows the absolute structure for non-centrosymmetric crystals to be correctly assigned, with excellent lateral resolution[18].

All characterization techniques – in combination with state-of-art preparation - play a key role in the systematic studies on the relationship between chemical composition, crystal structure and bonding and enabled the discovery of new heavy-fermion and thermoelectric materials in the reported period.

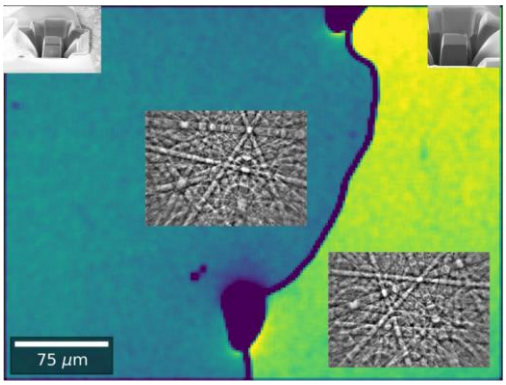

Fig: 9. EBSD pattern of single-crystalline grains of CoSi reveals the different orientation of the crystals on the left and right side of the grain boundary. Different colors reflect different values of mean correlation coefficient for the Kikuchi pattern.

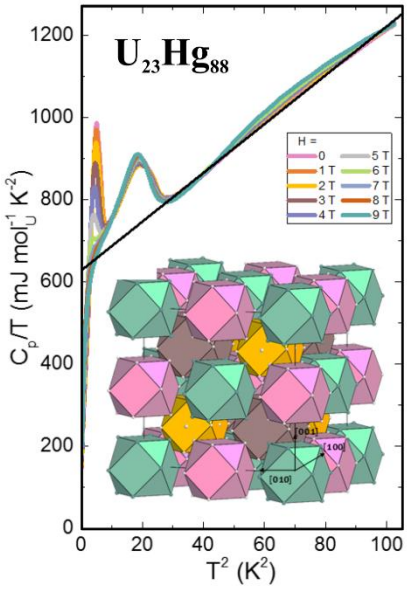

Fig. 10: Crystal structure (bottom) and specific heat of the heavy fermion $U_{23}Hg_{88}$ as Cp/T vs T^2 at different magnetic fields allowing estimation of the Sommerfeld coefficient of 630 mJ mol_U^{-1} K^{-2}.

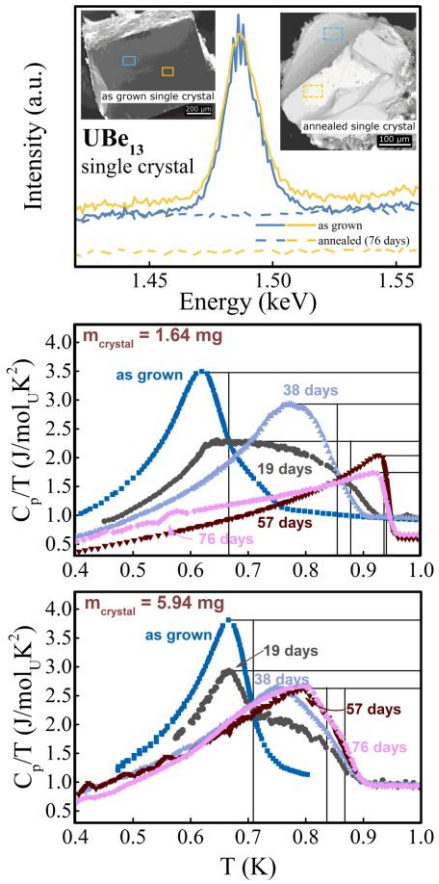

Fig. 11: (top) Aluminium incorporated into the crystal structure of UBe_{13} after crystal growth from Al melt leaves the material during the heat treatment. The superconducting temperature scales with the dimension of the crystal and increases with time of annealing.

The compounds of uranium are a fruitful field for discovering new heavy fermion systems. Dedicated preparation in the laboratory of high safety standards enabled synthesis of several compounds of uranium with the elements of the zinc group. Especially interesting behavior was found for the heavy-fermion antiferromagnet $U_{23}Hg_{88}$ (formerly reported as $U_{11}Hg_{45}$)[19]. The high value of the Sommerfeld coefficient suggests that this compound is one of the heaviest heavy-fermion materials among the U-containing substances. The compound displays features of both local and itinerant 5*f* magnetic moments, and is a candidate for the appearance of unconventional superconductivity (Figure 10).

Careful characterization of synthesis products was the key for explaining the superconducting behavior of single crystals of another uranium heavy fermion – UBe_{13}[19], which is famous for its unconventional superconductivity which is thought to condense from an incoherent metallic state. The manufacturing of single crystals of this compound is practically possible

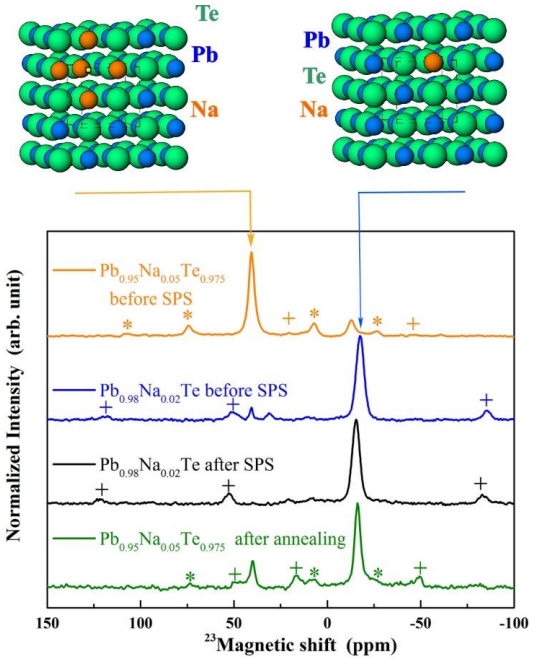

Fig. 12: Sodium substitution in thermoelectric PbTe: (top) local atomic configurations in the vicinity of Na atoms in the NaCl-type crystal structure; (bottom) MAS ^{23}Na NMR spectra for the substitution products.

only from aluminum melt. The role of aluminum in this process was not clear. The incorporation of Al into the crystal structure of as-cast polycrystalline samples $UBe_{13-x}Al_x$ is shown to be of the order 1-2 at% by means of X-ray single-crystal structure determination, HRTEM and ^{27}Al NMR[20] (cooperation with the Max-Planck Research Group 'Physics of Unconventional Metals and Superconductors'). Aluminum replaces Be atoms at the vertices of the Be_{12} icosahedrons, a basic structural unit of UBe_{13}. The aluminum solubility is strongly dependent on the temperature, it can diffuse and leave the structure upon annealing. Annealing strongly influences the low-temperature behavior of $UBe_{13-x}Al_x$ single crystals (Figure 11). The annealing time - required to reach the highest T_c - scales with the crystal dimensions, and confirms that Al diffuses and leaves the crystal rather than ordering locally on a specific site. However, prolonged annealing may lead to a degradation of the structure due to the relatively high Be vapor pressure[21].

Careful microstructural characterisation is also important for understanding and optimising thermoelectric materials[22]. For example, the sodium substitution in PbTe depends on material balance: the substitution according to the electronically non-balanced scheme $Pb_{1-x}Na_xTe$ is markedly smaller in comparison with the electron balanced replacement $Pb_{1-x}Na_xTe_{1-x/2}$ (Figure 12). A homogenous distribution of sodium is achieved by thermal treatment. The local

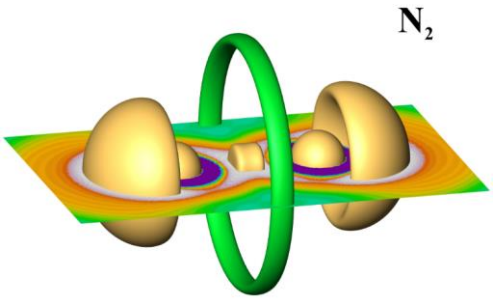

Fig. 13: PUC distribution for the N_2 molecule reflects the core and lone-pair regions for both atoms, as well as two bond regions between the nuclei.

atomic configurations with and without Te vacancies were proven by ^{23}Na NMR[20]. Thermoelectric properties change monotonically within the homogeneity range of the solid solution and change non-systematically in the multi-phase samples. Similar behavior is observed also in Eu-substituted PbTe [23].

Advanced preparation techniques in combination with the in-depth characterization of synthesized materials form the basis for the inter-departmental projects like studies on $FeGa_3$ and its substitution variants (with PQM department)[24] or on iron telluride (with PCM department)[25].

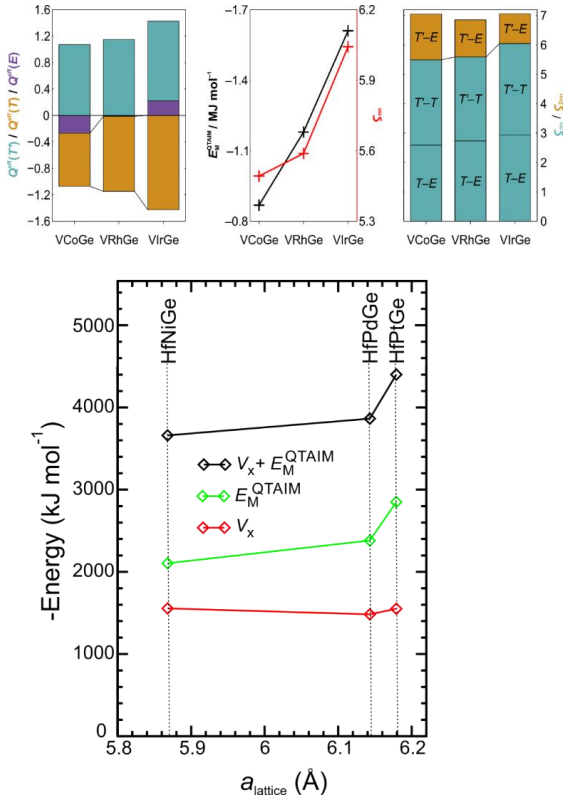

Fig. 14: QTAIM charges (top left), QTAIM Madelung energy E_M^{QTAIM} (ionicity) and nearest neighbor sharing ζ_{nn} (covalency, top middle), the second nearest neighbor sharing ζ_{2nn} (top right) and the contributions to the total energy for the VTGe (top) and HtTGe (bottom) compounds.

As it was shown above, analysis of chemical bonding is a key part of the research on intermetallic compounds. Several developmental studies were performed on new tools for bonding visualization and analysis[26]. The electron density represents the most basic property on which the investigation of chemical bonding in position space is based. The next step of complexity represents the pair density, and a today's understanding of chemical bonding in position space is achieved only with a combination of these two. With this in mind, identification of new powerful bonding indicators relying only on the electron density is an important field of development. The newly proposed indicator PUC (position uncertainty curvature) is connected with the uncertainty in the prediction of the position of an electron and represents an effort along this direction[27]. Its spatial distribution resolves the shell structure for most atoms up to Xe and yields reasonable shell populations. The PUC distribution for the N_2 molecule reflects the triple-bond character of the interaction (Figure 13).

The previously proposed bond delocalization ratio is based on three-center delocalization indices derived from the pair density[28]. It has developed into an important tool to quantitatively investigate complex bonding situations between two-center localized bonding A-B and perfect three-center wise delocalization toward formation of an A-B-C three-center bond. The tool has been recently employed to uncover the nature of B-B bonding in a B_{20} cage molecule in $SnNi_{21}B_{20}$. It turned out to be described as

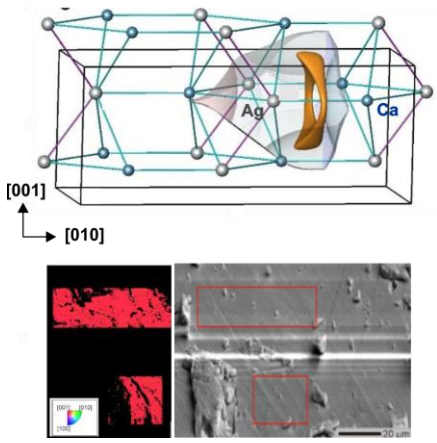

Fig. 15: Crystal structure and bonding in CaAg: (top) Ca-Ag bonding attractors are located within the QTAIM atomic basin indicating the formation of lone pairs layers perpendicular to [010]; (bottom) EBSD analysis of the cleaved (010) surface of CaAg particles.

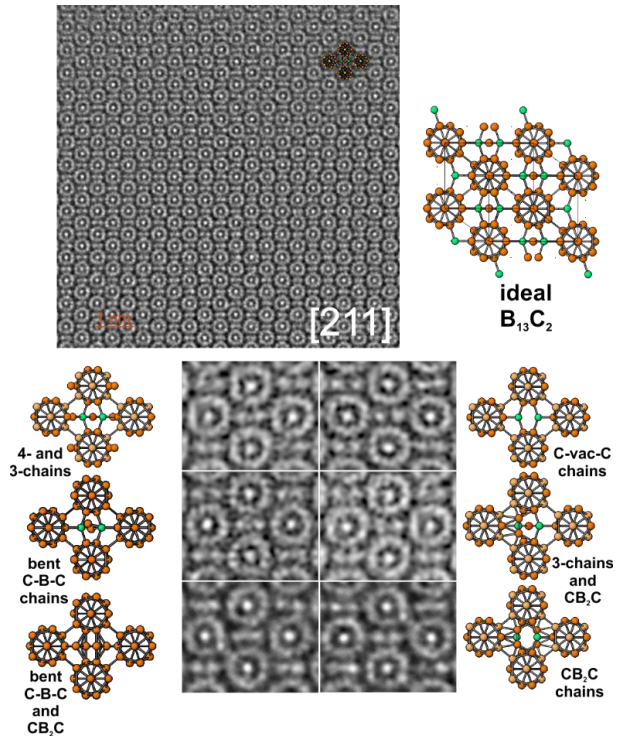

Fig. 16: High-resolution transmission electron microscopy of boron carbide: (top) TEM image and the view of the ideal crystal structure $B_{13}C_2$ along the [211] direction; (bottom) local atomic arrangements in the chain region.

a nesting of four B-B-Ni three-center bonds at the common B-B edge [29]. This bonding motif can be found in many intermetallic borides with boron chains in trigonal prismatic transition metal coordination, e.g. in CrB- and AlB_2-type of borides.

Further progress in the bonding analysis in intermetallic compounds was achieved by real-space definition of ionicity and covalency of bonds and contributions of these types of interactions to the total energy[29]. Applying this methodology, six compounds among the 18 analyzed *TT'*Ge compounds (*T* -transition metal) in a composition range dominated by the TiNiSi-type crystal structure, were selected as most likely exhibiting the MgAgAs-type (Figure 14). Two of them - TaIrGe and *lt*-TiPtGe - were already mentioned in the literature; another two - *lt*-HfPtGe and VIrGe - were reported for the first time[30].

The recently implemented theoretical tools were applied in combination with characterization techniques for the study on chemical properties of intermetallic compounds[31,32]. As a new research direction, the chemical stability of Ca-Ag compounds under ethylene epoxidation conditions was investigated. For the compound CaAg, analysis of the chemical bonding reveals strongly polar Ca-Ag interactions which can be understood as the formation of lone-pairs on silver atoms (Figure 15). The layered arrangement of silver anions yields the cleavage planes in the structure perpendicular to the [010] direction. Powdering therefore results in plate-like particles with surfaces determined by energy minimization. Further modelling reveals the formation of a stable oxygen-containing layer and thus the stabilization of the surface. Indeed, the particles are stable under epoxidation conditions for hundreds of hours.

Concerted application of ab-initio computational studies, precise crystal structure determination from diffraction experiments and state-of-art high-resolution transmission electron microscopy shed light on the real structure of boron carbide, the simple chemical combination of boron and carbon, one of the best-known binary ceramic materials[33]. This investigation reveals hitherto unknown local structure modifications together with the known structural alterations. Structural modifications reduce the electron deficiency of the pristine structure $CBC+B_{12}$ introducing new electronic states within the band gap which allow a better understanding of the physical properties of the material[34].

The understanding of the chemical nature of the intermetallic compounds was the main driving force and the main goal of the research at the department Chemical Metals Science. Experience of the recent years reveal the multi-layer complexity of these substances. Their compositions and crystal structures show often tiny deviations from the (previously known) ideal variants. Exactly these deviations may define the chemical and physical behaviors and allow to find new ways toward the understanding. Obtaining of the coherent picture of this family of inorganic compounds seems to be possible only by in-depth development of experimental and theoretical techniques for preparation, characterization and bonding analysis. This will be in focus of the work of the department in the future.

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Physics of Correlated Matter

Director: L.H. Tjeng

Group leaders: Simone Altendorf, Chun-Fu Chang, Zhiwei Hu, Alexander Komarek, Andrea Severing, Oliver Stockert and Steffen Wirth

The spectacular physical properties often observed in transition metal and rare-earth compounds challenge our understanding of solid state physics. These properties include superconductivity, unusually large magneto-resistance, metal-insulator transitions, heavy-fermion behavior, multiferroicity, and phenomena involving topologically protected states. We would like to understand how the electrons in such materials interact with each other to generate those unusual quantum phenomena.

The activities of our department are carried out by eight group leaders with specific and complementary expertise. They lead their own groups and follow their own scientific interests both independently and as part of an overall team that carries out projects in a collaborative manner on various aspects of correlated materials. Highlights of their research activities will be described below.

In terms of personnel and career development, we would like to mention that Maurits Haverkort (group leader) has left us in Oct. 2016 to accept a full professorship position (W3) at the Institute for Theoretical Physics of the Heidelberg University, and that Zhiwei Li and Wei Liu (senior postdocs) have accepted associate professorship positions at the University of Lanzhou and the Wuhan University of Technology, respectively.

1.2.1. Objectives and Strategy

The research activities of our department are focused on the investigation of the electronic structure of the materials, using both spectroscopic tools as well as material specific many body calculations. This combination of experimental and theoretical work is a fruitful strategy to identify the most suitable working models. The experimental activities also have a strong material development component: new materials, both in bulk as well as in thin film form, are synthesized in order to tune the relative strength of the relevant interactions. With exact solutions to the many-body problem out of reach, the objective of our Department for Physics of Correlated Matter is to find smart approximations by which we can capture the essentials. It is likely that we need to develop and use different theoretical starting points for different materials. Guided by the various approximations developed, we also aim to optimize the properties for applications and we hope to even discover new phenomena.

1.2.2. Selected research highlights

Members of our Department for Physics of Correlated Matter have coauthored 201 publications in the May 2015 – Apr 2018 census period (161 publications in the previous three year census period). In the following we will present highlights that are representative of our research program.

Role of spin and orbital degrees of freedom in phase transitions of correlated materials (Hu, Chang, Severing, Tjeng):

The fascinating properties and the complexity of the phase diagrams of strongly correlated systems can be traced back to the richness offered by the multiplet structure of the relevant atoms and how this is affected by the crystal. We will elucidate the importance of these aspects for the case of the metal-insulator transition (MIT) in Ti_2O_3 [1] and for the hidden order in URu_2Si_2 [2].

Ti_2O_3 has a corundum crystal structure and exhibits, upon lowering the temperature, a gradual MIT with neither a structural transition nor magnetic ordering. According to standard band theory, the low temperature phase is metallic with the Ti $3d^1$ ions having a mixed a_{1g} and e_g^{π} orbital occupation.

Our photoemission study (see Fig. 1) shows a clear insulating state for the low temperature phase. Moreover, it exhibits a Ti *3d* double peak structure that can only be explained using a double Ti-site cluster. This establishes that the Ti dimer configuration is not only structurally but, above all, also electronically present. Using x-ray absorption spectroscopy (XAS), we demonstrated that the orbital occupation is of the pure a_{1g}-a_{1g} molecular singlet type. By going to higher temperatures, we revealed that the occupation changes

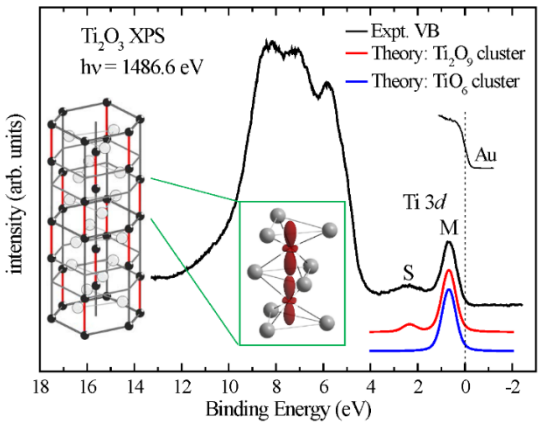

Fig. 1: Valence band photoemission spectrum of Ti_2O_3 in the low temperature phase.

and that the e_g^{π} orbital also becomes occupied. The insulator metal transition may thus be viewed as a transition from a solid of isolated Ti-Ti molecules into a solid of electronically partially broken dimers, where the Ti ions acquire additional hopping in the *a-b* plane via the e_g^{π} channel. This break-up, however, requires the consideration of the multiplet structure of the effective on-site Coulomb interaction: U_{eff} is much smaller for a triplet $a_{1g}e_g^{\pi}$ configuration than for the ground state dimer singlet $a_{1g}a_{1g}$. In other words, in the high temperature phase the increased band width (due to e_g^{π} channel) can become larger than the reduced U_{eff} and stabilize the metallic state. We were also able to argue that the differences in the total energies of the low and high temperature configurations are small so that they can be overcome by entropy, allowing the transition to take place.

The *hidden order* (HO) phase transition at 17.5 K in the heavy fermion superconductor URu_2Si_2 is a long standing puzzle despite tremendous theoretical and experimental efforts. By now it is generally accepted that the symmetries of the 5*f* electrons involved are key for understanding the HO phase. Their determination is therefore a necessity.

We have carried out a non-resonant inelastic x-ray scattering experiment (NIXS) with hard x-rays (≈10keV) at the U $O_{4,5}$ edge of URu_2Si_2. The first experimental result is shown in Fig. 2, together with an atomic multiplet simulation for the U ion in the $5f^2$ configuration. The agreement between experiment and theory is remarkable for several reasons. First, it is for the first time that one can observe atomic multiplet structures in a core level experiment for an itinerant metallic U compound. Usually, in XAS experiments the core level spectra are are broad and featureless. This is contrasted by our NIXS data that probe final

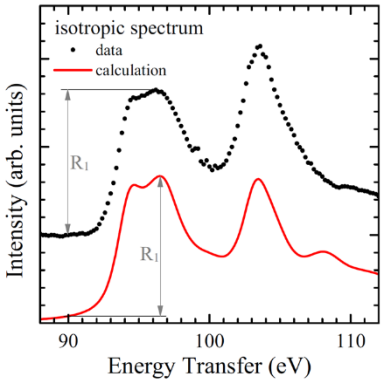

Fig. 2: Uranium $O_{4,5}$ NIXS spectrum of URu_2Si_2.

states with higher quantum numbers that are lower in energy, i.e. less mixed with the continuum states and therefore more excitonic. This can be achieved by working with high momemtum transfers (≈10Å^{-1}) so that higher than dipole transitios are operative. The second remarkable aspect of seeing multiplet structures is that the electronic properties of this itinerant system have apparently a strong local atomic character. This thus gives credit to theoretical approaches that use local atomic wavefunctions in their *Ansatz.*

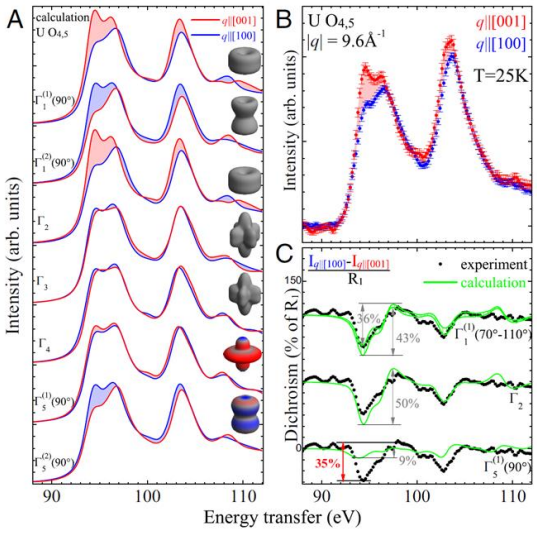

Fig. 3: Directional dependence of the U $O_{4,5}$ NIXS spectrum of URu_2Si_2 together with simulations.

We then measured the directional dependence of the NIXS spectra and compared them with simulations for the various wavefunctions scenarios proposed in the literature, see Fig. 3. This allowed us to show that the predictions of an LDA + DMFT calculation are close to our data. Futhermore, our findings thus exclude many HO scenarios proposed in literature.

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Strongly correlated topological insulators (Wirth, Severing, Tjeng):

SmB_6 has become of enormous topical interest because it is considered a candidate to be the first strongly correlated material with non-trivial topology. If true, this also will solve a long standing mystery concerning its residual conductivity at low temperatures, which would be caused by the topologically protected surface states. Here we report our results on the symmetry of the Sm *4f* ground state wavefunction using NIXS [3] and our finding of an additional low energy scale at low temperatures using scanning tunneling spectroscopy (STM) [4].

Knowing the symmetry of the 4*f* ground state wave function that is involved in the hybridization with the conduction *d* bands is of great importance, especially since the topological properties of the surface are fully determined by the bulk. In SmB_6 the ground state is a mixture of Sm^{2+} and Sm^{3+}. However, the Sm^{2+} is not crystal-field split and hence, the problem reduces to determining the symmetry of the crystal-field wave function of Sm^{3+}. Due to the cubic crystal structure the question is whether the ground state is the Γ_8 quartet or the Γ_7 doublet. Conventional methods like neutron scattering were unsuccessful, probably due to the high absorption of Sm and B in combination with broadened magnetic excitations in the energy range of phonons.

We carried out NIXS experiments at the Sm N-edge, i.e. we probe the 4*f* states directly via the core hole 4*d*→4*f* excitation. The direction dependence of the scattering function $S(\vec{q},\omega)$ gives insight into the ground state symmetry: asymmetries can be detected even in a cubic environment since we are making use of high momentum transfers, thereby allowing for higher multipole contributions in the scattering.

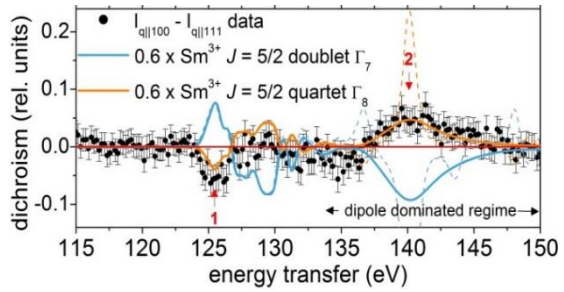

Fig. 4: Dichroism in the Sm $N_{4,5}$ NIXS spectrum of SmB_6 and simulations for the Γ_8 and Γ_7 scenarios.

Fig. 4 shows the main result of the NIXS experiment: the experimental dichroic spectrum (black dots) and simulated dichroic spectra for the Γ_8 quartet (orange) and Γ_7 doublet (light blue) scaled by a factor of 0.6 to account for the Sm^{3+} component of the ground state; dashed lines with energy independent broadening, solid lines with extra broadening in the dipole region. We can directly conclude from the good quantitative agreement that the ground state is the Γ_8 quartet. In fact, the opposite dichroism at 125 eV and 140 eV (see red arrows) reduces the experimental challenge to a simple yes-no exercise. The finding that the ground state is the Γ_8 and not the Γ_7, contradicts all existing band structure calculations and illustrates in a sobering manner the difficulties in making reliable predictions for the properties of correlated systems. Our findings point out that future calculations of the low-energy properties of SmB_6 should be performed within a reduced basis of only Γ_8 states. This is of direct importance for the prediction of the spin texture of the topological surface states. Moreover, it is remarkable that the Γ_8 polarization of the Sm^{3+} component is so complete despite the fact that the system is itinerant, indicating that the 4*f* band width must be much smaller than that indicated by band theory. We ascribe this to fractional parentage aspects involved for the charge hopping (*s=1/2*) between the Sm^{2+} (*J=0*) and Sm^{3+} (*J=5/2*) configurations.

In our scanning tunneling microscopy (STM) experiments we found differently terminated surfaces with correspondingly different dI/dV-spectra. Nevertheless, all spectra pointed to the existence of a hybridization gap at the Fermi energy, and, most importantly, displayed a finite zero-bias conductance of considerable magnitude which confirms the robustness of the metallic states and is in line with the proposal of SmB_6 being a topological insulator. Interestingly, the tunneling spectra become much more detailed for T < 5 K, suggesting not only a bulk contribution but also a contribution from a metallic surface state. Fig. 5 shows the temperature evolution.

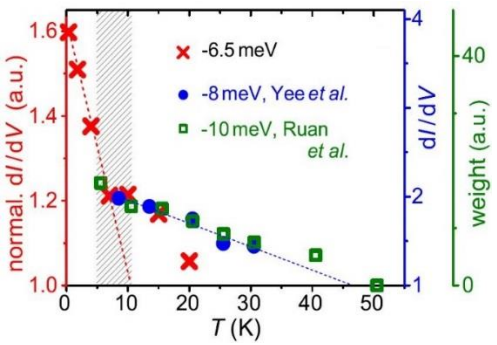

Fig. 5: Temperature dependence of the low energy peaks in the scanning tunneling spectra of SmB_6.

We can clearly observe the existence of an additional energy scale at low temperatures. Recently, a surface Kondo breakdown scenario was proposed based on the reduced screening of the local 4*f* moments at the surface. In consequence, the Kondo temperature of the outmost layer, T_K^S, can be strongly suppressed, resulting in a modified band structure. Based on our experiments, we infer that T_K^S is around 7 K, an order of magnitude smaller than the bulk T_K of about 50 K. The presence of such a low energy feature will then lead to heavy quasi-particle surface states.

http://www.cpfs.mpg.de/pcm/correlated-TI

High-oxidation state materials (Komarek, Tjeng):

In transition metal (TM) oxides the charge transfer energy for transferring electrons from the oxygen *2p* states to the TM *3d* states can be negative when the oxidation state of the TM ion is high. Hence, within these materials the charge carriers could be made of O *2p* holes. The superconducting cuprates and cobaltates may be considered to belong to this class of materials, as well as ferromagnetic metals like CrO_2. In this project we were interested in synthesizing high oxidation state materials, especially in single crystalline form, in order to study their physical properties – with a focus on nickelates [5].

The rare earth nickelates $RNiO_3$ (R = rare earth, Y) with a Ni^{3+} oxidation state, have continued to attract enormous interest over the last decades due to their famous bandwidth-controlled metal-insulator transition and associated unusual charge and spin-ordering phenomena, together with the prediction of multiferroicity and even superconductivity in thin film hetero-structures. The description of the underlying physics of these phenomena turned out to be a true intellectual challenge, and theoretical concepts have been, and still need to be, developed. Regarding the $RNiO_3$ phase diagram the question of why $LaNiO_3$ seems to be the only nickelate that stays metallic and paramagnetic down to lowest temperatures also arises. Across the $RNiO_3$ series, the octahedral tilts become smaller with increasing R-ionic radius, thus the Ni-O-Ni bond angles become smaller and the magnetic exchange interactions larger. With La having the largest ionic radius of the series the strongest antiferromagnetic properties could be expected for $LaNiO_3$. Instead, $LaNiO_3$ seems to stay paramagnetic, thus violating the trend.

The vast majority of studies reported are based on powder samples. So far, no growth of sizeable impurity-free single crystals has been reported for these intensively studied materials. Using a high pressure mirror furnace, we were able to grow large, cm^3 single crystals of $LaNiO_3$. Electrical resistivity and Hall effect measurements reveal that $LaNiO_3$ is intrinsically not a bad metal as recently discussed for the $RNiO_3$ (R = Pr-Lu, Y) compounds in their paramagnetic phase. Instead, we found that $LaNiO_3$ has a high conductivity – higher than reported for the $LaNiO_3$ samples in literature so far. Furthermore, in our neutron scattering experiments we observed clear antiferromagnetic correlations (see the left panels in Fig. 6), and their corresponding signatures in magnetization and specific heat measurements, all indicating a magnetic ordering temperature of 157 K.

Thus, $LaNiO_3$ appears to be a highly metallic and antiferromagnetic transition metal oxide - a rather rare combination of properties in oxides. It is also very close to an insulating state, making $LaNiO_3$ an intriguing material as there is a competition of local electronic correlations and Fermi surface effects. We now can draw a new phase diagram for the $RNiO_3$ system (see the right panel in Fig. 6).

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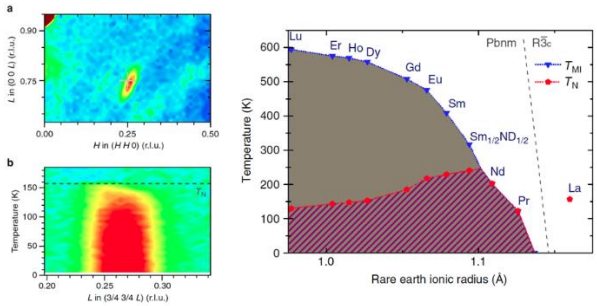

Fig. 6: Neutron diffraction data on $LaNiO_3$ single crystals revealing (a) quarter-integer peaks which (b) appear below T_N = 157 K, together with (c) the now modified phase diagram of $RNiO_3$.

Phase transitions in thin films: influence of strain, domain size, and surface termination (Altendorf, Chang, Hu, Tjeng):

The properties of many materials are governed by the interplay of complex correlations. Thin films and heterostructures offer a broad platform to tune these correlations, e.g. by strain, domain size, screening, and doping. This can provide important insights into the fundamental mechanisms that determine the properties of a material, and enables us to manipulate the characteristics of a material, for instance by inducing or suppressing phase transitions. Here we report on our

studies on the control of the properties of Fe_3O_4 thin films by substrate matching [6], on the growth of thin films with polar surfaces and interfaces without electronic reconstruction [7], and on the design of single domain multiferroic thin films [8].

Fe_3O_4 (magnetite) is one of the most studied quantum materials. Numerous studies have been devoted to understand its enigmatic Verwey transition. The theoretically expected half-metallic behavior also generates high expectations that magnetite thin films can be used in spintronic devices such as spin valves and magnetic tunnel junctions. However, up to now, in the twenty years of intensive research, the Verwey transition in Fe_3O_4 thin films is extremely broad and occurs at substantially lower temperatures than those in bulk single crystals. It is not at all clear why.

We have succeeded in growing magnetite thin films which not only have the Verwey transition as sharp as in the bulk, but also show transition temperatures that are substantially higher than the bulk, see Fig. 7.

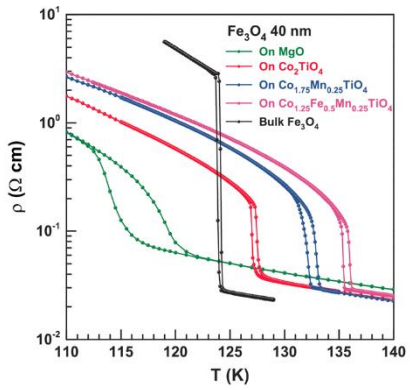

Fig. 7: Resistivity as a function of temperature of 40 nm Fe_3O_4 thin films grown on various substrates and of single crystal bulk Fe_3O_4.

The key issue here is the realization that the substrate is as important as the Fe_3O_4 thin film. We have identified the $Co_{2-x-y}Mn_xFe_yTiO_4$ system as the material of choice, and have made special efforts to grow single crystals of this for the fabrication of the substrates. Using these tailor-made substrates, our record high for the Verwey transition temperature so far is 136.5 K, about 12 K higher than that of bulk single crystals and about 25 K higher than that of the epitaxial thin films reported so far in the literature. The main principle behind this result is to obtain thin films with sufficiently large domains and sufficiently small domain-size distribution. This is a principle that should be used also for the study of other thin film materials that have first order transitions. Once the domain conditions are fulfilled, one will be able to tune the transition temperature in a controlled manner by exerting externally applied strain, either tensile or compressive. Moreover, in view of the strong anisotropy exerted by the strain, it is interesting to study the type of orbital and charge ordering across the Verwey transition in such films.

Physical properties of surfaces and interfaces of solids can markedly differ from those in the bulk, especially in cases when the surface or interface involves non-neutral crystal planes. For insulators, the stacking of such polar planes causes the electrostatic potential to diverge, and forces the surface or interface to behave very differently than the bulk. A representative example is the interface of $SrTiO_3/LaAlO_3$ as well as that of $SrTiO_3/RETiO_3$ (RE = rare earth). The formation of a two-dimensional electron gas and the occurrence of even superconductivity in this interface between two insulating materials has generated frantic research efforts worldwide. However, the growth process of these interfaces and polar interfaces in general remains a mystery. Here we take the case of Fe_3O_4 thin film growth as a model system. How do the atoms move during the deposition or growth such that a well ordered and smooth interface is formed, and stay insulating, despite the destabilizing forces due to the catastrophic electrostatic potential?

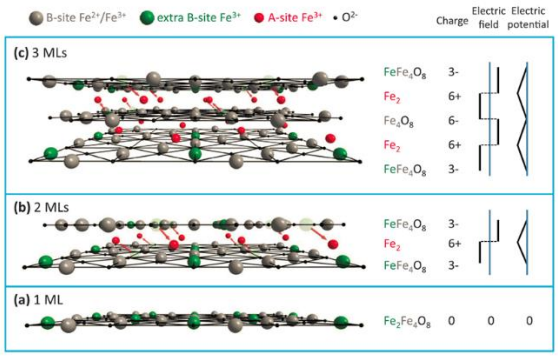

Fig. 8: Growth process of polar Fe_3O_4 (001) films. The A-site Fe^{3+} ions are missing in the first Fe_3O_4 layer and the growth process involves movements of not only the surface but also the subsurface Fe ions.

We carried out XAS measurements on MBE grown Fe_3O_4/MgO (001) films as a function of film thickness, and discovered that the so-called A-site Fe ions are missing in the first Fe_3O_4 monolayer. This is apparently the solution that nature takes to solve the polar catastrophe problem. From data on thicker films, we are able to develop a growth model in which during deposition not only the surface but also the sub-surface Fe atoms are constantly on the move to solve the divergent electrostatic potential problem, thereby

ensuring epitaxy and stoichiometry at the same time, see Fig. 8. Having identified this 'dynamic atomic reconstruction' growth principle, we then can conclude that we really have to think differently about how polar interfaces can grow: apparently, nature offers us a much wider range of opportunities to prepare unstable polar interfaces than previously thought.

The coupling between antiferromagnetism and ferroelectricity at room temperature found in $BiFeO_3$ generates high expectations for the design of new technological devices. However, the multi-domain nature of the material tends to nullify the properties of interest and complicates the thorough understanding of the mechanisms involved.

Here we report the realization of a $BiFeO_3$ material in thin film form and as a single domain: the entire film has its antiferromagnetic axis aligned along the *b*-axis as determined by magnetic linear x-ray dichroism measurements, and with its ferroelectric polarization along the *c*-axis as revealed by the piezo response force microscopy experiments.

In order to achieve such a single domain state, we have utilized (1) the in-plane compressive strain as well as the in-plane anisotropic strain exerted by the $NdGaO_3$ substrate with non-identical *a*- and *b*- axis to fix the antiferromagnetic spin axis along the *b*-axis, and (2) the presence of an $LaNiO_3$ bottom electrode to help direct the ferroelectric polarization to point along the *c*-axis. We were also able to show that a Co film deposited on top of such a film shows a magnetic hysteretic loop with very clear magnetic anisotropy where the easy axis is aligned along the *a*-axis, that is, perpendicular (parallel) to the AFM axis (FM moment) of the $BiFeO_3$ film. This shows that we indeed can make use of the unique properties of the single-domain $BiFeO_3$ film to steer the magnetic orientation of a ferromagnetic material.

http://www.cpfs.mpg.de/pcm/thin-films

New multiferroic materials (Komarek)

Spin-driven multiferroics have attracted substantial attention in the past decades because of their potential for applications in electronic devices, which arises from the intrinsic coupling between magnetic and ferroelectric ordering parameters. After the initial finding of spin-induced ferroelectricity below ~28 K in $TbMnO_3$ the race is on for discovering new multiferroics with higher ordering temperatures and magnetoelectric couplings for applications. Here we report on our successful search for multiferroicity in oxihalides [9].

Quasi–two-dimensional (2D) transition metal (TM) oxychlorides *M*OCl (*M* = Sc, Ti, V, Cr, Fe) have been studied recently because of their exciting magnetic and electronic properties such as pressure-induced insulator-to-metal transitions in TiOCl and a crossover from a spin-Peierls at ambient pressure to a Peierls transition at high pressures. However, so far no multiferroic properties have been reported in oxihalides. For copper the system crystallizes in the 'melanothallite' structure: the Cu^{2+} is coordinated by four chlorine and two oxygen ions. The structure is not anymore quasi-2D, but consists of edge-sharing CuO_2Cl_2 squares forming chains (in the [110] and $[\pm 1 \mp 10]$ direction) that are inter-connected via common oxygen ions in the *c* direction as well.

Cu_2OCl_2 orders antiferromagnetically below ~70 K. In dielectric measure-ments we discovered an anomaly at the Néel-temperature. Moreover, we observed an electric polarization of ~40 µC/m² in pyroelectric measurements. This polarization can be inverted by reverse poling, thus revealing the ferroelectric properties of Cu_2OCl_2. Using neutron diffraction measurements we observed an incommensurate magnetic structure which corroborates our scenario of spin-driven multiferroicity in this system. Hence, oxihalides turn out to be a new class of spin-driven multiferroic materials with exceptionally high critical temperatures (compared to $TbMnO_3$ and many other spin-driven multiferroics) and with promising perspectives for discovering further, new multiferroic materials within this class.

http://www.cpfs.mpg.de/pcm/multiferroics

Spin-orbit interaction in iridates and ruthenates (Hu, Tjeng)

Frustrated magnetic systems realized in actual materials usually deviate from idealized theoretical models such as the famous Kitaev compass model. A fundamental prerequisite for the Kitaev model is the realization of the many body $J_{eff} = 1/2$ state. Here we report on our experimental study using x-ray spectroscopy on Sr_2IrO_4 [10] and α-$RuCl_3$ [11] in order to address whether such a condition can be fulfilled in real materials.

We have carried core-to-core RIXS measurements on Sr_2IrO_4 and found out that Sr_2IrO_4 and iridates in general are negative charge transfer systems with large covalency and a substantial oxygen ligand hole character in the Ir t_{2g} Wannier orbitals. This has the important consequence that the spatial extent of the low-energy or effective t_{2g} orbitals is large, see Fig. 9, thereby reaching the nearest neighbor Ir atoms and

beyond, with the consequence that the effective low-energy Hamiltonian has long range terms, thereby also creating strong orbital anisotropies depending on the lattice structure. These findings set conditions for the design of d^5 materials that can host compass-like magnetic interactions.

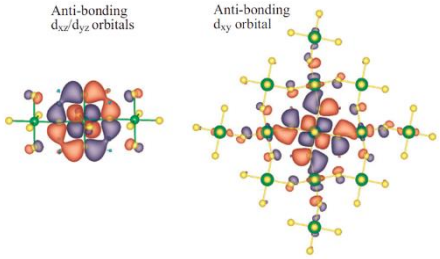

Fig. 9: *Charge density plots for Sr_2IrO_4 of the antibonding Ir $d_{yz/xy}$ orbitals*.

Recently, α-$RuCl_3$ has been suggested as a promising Kitaev-candidate. Excitations observed via Raman and inelastic neutron scattering indeed provide evidence that the system may be close to a quantum spin-liquid ground state. A key issue concerns the degeneracy of the Ru *4d* t_{2g} orbitals. Quantum chemistry calculations proposed a trigonal splitting of about 70 meV, i.e. not small compared to the spin-orbit coupling constant of 150 meV. A large splitting was also estimated from the large anisotropy shown by high-field magnetization measurements. If true, such large splittings would inhibit the presence of Kitaev-physics.

We carried out a polarization dependent XAS experiment at the Ru $L_{2,3}$ - edge of α-$RuCl_3$ to determine quantitatively the trigonal crystal field strength. We observed a vanishingly small linear dichroism indicating that, electronically, the Ru *4d* local symmetry is very close to cubic. Using full multiplet cluster calculations we were able to reproduce the spectra excellently and to extract the trigonal splitting of 12±10 meV, which is negligible as compared to the Ru 4d SOC. Consistent with our magnetic circular dichroism measurements, we found that the ratio of the orbital and spin moments is 2.0, the value expected for a $J_{eff} = 1/2$ ground state. We have thus shown that α-$RuCl_3$ is an ideal candidate for the realization of Kitaev physics. Indeed, very recent studies reveal the suppression of the magnetic order by magnetic fields, indicating the formation of a spin-liquid state in α-$RuCl_3$.

http://www.cpfs.mpg.de/pcm/spin-orbit

New routes to quantum critical materials (Stockert)

The study of quantum criticality in strongly correlated electron materials continued to be a central issue in current condensed matter physics. Here we are focusing our work on the influence of frustration, a new tuning parameter [12].

CePdAl is an antiferromagnetically ordered heavy-fermion compound with a Néel temperature of 2.7 K. Due to the arrangement of the cerium atoms on a distorted kagome lattice, geometrical frustration is present and subsequently only two thirds of the magnetic moments take part in the magnetic order while one third of the moments remains disordered at lowest temperatures.

In neutron diffraction at very low temperatures an unusual broadening of magnetic peaks is visible in CePdAl, likely as a result of competing interactions. Our measurements indicate that frustration is also present in $CePd_{1-x}Ni_xAl$, and even might become stronger when approaching the QCP. In CePdAl we performed thermodynamic measure-ments and studied the magnetic $B - T$ phase diagram and the evolution of the entropy with magnetic field. While at low temperatures and zero magnetic field the frustrated moments are screened by the Kondo effect, upon increasing the magnetic field the Kondo effect is suppressed with enhanced magnetic entropy and subsequently a strongly increased frustration. Our experiments showed a large magnetic field range where frustration in CePdAl plays an important role. In addition, the field range around the maximum in the frustration might be a candidate for a possible quantum spin liquid phase sought for a long time in metallic systems.

http://www.cpfs.mpg.de/pcm/QCP-PCM

FeSe/FeTe competing orders (Wirth, Schwarz), Heavy fermion materials (Wirth, Steglich), and novel Osmate materials (Jansen, Felser, Tjeng) are projects in collaboration with the other departments, see sections 1.6.1-1.6.3 and the report by F. Steglich.

http://www.cpfs.mpg.de/pcm/FeSe-Wirth-Schwarz

http://www.cpfs.mpg.de/pcm/HF-Wirth-Steglich

http://www.cpfs.mpg.de/pcm/Os-Ir

1.2.3. Future directions

One of the scientific revelations that we encounter in the 2015-2018 period is how powerful core-level NIXS (non-resonant inelastic x-ray scattering) actually is for the investigation of the symmetry of local atomic wavefunctions. Accordingly, we have spent considerable amount of effort to build our own NIXS end-station at the P01 beamline at PETRA-III. The set-up is now running and producing spectra.

Using this new spectroscopic method, we have been able to determine the in-plane *orientation* of 4*f*-orbitals, to distinguish Γ_8 from Γ_7 4*f*-wavefunctions in *cubic* systems, and even to identify the 5*f* ground state wavefunction in highly *itinerant* U materials. This is thanks to the high multipole transition matrix elements being operative due to the large momentum transfers used as explained in the previous sections.

Very new (unpublished) and exciting is our discovery that we can directly image the shape of the relevant local orbital or wavefunction without doing any spectroscopic analysis, simply by measuring the total integrated NIXS intensity from an *s*-core-level. We have done a test experiment using NiO: we collect the Ni M_1-signal ($3s \rightarrow 3d$) at a fixed scattering geometry and rotate the crystal as to vary the transferred momentum direction with respect to the crystal axes.

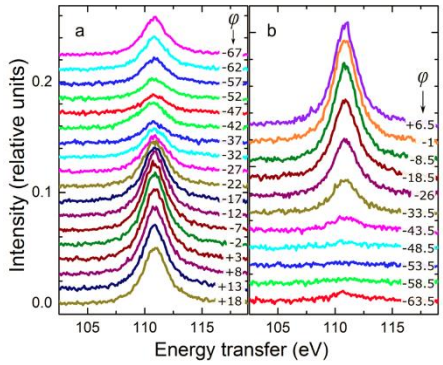

Fig. 10: Angular or directional dependence of the Ni M_1 ($3s \rightarrow 3d$) NIXS signal of NiO.

The spectra for the scattering in the [001]-[100] and [001]-[110] planes are shown in panels (a) and (b), respectively, of Fig. 10. We can clearly observe the strong intensity variations as function of angle. To quantitatively analyze the data, we simply make a polar plot of the measured integrated intensity as a function of the angle of rotation, see Fig. 11. Remarkably, the intensity distribution falls accurately on top of the orbital shapes which are 'cuts' through the [001]–[100] (orange) and [001]–[110] (green) planes of the three-

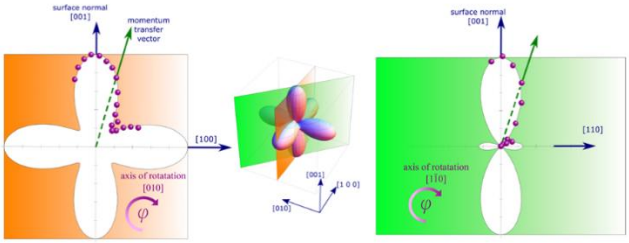

Fig. 11: Polar plot of the experimental angular intensity distribution of the Ni M_1 NIXS of NiO and the theoretical $3d^8$ $(x^2-y^2)(3z^2-r^2)$ hole density.

dimensional hole density distribution of the Ni high-spin $3d^8$ configuration, i.e. the $^3A_2$ $(x^2-y^2)(3z^2-r^2)$. The result is evident: The directional dependence of the integrated *s*-NIXS intensity directly maps the ground state local hole density of the ion. There is no need to do a multiplet analysis of the spectra to extract such information, in contrast to the standard $L_{2,3}$, $M_{4,5}$, $N_{4,5}$ XAS. The reason is fundamental: The quadrupole $3s \rightarrow 3d$ excitation process involves a spherically symmetric *s* orbital, so the angular distribution of the intensity is solely determined by the hole charge distribution in the initial state with respect to the momentum transfer.

To our knowledge, this result is the first direct experimental demonstration of the shape of a local quantum mechanical orbital. The potential of the method is obvious: we can now determine directly the relevant local (hole) charge density without the need to do spectroscopic analysis. This is extremely valuable for solid state chemistry in general and for strongly correlated phyiscs systems where band formation prevent the use of single-site approaches. More on our plans will be presented during the Scientific Advisory Board site visit in Nov. 2018.

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Physics of Quantum Materials

Director: Andy Mackenzie

Group leaders: Michael Baenitz, Manuel Brando, Christoph Geibel, Clifford Hicks, Michael Nicklas, Takashi Oka and Helge Rosner

The overarching goal of the Physics of Quantum Materials department is to advance understanding of the behavior of interacting electrons in solids. From the viewpoint of conductivity in the limit of low temperatures, we know of only three distinct equilibrium ground states – metals, superconductors and insulators. Our interests focus mainly on the first two of these, but the inter-relationship with insulating states is sometimes key to understanding metals and superconductors, and is something that we study where appropriate. In the spirit of the Institute we profit from working at the interface between physics and chemistry, either in the form of direct collaborations with the Chemistry departments or by developing new technologies or materials that have both chemical and physical relevance.

An important aspect of our working philosophy is breadth. Half a century's experience of the interacting electron problem shows that discoveries are often made at the borderline between localized, magnetic systems and broader band metals. It is difficult to predict with certainty where the next breakthrough will come, so we believe that maintaining a broad base of expertise is the wisest strategy. For this reason we retain an interest in modern problems in magnetism, in tandem with unconventional superconducting and metallic states. A particular theme is material purity. Observation of some of the most interesting new states relies on minimizing electronic scattering from defects, so we try to specialize in working with materials that have extremely low defect levels, and in developing new experimental techniques optimized for working on ultra-clean materials.

In the following sections we outline highlight areas of our research since 2015. Among these we particularly flag four achievements which we believe are of broad significance, and were surprising discoveries that present a challenge to received wisdoms:

1. Discovery of hydrodynamic electronic flow in ultra-pure layered metals [1]; see also Perspective by J. Zaanen, *Science* **351**, 1026 (2016).
2. Explicit tuning of a charge density wave system to superconductivity [2].
3. Tuning of an unconventional superconductor through a topological Lifshitz Fermi surface transition using bespoke uniaxial stress techniques, thereby increasing its transition temperature by a factor of 2.3 [3,4]; see also Perspective by K.M. Shen, *Science* **355**, 133 (2017).
4. Gaining a chemical physics understanding of the circumstances in which Rashba-split states can be created at surfaces and interfaces, and creating a record splitting for a transition metal based state [5]; see also News and Views by Z.-X. Shen & J. Sobota, *Nature* **549**, 464 (2017).

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

Electronic hydrodynamics (Mackenzie, Schmidt, collaboration with Moll)

The flow of electrons in more or less every known metal is described by Ohm's law, but that is an empirical law based on observation. Perhaps surprisingly, it implies flow patterns that are very different from the way that water would flow in a river or normal ^{3}He in a tube. The reason is that by far the dominant scattering processes in most materials relax the electron fluid's momentum strongly in the bulk of the host lattice. In hydrodynamic flow, boundary scattering dominates the relaxation unless one specifically inserts scattering centres in analogy to rocks on a river bed.

As pointed out over fifty years ago in theoretical work by Gurzhi, the first prerequisite for reaching the hydrodynamic limit in a metal is extremely high purity. Almost every known material is simply far too dirty. Experimental progress was made in the 1990s using artificial two-dimensional electron gases, but no convincing evidence had been seen in bulk materials. Noting that $PdCoO_2$ has astonishingly high conductivity, with mean free paths of tens of microns

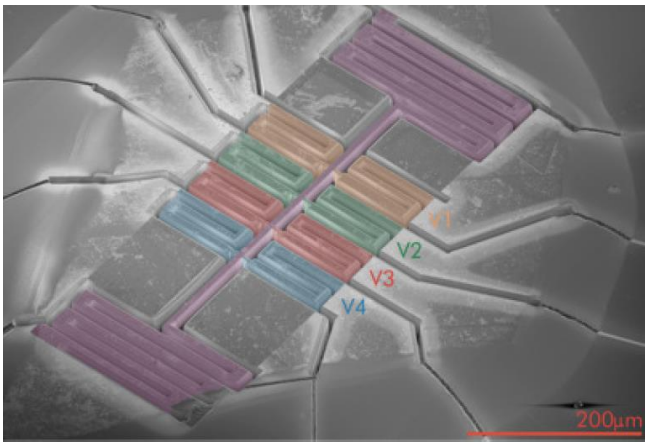

Fig. 1: A $PdCoO_2$ single crystal mounted on a drop of epoxy and sculpted with a focused ion beam to produce a width-restricted conducting channel for electron hydrodynamic studies [1].

at low temperatures, we found hydrodynamic signatures in mesoscopically patterned single crystals (see Fig. 1), in a collaboration with Philip Moll that we began about 18 months before he joined the Institute. These developments are topical, especially since a host of other extremely high conductivity compounds are now being discovered by those searching for topological metals, with Claudia Felser's department playing a leading role in those searches. Although basic physics of metals was thought to be understood, it seems that there is much more to discover.

A feature of electronic hydrodynamic research is a close interplay between experiment and theory. Our first paper contained fairly substantial kinetic calculation performed in-house by Dr. Burkhard Schmidt, and we have extended this approach to incorporate magnetic fields in collaboration with Dr. Thomas Scaffidi at Berkeley [6]. Unpublished experiments on $PdCoO_2$ from the thesis work of Nabhanila Nandi show evidence for 'electron magneto-hydrodynamic' effects, and work by other groups on graphene is also progressing rapidly. In Dresden, Roderich Moessner decided to form a hydrodynamic theory group at MPI-PKS after learning of our experimental work. Regular joint discussion meetings are now held, and are generating ideas for further experiments. We are optimistic about further progress in what is becoming a new field, and glad to have played a role in establishing it.

For further reading on this research see
www.cpfs.mpg.de/pqm/hydrodynamics

Unconventional superconductivity (Mackenzie, Hicks, Geibel, Brando, Nicklas, collaboration with Grin and Hassinger)

Superconductivity has a special place in materials physics because of its richness as a phenomenon, and the ever-present hope that room temperature superconductivity will one day be attainable. Work from the MPI for Chemistry in Mainz on H_3S has famously showed that it can now be achieved at temperatures (-70 C) that are found on the earth's surface, but at pressures that have more in common with planetary interiors. The underlying mechanism for this exciting new superconductivity appears to be conventional, in the sense that it is driven by phonons. However, that should only increase the urgency to understand the mechanisms of unconventional superconductivity, for which there is theoretical evidence that the underlying energy scales are even higher than in compounds like H_3S. The best strategy is to work with model systems and try to understand their phase diagrams. A high T_c is not an absolute prerequisite for such experiments since what is learned at one energy scale can often be transferred to another, and the field still faces fundamental challenges – we have no agreed theory for the mechanism of unconventional superconductivity in most superconductors.

Since 2015 we have made progress on several fronts. We have shown that $YbRh_2Si_2$ is a heavy fermion superconductor, culminating many years' research in our department on this system [7]. An exciting collaboration on noise spectroscopy with colleagues at the University of London is allowing extension of study in this challenging mK temperature regime, and the full phase diagram is being established. The full mystery of heavy fermion superconductivity is highlighted by new experiments revisiting the superconductivity of $CeCu_2Si_2$ [8,9], and our colleagues in Juri Grin's department are working on a new generation of crystals of UBe_{13} using previously untried growth routes, in collaboration with our department and the group of Elena Hassinger. In a particularly intriguing development, a collaboration led by the group of Philip Moll has shown that microstructured $CeIrIn_5$ single crystals feature unidirectional superconductivity over part of their phase diagram. Although anomalous superconducting behavior had been seen in this compound for many years, the new microstructuring techniques pioneered in our Institute are enabling new classes of experiments to find out what is really happening. The work is on-

going, in collaboration with scanning SQUID microscopy on the same samples, by the group of Katja Nowak at Cornell.

At the other end of the T_c spectrum, we have also obtained important results on cuprate superconductors. A collaboration with the Cornell group of Seamus Davis, mediated by joint PhD student Stephen Edkins, has investigated the interrelationship of charge- and Cooper pair-density waves with homogeneous superconductivity [10,11]. This work opens the possibility of unified theories in which one mechanism determines the formation of all three kinds of order, opening the way to tuning the balance between them and understanding entirely new classes of physics.

Arguably the highlight of our work on superconductivity is a series of experiments on Sr_2RuO_4, a benchmark system for unconventional superconductivity because of its extreme purity, the relative simplicity of its Fermi surface and its proximity to a Fermi liquid metallic state. We have discovered an extreme sensitivity of the superconducting state to uniaxial pressure, motivating us to develop new methods of performing such experiments (see Fig. 2). In work led from our department, we have demonstrated the existence of a maximum in T_c a full factor of 2.3 higher than that in ambient conditions, and shown that this occurs at close to the strains required to drive the Fermi surface through a topological Lifshitz transition. Our work also provides the cleanest data ever acquired on the evolution of the metallic properties across such a transition [4]. Our measurements of superconducting critical fields are now complemented by high precision studies of the electronic specific heat under uniaxial pressure, and challenge the widely-held belief that Sr_2RuO_4 is a p-wave superconductor with a two-component order parameter [12]. The final chapter on Sr_2RuO_4 is evidently still unwritten, but we believe that our work has opened a new route to the study of unconventional superconductivity in this material and beyond. It is not the only superconductor proposed to have a two-gap triplet state; it will be interesting to see how other materials under study by the department such as $LaNiGa_2$ [13] react to uniaxial pressure.

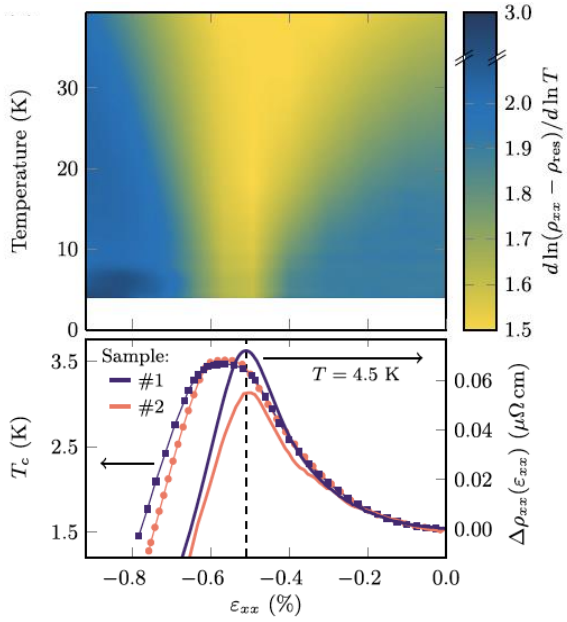

Fig. 2: Correlation between maximized T_c and value of low temperature normal state resistivity with depression of the power law governing the temperature dependence of the resistivity in Sr_2RuO_4, all as a function of lattice strain produced in one of our bespoke uniaxial pressure rigs [3,4].

Further information can be found at
www.cpfs.mpg.de/pqm/superconductivity

Advancing quantum criticality (Brando, Geibel, Nicklas)

Quantum criticality, in which a continuous phase transition is tuned to low temperatures using some external control parameter, is a central concept in correlated electron physics. It is used as a tool to amplify response functions in the vicinity of the

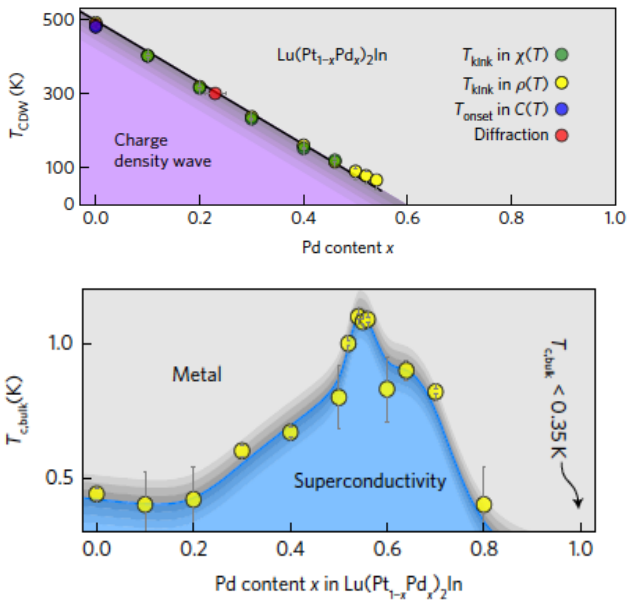

Fig. 3: The temperature-composition phase diagram of the quantum critical charge density wave system $Lu(Pt_{1-x}Pd_x)_2In$ (top panel) and a zoom-in showing how the superconductivity peaks around the quantum critical point (bottom panel) [2].

transition, and to stimulate the formation of novel forms of order. Our Institute has been at the centre of research in the field over the past two decades, and rather than continue with mature avenues of research such as antiferromagnetic systems, we are concentrating on moving the field to new areas. Department members have contributed a major review on ferromagnetic quantum criticality [14], the experimental discovery of quantum tricriticality [15], and extended research towards multipolar criticality [16].

A particular highlight has been work on $Lu(Pt_{1-x}Pd_x)_2In$ in which a charge density wave transition has been tuned towards zero temperature, resulting in superconductivity thought to be mediated by a soft mode associated with the criticality [2] ; see Fig. 3. Since understanding the interplay of charge density wave physics and unconventional superconductivity is of strong topical interest in systems such as the cuprates (see above), this first clear example of superconductivity explicitly related to density wave fluctuations is of particular significance. We are now studying the relevant excitations using newly developed high resolution inelastic XR scattering techniques, in cooperation with Hao Tjeng's department.

Further information can be found at
www.cpfs.mpg.de/pqm/quantum-criticality

Fundamental magnetism (Baenitz, Sichelschmidt, Brando, Rosner, Schmidt, Hicks, Mackenzie, Oka, Nicklas, Geibel)

Magnetism is one of the oldest fields in the physics of solids, but it continues to surprise and delight. By maintaining our expertise in magnetism we have an excellent foundation from which to contribute to forefront developments. For example, over the review period we have contributed to the understanding of incommensurate order stimulated by the application of static fields [17], to constructing the appropriate Hamiltonian for the study of spin ice physics [18], and to understanding chiral lattice ferrimagnets [19] and Dzyaloshinsky–Moriya molecular magnets [20].

The above work mainly resulted from applying our pre-existing expertise to relevant collaborations, but we have also initiated themed research in two major topical areas, namely the search for unconventional magnetic ground states (e.g. spin liquids) in 3d-, 4d- and 5d- quantum magnets, and magnetically textured surface states. In the spin liquid programme we produced one of the foundational papers on

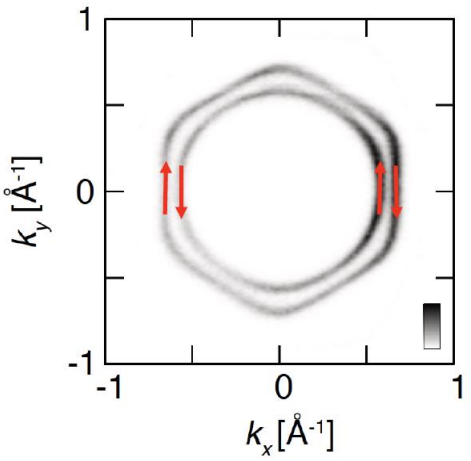

Fig. 4: Rashba-split spin-textured surface states in $PdCoO_2$. The red arrows indicate the relative spin orientations. Similar data were obtained from $PtCoO_2$ and $PdRhO_2$ [5].

$RuCl_3$ [21] and carried out spectroscopic investigations of candidate spin liquids such as $PbCuTe_2O_6$ [22] and Ba_2CuTeO_6, and are currently studying Yb-Na-sulphides with the same delafossite structure as that of the oxides on which we have studied hydrodynamic conduction.

The same delafossite oxides yielded an unexpected and potentially important result in terms of surface magnetic texturing. Starting from the observation of anomalously large Rashba-like splitting of Co-based surface states in $PtCoO_2$ (Fig. 4) we realized that, contrary to the previous received wisdom of the field, the key to obtaining large Rashba splittings is not simply to work with heavy elements with large atomic spin-orbit coupling. The ideal condition to achieve is an energy scale for inversion symmetry breaking that is larger than the atomic spin-orbit coupling scale of the surface atom, because then the bare atomic spin-orbit energy is fully utilized in the Rashba splitting [5]. Using this insight it was possible to achieve 150 meV Rashba splitting at the surface of $PdRhO_2$, a compound for which we grew the first single crystals.

This discovery themes particularly well with the goals of the Institute, because the reason that such large inversion-breaking scales can be found in the delafossites is their unusual crystal chemistry, in which the layers are parallel to one of the triangular surfaces of the transition metal octahedra, not to the square basal plane. Also, the growth of the $PdRhO_2$ crystals used to validate the theory that we had developed was done in close collaboration with colleagues from Juri Grin's department, while important contributions to

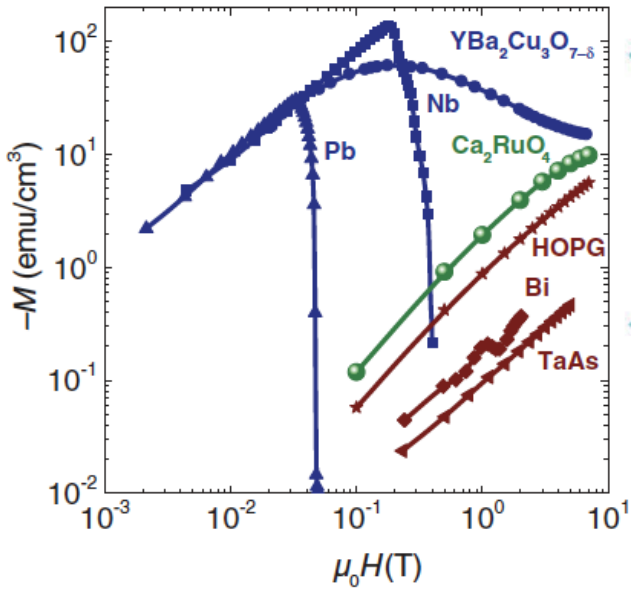

Fig. 5: The remarkable diamagnetism of the current-induced state of Ca_2RuO_4 which our theoretical work predicts to be a 'Mott semimetal' [23].

the electronic structure calculations came from colleagues in Hao Tjeng's department [24].

The final notable research into exotic magnetism is theoretical work into an astonishing phenomenon in which passing very modest currents through the Mott insulator Ca_2RuO_4 creates a completely unanticipated insulator – conductor transition, accompanied by a huge structural change. Even more surprisingly, the resultant state, for which we have proposed the name 'Mott semi-metal', has the largest diamagnetic susceptibility of any known non-superconductor, and bigger than that of almost all superconductors as well by the time the applied field reaches 10 tesla (Fig. 5). A simple model accounts for key features of the diamagnetism, which has its roots in the strong correlations of the original Mott state [23].

More information on this topic is available at
www.cpfs.mpg.de/pqm/spin-liquid
www.cpfs.mpg.de/pqm/delafossites
www.cpfs.mpg.de/pqm/fundamental-magnetism

Practical magnetism (Nicklas, Brando, Baenitz, Oka, collaboration with Felser)

Although our main goal is fundamental research, and the borderline between fundamental and applied science work is often blurred, we include this section separately in this report to emphasize the fact that we also have some projects aimed at direct exploitation of findings made while conducting basic research. Building on our work on magnetic quantum criticality, we are developing materials for magnetic cooling at very low temperatures [25], and working in collaboration with Claudia Felser's department to refine Heusler compounds with room temperature applications in mind [26,27] (Fig. 6). Some of our theoretical work also has technology development as its motivation; a notable example is the prediction of how to drive spin currents on ultra-short timescales [28].

See also
www.cpfs.mpg.de/pqm/magnetic-cooling
www.cpfs.mpg.de/pqm/magnetic-heusler

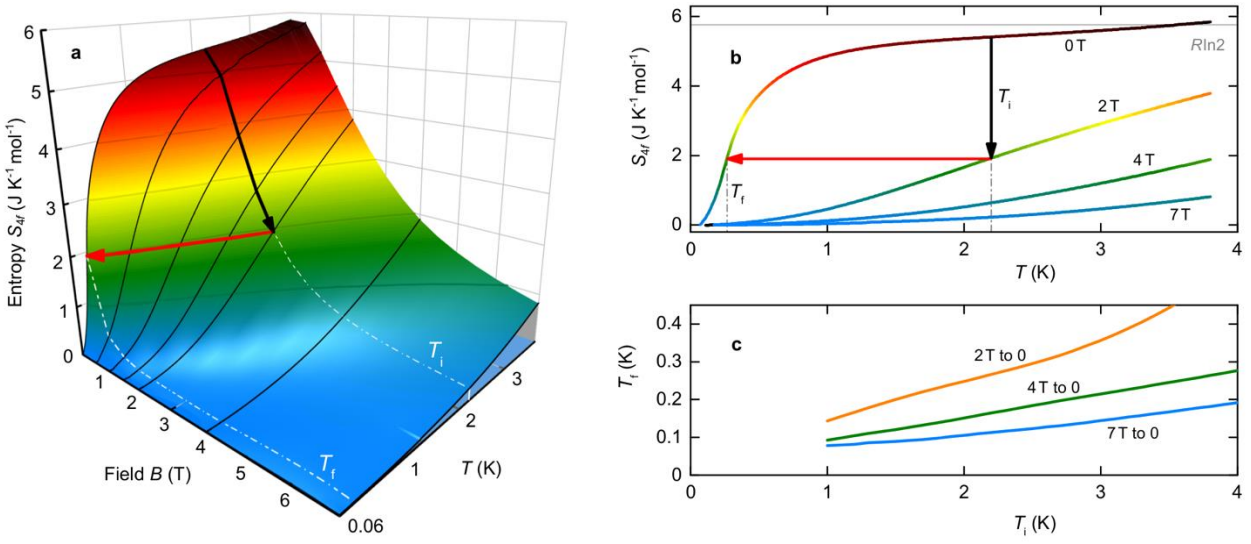

Fig.-6: a) Colour map of the 4f-electron magnetic entropy of $YbPt_2Sn$ and (b and c) the way in which the entropy can be exploited to achieve magnetic cooling [25].

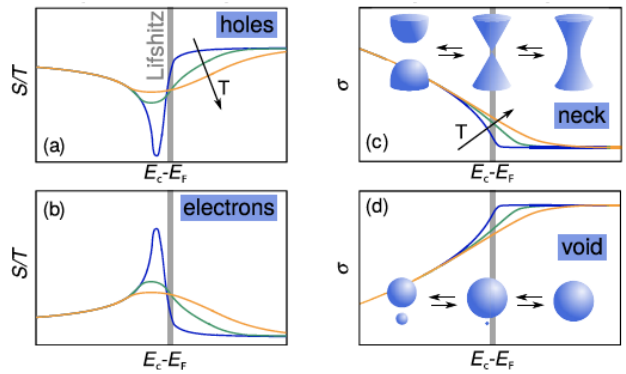

Fig. 7: Expected signals in thermopower (S) and conductivity (σ) for different classes of Lifshitz transition seen in $YbNi_4P_2$ [30].

Topological Fermi surface transitions (Hicks, Brando, Mackenzie, Nicklas, Rosner, collaboration with Moll)

Topology has become a major research area in the physics of metals thanks to the discovery, for example, of Weyl semi-metals (see below). However, this is not the only topological physics relevant to metallic systems. Zero temperature Lifshitz transitions also require a topological classification. As well as work on Sr_2RuO_4 [3,4,29], we have demonstrated the importance of Lifshitz transitions in controlling many-body effects in $YbNi_4P_2$ [30] (Fig. 7) and the FeTe system [31], and believe that they may play a role in the intriguing metamagnetic/nematic physics of $Sr_3Ru_2O_7$ [17] and $CeRhIn_5$ [32] as well.

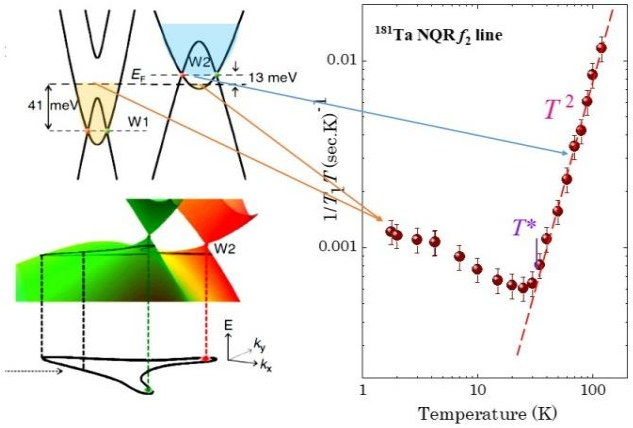

Fig. 8: The first measurements of nuclear relaxation signatures characteristic of Weyl semi-metals, as observed in ^{181}Ta nuclear quadrupole resonance experiments on TaP [35]*. The T-dependence of $1/T_1T$ (right hand panel) shows the T^2 behaviour characteristic of Weyl fermion excitations from a W2 point (dashed line) above T* = 30 K. For T<T* the signal is dominated by Korringa relaxation with a temperature dependent chemical potential.*

Fully understanding the significance of this class of topological transitions is still an open challenge, but the high-precision experiments that we have performed are helping to build a data-base of relevant observations, and since uniaxial pressure is an ideal tuning parameter for Lifshitz transition physics, we anticipate further research in this area in future.

Collaboration on Weyl semimetal physics (Baenitz, Nicklas, collaboration with Felser, Hassinger)

Weyl semi-metals have become a huge field of research, extensively studied in Claudia Felser's department as described in their section of this report. For some studies joint work with our department and the group of Elena Hassinger has enabled more rapid progress. We strongly encourage such collaborations, which have led to a number of high-impact publications in the field [33,34]. In several cases we lead the work, such as the recent quadrupole resonance (NQR) studies on TaP [35] (Fig. 8), which we believe to be the first discovery of NQR signals from a Weyl dispersion.

Further information can be found at www.cpfs.mpg.de/pqm/weyl-fermions

Development of bespoke technical platforms (Hicks, König, Mackenzie, collaboration with Moll and Hassinger)

As well as performing the experiments outlined above, we see one of our core missions as being to develop experimental techniques that are either entirely new or allow large increases of resolution over those in use in other institutions around the world. Of particular interest to us are developments that help physics and chemistry to overlap. We have done this in several ways. One of our major development efforts is the design and construction of novel apparatus for the application of uniaxial pressure.

These techniques, invented by members of our department, were key to the success of a number of the experiments described above [3,4,17], and have been successfully commercialized via a licensing agreement with Razorbill Instruments negotiated by Max Planck Innovation (Fig. 9). Nearly seventy uniaxial pressure rigs have now been sold world-wide, and orders are coming in at a rate of approximately three per month. The published experiments and the commercially available rigs are based on designs several generations behind our current state-of-the-art, and we anticipate further discoveries using our newer apparatus (for example Fig. 10).

The uniaxial pressure work overlaps with chemistry because we can achieve lattice parameter changes, currently, of up to 1.5%, and anticipate up to a factor of three increase in future in certain materials. This is the equivalent of creating new compounds, often unavailable to equilibrium chemistry, using an external tuning parameter. Complementary developments were made on the design and construction of our high-resolution thermal expansion cells to be able to measure thermal expansion and magnetostriction under large uniaxial pressures and very high magnetic fields [36,37]. With these new designs, which have also been made commercially available (http://www.dilatometer.info/), thermodynamic properties could be studied under uniaxial stress up to 3 kbar and in magnetic fields up to 37.5 T [38].

The second main way in which we are working at the interface with chemistry is in our development of focused ion beam microstructuring techniques and ultra-sensitive measurement apparatus to free experimental physics from the need to work with large single crystals, and enable experiments to be performed at mesoscopic length scales on the complex quantum materials that are produced by an institute like ours. Often working in collaboration with the Max Planck Research Groups of Philip Moll and Elena Hassinger, our microstructuring capabilities have proved vital to the success of some of our key projects [1,30,32], and our ambitious uniaxial pressure goals are being tackled by using microstructuring techniques to produce miniaturized samples and pressure apparatus. In combination with this, we have continued our development and use of ultra-sensitive dilatometers [38], and collaborated with the Hassinger group on calibrating their SQUID-based torque magnetometry setup [39].

Fig. 9: Figure from Razorbill Instruments literature (https://razorbillinstruments.com) showing some of the product range of uniaxial pressure cells that they have developed based on our designs.

Further information on these projects can be found at www.cpfs.mpg.de/pqm/technical-plattforms

Future plans

One of the major attractions of the Max Planck Society is the possibility to do opportunity-driven research without the need to provide detailed advance plans, and we will certainly continue to enjoy and take advantage of this unique environment. However, that does not mean working entirely without a strategic vision, and we foresee focused efforts in several areas. We will continue to invest heavily in development of uniaxial pressure apparatus, in which we believe we have a world lead, and broaden the range of uniaxial pressure experiments that are performed, sometimes in-house and sometimes in collaboration. The hydrodynamic work on delafossites has highlighted their broader potential as a materials class, and we plan both to perform hydrodynamic and ballistic experiments on the existing materials, and to attempt to fabricate others with similar levels of crystalline perfection to that achieved on the known materials. We aspire to a considerable expansion of our joint work with Professor Molenkamp, with whom we share a number of interests, not least in the development of noise spectroscopy as a low temperature measurement tool. The groups of other existing collaborators, Prof John

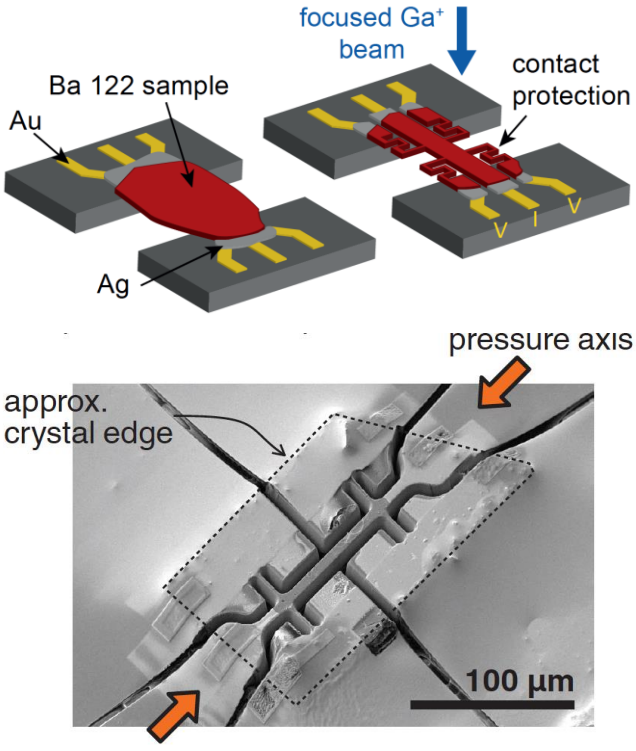

Fig.-10: Focused ion beam microstructured strain apparatus – concept (upper panel) and feasibility study on $Pr_2Ir_2O_7$ (lower panel).

Saunders in London and Prof Séamus Davis at Cornell, are also making rapid developments in noise spectroscopy, and we hope that we can join them in pioneering some novel capabilities in this field of research.

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Solid State Chemistry

Director: Claudia Felser

Group leaders: Peter Adler, Chandra Shekhar, Gerhard H. Fecher, Chenguang Fu, Johannes Gooth, Nitesh Kumar, Anastasios Markou, Sergey Medvedev, Walter Schnelle and Yan Sun

The main goal of the solid-state chemistry department is the rational design of new Heusler compounds and intermetallic compounds with related structure types. The wide range of tunable materials is combined with our recent focus on topology [1]. Topology is a global aspect of materials, leading to fundamental new properties for compounds with large relativistic effects. The incorporation of heavy elements gives rise to strong spin-orbit coupling (SOC), and non-trivial topological phases of matter, such as topological insulators (TIs), have been discovered. Dirac and especially Weyl semimetals were in focus of the last 3 years. The interplay of symmetry, SOC and, in magnetic materials, the magnetic structure, allows for the realization of a wide variety of topological phases through Berry curvature design. The Berry curvature describes the entanglement of the valence and conduction bands in an energy band structure, or in words of a chemist: the crossing of the outermost atomic s orbital (inert pair effect) with the valence band. Weyl points and nodal lines can be manipulated by various external perturbations, which results in exotic local properties such as the chiral or gravitational anomaly, and large anomalous, spin and topological Hall effects.

In our institute, the unique combination of solid state chemistry and single crystal growth facilities allows for the synthesis of high quality single crystals of nearly any type of compound such as oxides, semiconductors and metals, preconditions to be a world leader in the field of topological materials. The scientific goal of the solid state chemistry group is the investigation of these new topological materials as high quality single crystals, and studies of the Hall effect and magneto-transport properties as a function of external stimuli and defects and doping in close collaboration with the groups in physics at the CPfS. Recently our team has completed the thin-film growth laboratory by adding one molecular-beam epitaxy chamber, in-situ ARPES, in-situ scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) to the two sputter chambers. All chambers are connected by a vacuum tube, providing a unique combination of equipment which enables us to grow films of many different materials and thereby explore all quantum Hall effects.

In the following report, we summarize our major achievements since 2015, including three major highlights which will likely have a big impact in the scientific community and beyond:

In Heusler compounds, the variety of accessible electronic and magnetic properties, together with the existence of a topological band order, generates highly tunable and versatile multifunctional properties such as topological insulators, Weyl and nodal line semimetals, topological superconductivity and spin-structured topological states, such as antiskyrmions [2]. Antiskyrmions were observed for the first time in the inverse tetragonal acentric Mn-Pt-Sn Heusler compound with D2d symmetry by Lorentz transmission electron microscopy (LTEM) over a wide temperature range beyond room temperature carried out in the Max Planck Institute for Microstructure Physics in collaboration with Parkin's new department [2]. Previously, skyrmions have been reported in various ferromagnetic materials, but anti-skyrmions are predicted to exist only in materials whose crystal structure symmetry supports a Dzyaloshinskii-Moriya vector exchange interaction that has different signs along different crystal axes. Just like skyrmions, anti-skyrmions arise from a helical magnetic structure but the anti-skyrmions appear to be more stable. By varying the magnetic field and temperature both single and hexagonal lattices of anti-skyrmions are formed.

One important breakthrough in collaboration with Bernevig et al. is the recent development of a quantum topological chemistry. More than 200,000 inorganic compounds have been made by chemists or material scientists or are known in nature. From the view-point of topology, it is now possible to classify all these existing compounds as well as those to be discovered in the future, as: trivial compounds; topological insulators; Weyl; and Dirac semimetals; or topological metals, including new Fermions with x-tuple points in their band structure [3]. Soon with a single click in a data

base, such as the Bilbao Crystallographic Server (http://www.cryst.ehu.es/), a scientist will be able to learn about the topology of a new compound, or will be able to identify many previously undiscovered families of candidate topological materials. Based on a new complete electronic band theory, topological quantum chemistry provides a description of universal topological properties based on: (i) a graph-theoretic description of reciprocal space, (ii) a group-theoretic description of real space, and local orbitals for all 230 space groups. Quantum chemistry adds two ingredients to the Bloch theory, namely (i) band topology and (ii) orbital hybridization [3]. These concepts can and will be extended to magnetic space groups, phonons etc. in the future.

Solutions of the Dirac equation which naturally occur in high energy- and astrophysics are experimentally much more easily accessible in excited states of solids. This, in principle, allows table top experiments to address important questions in high energy and astrophysics via the investigation of properties of specially designed materials. Examples are the chiral anomaly and the axial-gravitational anomaly [4], invoking massless chiral fermion particles. These quantum anomalies are the violation of a classical conservation law, which dictates that the numbers of massless fermions of different chirality (relative orientation of linear momentum and spin) are separately conserved. However, in a Weyl semimetal when the current and an applied magnetic field are parallel with each other, the left- and right handed quasi particles are not conserved in the quantum limit due to the chiral imbalance induced by the quantum anomaly. By analogy to the underlying curved space-time of the universe, which provides the contribution to the chiral imbalance close to a Black hole, a temperature gradient in a Weyl semimetal in the case of the gravitational anomaly and a voltage gradient in the case of the chiral anomaly can give a rise to an analogous effect. Johannes Gooth, the first author of ref. 4, and leader of his recently funded independent Max Planck Research Group was and will be in charge of this research, which will inspire our materials design effort. His keen interest and knowledge of both cosmology and condensed matter physics has rendered this new research direction possible.

1. Magnetic antiskyrmions above room temperature in tetragonal Heusler materials [2]
2. Topological quantum chemistry [3], see also News & by Gregory A. Fiete, *Nature* **547**, 287 (2017) and feature by Davide Castelvecchi, *Nature* **547**, 272 (2017) and cover
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Topological Quantum Chemistry (Felser)

For more than a decade, materials have been classified according to the topology of the underlying electronic structure. Topological insulators can be identified in the bulk band structure by calculating the Z2 topological invariants. As analogues of HgTe, the material in which the quantum spin Hall effect was first realized, half-Heusler compounds were identified as topological insulators with promising additional functionalities such as superconductivity. Dirac cone surface states were recently observed in half-Heusler compounds by angle resolved photoemission (ARPES) [5]. Dirac and Weyl semimetals have recently emerged as a new focus in solid state physics and chemistry [6]. These materials are characterized by band-touching points with linear dispersion, similar to massless relativistic particles. Weyl semimetals require broken inversion symmetry or time-reversal symmetry (via magnetic order or an applied magnetic field). These band-touching points are monopoles of the Berry curvature and are topologically protected by their monopole charge, which is given by a Chern number. In addition to doubly degenerate Weyl points several new and unconventional Fermions were predicted by Bernevig, Felser et al. [7]. Here the guiding principle was to look for linear and quadratic 3-, 6- and 8- band crossings stabilized by space group symmetries for all 230 space groups. A logical next step after identifying topological insulators and semimetals is looking for topological metals. It has been realized that gold and platinum are examples of topological metals [8]. The only limitation of the "topological quantum chemistry" are that properties that can be predicted are based on a single particle picture. However, the interest of many physicists center on precisely those exceptions from the single particle picture, e.g. electron-electron correlations. The

first step in the direction of correlation in topology is the systematic understanding of magnetic compounds, which is a new focus of the solid-state chemistry team in collaboration with Bernevig and co-workers.

Theoretical study of topological materials (Sun, Felser)

www.cpfs.mpg.de/ssc/theoretical-TI

Much of the progress in new topological materials and new topological properties is driven by theory. Therefore, the theory group plays an important role, and has a very close collaboration with the experimental groups. By applying topological band theory, Sun et al. have studied systematically a series of topological materials from topological insulators to metals. Extending the topological band theory to semimetals and metals, several new compounds with a linear band crossing due to Weyl points have been identified. These points behave as monopoles of Berry curvatures and give rise to new topological properties, even to properties that break fundamental conservation laws. The first experimentally discovered type-II Weyl semimetal, $MoTe_2$ was predicted by us [9] and subsequently verified by ARPES [10]. Weyl points generated via time reversal symmetry breaking were predicted and realized in ferromagnetic $Co_3Sn_2S_2$ [11,12]. Weyl points can be only defined in three dimensions, but by breaking the translation symmetry along one direction, we realized that quantized anomalous Hall effects can be achieved in the two-dimensional limit of Weyl semimetals, such as a monolayer of $Co_3Sn_2S_2$ [13]. Guided by the Berry curvature, it was possible to identify new materials with large spin Hall effect (SHE) or spin transfer torques as electrodes for magnetic random access memory (MRAM): examples are TaAs [14], Mn_3Sn [15] and other Weyl semimetals. The SHE in non-magnetic materials, the anomalous Hall effect (AHE), and the anomalous Nernst effect (ANE) are enhanced near Weyl points and nodal lines close to the Fermi energy. This is a paradigm change since it had been believed that antiferromagnets and compensated ferrimagnets should display no AHE and that, rather, the AHE scales with the net magnetisation. By designing materials with a certain symmetry of the Berry curvature, it was found that the AHE can even exist with zero net magnetisation in the absence of symmetry operations that change the sign of the Berry curvature, while the AHE can be zero in strong magnets by adding symmetry elements, which lead to a compensation of the Berry curvature. Following this guiding direction, we have observed a strong anomalous Hall effect in the noncollinear antiferromagnets Mn_3Ge/Sn [16,17] and in compensated magnets like Ti_2MnAl [18]. Replacing the electrical field by temperature gradient, transverse charge current and spin current can also be observed due to anomalous and spin Nernst effect [19].

Exceptional transport properties of topological semimetals and metals (Shekhar, Kumar, Manna, and Felser in collaboration with Schmidt and Hassinger)

www.cpfs.mpg.de/ssc/TM-transport.

Semimetals are a well-established field of research in solid state science, but topology has given us a new perspective on old and newly predicted semimetals. Inspired by the work of the Princeton groups, we started our activities in the area of Weyls semimetals with NbP [7]. The conductivity is high at cryogenic temperatures and the mobility even better than graphene. The easy access of high quality single crystals, crystals grown by vapor transport are grown in collaboration with Marcus Schmidt (CM) enabled us to publish a series of high impact papers immediately [20-22]. The four members of TaAs family allowed for a systematic study of the influence of SOC on the topological properties. Inspired by this success we searched for other phosphides with even better properties. WP_2 was predicted to be an extremely stable Weyl semimetal with Weyl points of the same chirality as closest neighbours. As a consequence, the transport properties were superb, consistent with a very large mean free path of the conduction electrons of 0.5mm [24]. However, the growth conditions were not very special, so WP_2 is a unique material for quantum properties and devices. MoP is an example of a material with a triple point in addition to the Weyl points close to the Fermi Energy, and is also a highly conductive material with large magneto-resistance effect and large mean free path [25].

The inverted band structure in Half-Heusler compounds LnPtBi (Ln=Lanthanide) (see Fig. 1 a) gives rise to a variety of topological states. GdPtBi turns out to exhibit Weyl fermions via Zeeman splitting of the bands around the Fermi energy and seems to be, from our view point, the ideal material for the investigation of Weyl physics. In GdPtBi several characteristic signatures of Weyl physics, such as the chiral anomaly, an unusual intrinsic AHE, a non-trivial thermal effect and a strong planar Hall effect, as well as a linear dependence of the optical conductivity on the temperature, were observed [26].

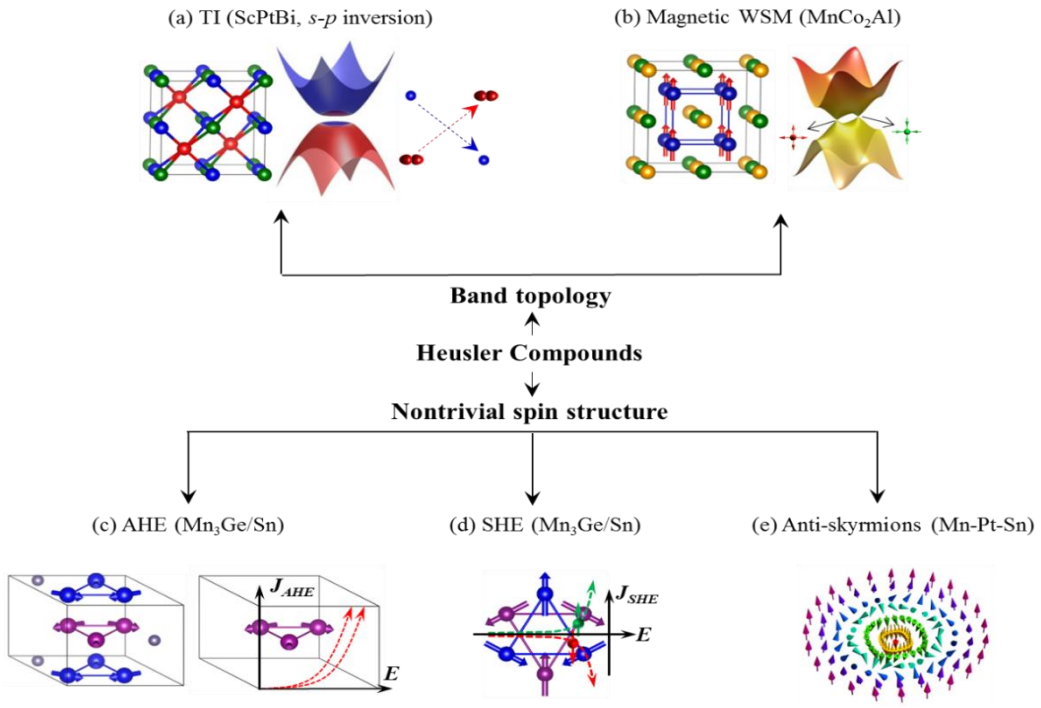

Fig 1: Various topological states realized in Heusler compounds, namely a) topological insulator, b) Weyl semimetal, c) Berry-curvature-induced anomalous Hall effect, and, d) spin Hall effect, and (e) antiskyrmion state [1].

Topological Magnetic Heuslers: Role of Symmetry and Berry Phase (Manna, Gooth, Shekhar, Sun, and Felser)

www.cpfs.mpg.de/ssc/heusler-topo

Heusler compounds are a constantly growing family of materials synthesized from combinations of more than 40 elements, with unique properties, which allows band structures with energy gaps for unexpected valence electron counts and combination of atoms. Most recently, our main emphasis was on Heusler family members which contain heavy elements that can give rise to strong SOC (spin orbit coupling), and thereby to design compounds with non-trivial topological phases of matter, including strong, (Fig. 1 a) and weak topological insulators and Weyl semimetals [27,28] (Fig. 1 b). The various topological properties of Heusler compounds and their connection to symmetry and Berry curvature are described in an invited Nature review article [1]. Already in 2012, a few years before linear crossings in topological semimetals were discussed as the origin of a Berry curvature, Kübler and Felser recognized that in some Heusler compounds a linear crossing leads to an enhanced Berry curvature and a large AHE.

In general, band crossings are common in many band structures but they must be positioned very close to the Fermi energy for the observation of topological physics. Co_2TiSn and Co_2MnGa are examples of half-metallic ferromagnets, for which topological surface states were recently predicted (Fig. 1 b). When bands of opposite eigenvalues cross, a nodal line is formed. Upon incorporating spin–orbit coupling, the electron spin is no longer a good quantum number, and the crystal symmetry changes depending on the

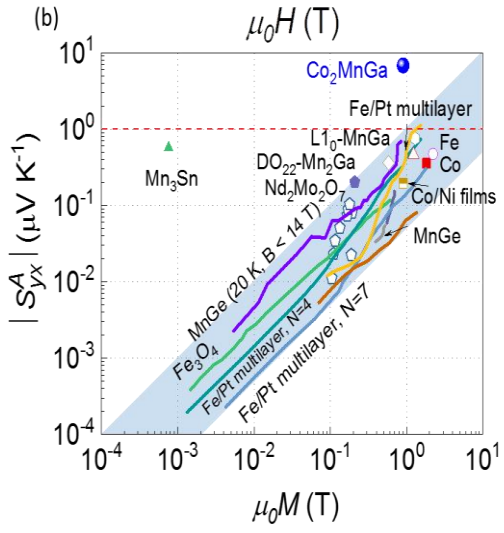

Fig. 2: A compared plot of the magnetization dependent anomalous Nernst thermopower (S_{yx}^{A}) of various ferromagnetic metals. Co_2MnGa single crystals show the highest value of beyond any magnetization scaling relation as highlighted by the blue shaded region.

direction of the magnetization. By applying a magnetic field, the nodal lines can turn into Weyl nodes, leading to an enhanced anomalous Hall conductivity. Co_2MnGa, the first three-dimensional topological magnet, shows one of the highest anomalous Hall conductivities and the highest known anomalous Hall angle [27] in any magnetic Heusler (up to 12% at room temperature). In addition, this compound exhibits a remarkably high anomalous Nernst thermopower, (S_{yx}^{A}) of ~6.0 μV K−1 at 1 T at room temperature [28,] which is beyond the magnetization-scaling relation in any compound reported so far in the literature (Fig. 2).

Through suitable engineering of the composition and thereby the symmetry of Heusler compounds, one can easily tune a half-metallic Weyl semimetal into a spin-gapless semiconductor with the same magnetization. Mn_2CoAl is an inverse-Heusler and has the same number of valence electrons (NV = 26) as the regular-Heusler compound Co_2TiSn. Mn_2CoAl belongs to the special class of materials known as spin-gapless semiconductors, in which the crossing (Weyl points) of the centrosymmetric Heusler structure becomes forbidden and thus an energy gap is possible for a compound made only from metallic atoms. Although the material has a high magnetic moment, the AHC is nearly compensated around the Fermi energy, which is in contrast with the longstanding belief that large magnetic moments always accompany a strong anomalous Hall effect (AHE).

The new topological viewpoint and the high tenability of Heusler compounds make them a rich source for the future discovery of new properties and phenomena. They can also act as benchmark materials for this rapidly developing field. Many of the concepts developed for Heusler compounds can be generalized and directly transferred to other large classes of materials such as double perovskites or Skutterudites [29].

Magnetic Weyl Semimetal (Liu, Sun, Kumar, and Felser)

www.cpfs.mpg.de/ssc/magnetic-weyl

In the family of Shandites with non-collinear spin structures we searched for skyrmions, but instead we found the first magnetic Weyl semimetal, $Co_3Sn_2S_2$, that has a Kagomé lattice of magnetic Co atoms. Since the Weyl points are very close to the Fermi energy, an intrinsic large anomalous Hall effect was observed, owing to the non-zero Berry curvature from the Weyl nodes. Two important signatures of Weyl physics, the

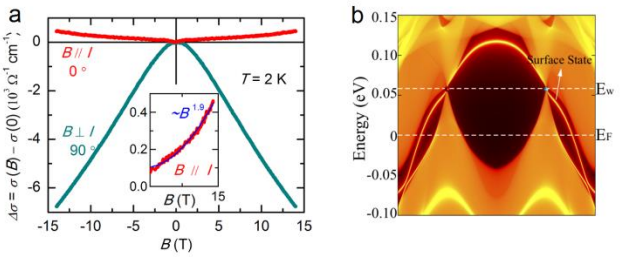

Fig.-3: a) Magnetoconductance at 2 K in both cases of B ⊥ I and B // I. b) Energy dispersion for the Sn-terminated surface along a k-path crossing a pair of Weyl points connected by a Fermi arc.

chiral anomaly and Fermi arcs on the surface were realized in in $Co_3Sn_2S_2$ (Fig. 3).

Additionally, due to the crystal anisotropy, the magnetic moments are oriented out of plane, a precondition for a quantum anomalous Hall effect (QAH). While observing the intrinsic anomalous Hall conductivity and giant anomalous Hall angle experimentally simultaneously, theoretical investigation predicted a QAH in this compound in the 2D limit (monolayer) [13]. The out of plane magnetisation and the relative high Curie temperature of $Co_3Sn_2S_2$ make it an ideal candidate for a high-temperature QAH and for application to spintronics devices.

Non collinear spin structures in Heusler compounds (Nayak, Felser, Kumar, and Shekhar)

Manganese rich Heusler compounds can be distorted along the 111 or 100 direction, resulting in hexagonal or tetragonal structures. For magnetic compounds these anisotropic crystal structures lead to a magnetocrystalline anisotropy and depending on the magnetocrystalline energy, the preferred magnetization orientation can be tuned from in-plane to out-of-plane directions and sometimes stabilizes in a complex non-collinear order. Non-collinear magnetism and evidence for skyrmions via a topological Hall effect were first found in Mn_2RhSn [31]. However, the visualisation of skyrmions is only possible with LTEM or with small angle neutron scattering and the systematic investigation became possible recently in a close collaboration with Stuart Parkin. This real space topological state, the anti-skyrmions was only realized in Heusler compounds with non-collinear magnetic structures and is seen in Mn_2RnSn as well as in a structure with ordered manganese vacancies, $Mn_{1,4}PtSn$ (Fig. 1 e) [2]. The combination of a non-collinear magnetic structure and a reciprocal space Berry curvature realized in

antiferromagnetic Mn_3Sn and Mn_3Ge [17] gives rise to a non-zero anomalous Hall effect (Fig. 1 c and d). The hexagonal distortion of the Heusler structure exhibits a triangular antiferromagnetic (AFM) structure with T_N above 365 K. A non-zero AHE is found only when the magnetic field is applied perpendicular to the *c* axis due to a non-vanishing Berry curvature. The AFM order observed in Mn_3Ge sketched in Fig. 1 d is of negative chirality and, therefore, will necessarily be accompanied by a small ferromagnetic component due to orbital magnetism.

Tunable multifunctional properties in thin films of Heusler and other intermetallic compounds (Markou, Fecher, and Felser)

www.cpfs.mpg.de/ssc/multifunctional

Thin films and devices using Heusler compounds are important for many applications, such as spintronics, including the recent direction of antiferromagnetic spintronics [31], racetrack memory with skyrmions, new permanent magnets etc. Since 2014, our thin film laboratory has been in operation to fabricate and study novel materials (Fig. 4). The morphological, structural, magnetic and magneto transport properties of thin films can be controlled through epitaxial growth and strain engineering, providing a new platform to study novel phenomena also in the quantum limit. With support of theory a fully compensated ferrimagnetic Heusler with a giant coercive field (6T) and a giant exchange bias was synthesised in the bulk [32]. In thin films the same effect could be achieved but then in a well controlled manner [33]. By partially replacing Mn in Mn_3Sn by Pt, the effective moment can be reduced to match to a fully compensated magnetic state. The sign change of the anomalous Hall effect above the compensation point is a further proof of the compensation state through Pt substitution. Thin films of topological materials, the non-collinear Mn_3Sn [34] and Mn_2RhSn [31] and the Weyl metal Co_2TiSn are available for anomalous Hall, Nernst devices and beyond. The project concerning molecular beam epitaxy (MBE) focusses on the QAH effect in Chromium doped Bi_2Se_3.

Fig. 4: (a) UHV cluster tool for the growth and characterization of thin films. (b) Two sputter deposition systems, (c) the MBE and ARPES systems and (d) the UHV scanning probe microscope.

High-pressure studies of topological materials (Medvedev, in collaboration with Felser, Sun)

www.cpfs.mpg.de/ssc/TM-pressure

The combination of pressure with magnetic field is an important external stimulus to probe the proprieties of topological materials. Last year, a miniature diamond anvil cell was designed in-house which can be used to achieve (ultra-) high pressures up to 100 GPa, even for Hall and magneto-resistance measurements. This enables us to measure the fundamental electrical transport properties of topological materials such as their carrier densities, oscillation frequencies, mobilities, and anomalous and topological Hall effects as high as ~100 GPa.

Transition-metal dichalcogenides are an ideal class of materials to study both topological effects and superconductivity under pressure. Ab-initio calculations have shown that Td-$MoTe_2$ is a type II Weyl-semimetal. [9] This theoretical prediction was subsequently confirmed by the experimental observation of Fermi arcs. [10] Our electrical resistivity measurements indicate that the Weyl Td-$MoTe_2$ becomes superconducting below 0.3 K at ambient pressure [35]. Thus, Td-$MoTe_2$ is a rare example of a material with both superconductivity and topologically nontrivial band structure. Further studies showed that the superconducting transition temperature, a

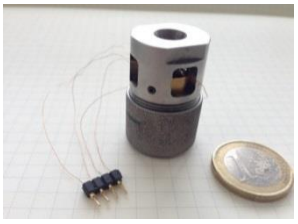

Fig. 5: Custom-designed miniature diamond anvil cell used for studies of structural, optical, magnetic, and electronic properties of materials at pressures up to 100 GPa.

superconductivity, T_c, can be enhanced up to nearly 9 K with pressure. This material exhibits a superconducting dome that is also very sensitive to doping, indicating unconventional superconductivity in Td-$MoTe_2$. In WTe_2, superconductivity can be induced by applying external pressure with suppression of the large magneto-resistance. Here we raise the question of the interplay between the large mobility of the electrons and superconductivity. Superconductivity emerges in $PdSe_2$ at the T_c ~ 14 K under pressure, another topological candidate from the big family of pyrite compounds [36]. With pressure as an additional tuning parameter we will be able to identify other topological superconductors.

Oxides with peculiar electronic and magnetic properties (Adler, Felser, in collaboration with Jansen, Komarek, Merz, and Prasad)

www.cpfs.mpg.de/ssc/oxides

The Functional Oxides group explores oxides with unusual electronic and magnetic properties that are a manifestation of the delicate balance between charge, spin, orbital, and lattice degrees of freedom. An important result was the discovery of a Verwey-type charge ordering transition in Cs_4O_6, a compound with mixed-valence negatively charged oxygen molecules in its crystal structure. Cs_4O_6 shows a structural transition from a cubic charge disordered to tetragonal charge ordered phase with distinct superoxide O_2^- and peroxide O_2^{2-} anions, which is accompanied by a drastic change in electrical conductivity. A similar transition was found for Rb_4O_6, where spin dimerization occurs at low temperatures, possibly driven by orbital ordering. The new layered oxoruthenates(V) with low-dimensional structural features, β-Ag_3RuO_4 and $AgRuO_3$, were synthesized by hydrothermal methods. While β-Ag_3RuO_4 exhibits cluster-like magnetism in the paramagnetic regime and magnetic ordering below 80 K, $AgRuO_3$ apparently lacks any long-range magnetic order despite strong antiferromagnetic exchange interactions.

Topological materials as efficient catalysts for hydrogen evolution reaction (Auffermann, Kumar, Li, and Felser)

www.cpfs.mpg.de/ssc/TM-catalysis

Catalysis is the most important area in chemistry. However, the process of heterogeneous catalysis is complex, and not well understood. One guideline are volcano plots: by plotting the reaction rate against the heat of adsorption of the reactant by the catalyst, Platinum is identified as an exceptional catalyst for redox reactions. Pt also exhibits a large Berry curvature. This observation inspired our approach to search for new catalysts by applying the concept of Berry curvature and topology to catalysis. Topologically protected surface states might have a positive impact on catalysis and also give rise to a stable supply of itinerant electrons at the surface. Semimetals with high mobilities of electrons and holes reduce the probability of recombination of the electron–hole pairs that are created in the redox process. By taking into account spin momentum locking and the chiral anomaly we believe that this might give us a new ways for even more complex catalytic processes. So far we have tested several topological materials such as the Weyl semimetals, 1T'-$MoTe_2$, NbP, TaP, NbAs and TaAs [37]; topological insulators (TI), Bi_2Se_3, Bi_2Te_2Se, Bi_2Te_3 and Sb_2Te_3 [38]; and the triple point metal MoP [39]. A first patent about the magnetic field dependence of catalytic activity has been submitted and several other compounds have already been successfully tested. The theory group is working on a theoretical model for the understanding of our results and collaborations with chemistry groups, Rao, List, and Schlögl have been initiated.

Thermal transport in topological semimetals (Gooth, in collaboration with Fu, Nitesh, Felser, and Shekhar)

www.cpfs.mpg.de/ssc/TS-transport

This topic was already mentioned as a highlight. Considering the richness of physics that electrical transport in topological bulk materials has provided recently, our group seeks to unravel thermal transport signatures of new emergent quantum phenomena in topological semimetals. Within the last three years, we have designed and built high-resolution thermal transport measurement equipment with sub-mK temperature resolution for bulk-, nano- and micro-structures that can be operated in the temperature range from 1.8 to 400 K and up to 9 T magnetic fields. Using this equipment, we have observed signatures of the mixed axial-gravitational anomaly in the Weyl semimetal NbP [4], hydrodynamic electron flow at the Planckian bound of dissipation WP_2 [40] and of the electron-phonon fluid in $PtSn_4$ [41].

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MPRG: Physics of Unconventional Metals and Superconductors

Group leader: Elena Hassinger

The MPRG's research concentrates on unusual ground states appearing in quantum materials at low temperature. We study materials called strongly correlated electron systems, where electrons interact with each other leading to emergent many-body phenomena. The second material class of interest to us are topological semimetals. In these, the bulk electrons behave as relativistic fermions due to their characteristic band structure and our aim is to observe their specific experimental signatures.

My group has specialized in the detection of quantum oscillations in metals. These oscillations are a direct consequence of the quantization of the electron orbits in a magnetic field. We measure thermodynamic and transport probes such as magnetization, torque or resistivity in which oscillations appear. However, their detection requires extremely pure materials and low noise detection methods. Hence, our working philosophy is to do careful measurements at low temperature and in high magnetic fields on clean metals. Once detected, quantum oscillations give information on the scattering processes and the interactions between charge carriers in the metal.

We apply this powerful technique but also standard low temperature probes to a variety of scientific problems as detailed below. In the following, I briefly summarize our group's main scientific achievements from the last 3 years.

Weyl semimetals (collaboration with M. Schmidt, B. Yan, M. Nicklas and C. Felser)

www.cpfs.mpg.de/has/weyl-FS

Chirality and topology of the Fermi surface

Weyl fermions are relativistic particles, first predicted as a solution of the Dirac equation when the mass of the fermion is zero. While lacking a realization as a free particle, their presence is predicted as fermionic excitations in metals when bands cross at points in reciprocal space, called Weyl nodes. In this case, the material is a topological semimetal, and a number of special signatures are predicted that differentiate Weyl fermions from normal electrons. Surface sensitive techniques such as angle resolved photo emission spectroscopy have proven their existence.

One important goal of my group is to find experimental signatures of Weyl fermions in bulk probes. A crucial precondition for the experimental detection of Weyl fermions is that the nodes need to be close to the Fermi energy. The best Weyl semimetal candidates where this energy difference is small are TaAs, TaP, NbAs and NbP. In the two first materials, we have established the Fermi surface via quantum oscillations and hence were able to determine the proximity of the band crossing points to the Fermi energy[1,2]. In TaP, the Fermi energy is so far from the nodes that chirality, a required property of Weyl fermions based on their spin structure, is not well defined. Therefore, the chiral anomaly is not expected in this compound.

In TaAs in contrast, our study revealed that chirality is well defined. This situation is equivalent to each Weyl node of a pair being surrounded by one Fermi surface pocket (see W1 and W2 pocket pairs in Fig. 1). With these studies, we have identified TaAs as the best

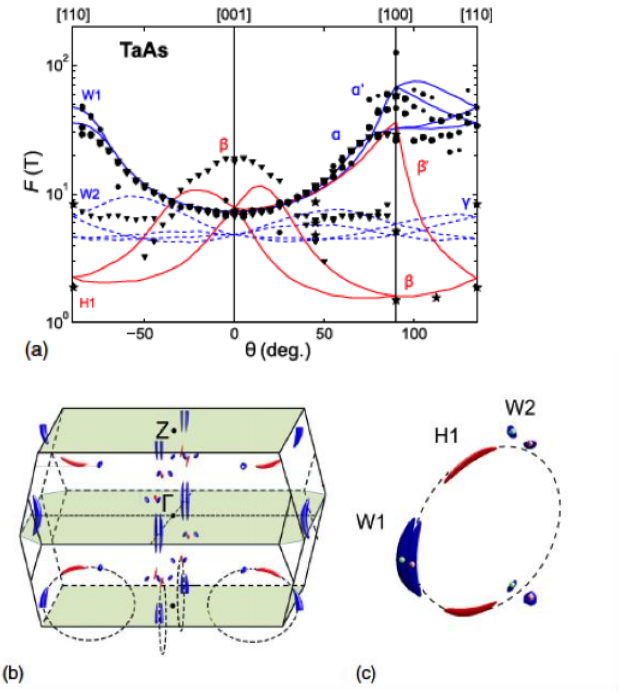

Fig. 1: a) Angular dependence of quantum oscillation frequencies in TaAs from magnetization, torque and resistivity data (stars, dots and triangles) and from band structure calculations (lines). b) Brillouin zone with resulting Fermi surface. C) Zoom on one element of b) with the three types of Fermi surface pockets [2].

candidate to date to study Weyl fermion physics in semimetals.

Longitudinal magnetoresistance of semimetals
The chiral anomaly is one of the main experimental signatures predicted for Weyl fermions. In Weyl semimetals it should induce a negative magneto-resistance, when the magnetic field and the current through the sample are parallel. However, our group has realized that this type of signal is often an artifact in this experimental configuration, caused by the extreme field-induced resistivity anisotropy typical for any compensated semimetal [1,3]. This brings into question published results which interpret the negative magnetoresistance as a sign of the chiral anomaly in Weyl semimetal candidates.

Fermi surface of delafossite metals (collaboration with Mackenzie)

Metallic delafossites are materials which show intriguing properties revealed over the past years. This includes ultra-high conductivity, unconventional magnetism, and hydrodynamic electron flow. Metallic delafossites have a structure consisting of triangular layers of transition metal atoms separated by nearly insulating oxide layers. Therefore, they are quasi 2-dimensional electron systems with an extremely large conductivity in the transition-metal layers barely influenced by the insulating oxide layers. The Fermi surface consists of cylinders with hexagonal cross sections. However, the interactions with the oxide layer influence the conductivity in and perpendicular to the plane and accordingly the Fermi surface shape. Our precise measurement of the Fermi surface *c*-axis dispersion allows for a closer understanding of these interactions in different materials of this family [4,5].

Unconventional superconductivity (collaboration with Leithe-Jasper, Grin, Moll and Mackenzie)

www.cpfs.mpg.de/cms/beryllium-compounds

Unconventional superconductivity remains one of the most intriguing phenomena in condensed matter physics. New pairing mechanisms and unconventional pairing symmetries are still actively sought. We have contributed to this area in three different materials.

Primarily, via directional thermal conductivity measurements carried out in the Taillefer lab in Sherbrooke, we showed that Sr_2RuO_4 has vertical line nodes [6]. This nodal structure is of strong relevance as it is *a priori* in contradiction with expectations of the chiral *p*-wave superconducting state proposed in this material.

An outstanding candidate for unconventional superconductivity is the material UBe_{13} since the superconducting state evolves out of a non-Fermi liquid state. However, crystal quality in this compound has always hindered a determination of the intrinsic properties and hence the physical understanding of this superconductor. Colleagues in Juri Grin's department are working on a new generation of higher purity crystals. In a first step, we have characterized how aluminium impurities and annealing affect the physical properties of single crystals, namely the specific heat, the lattice parameter and the lattice itself [7].

We also contributed to a recent study led by the group of Philip Moll on strain-influenced superconductivity in CeIrIn5 single crystals. Due to the small size of the microstructured samples, low-noise measurements in our cryostat were necessary to exclude a shift of the superconducting transition temperature T_c caused by noise-induced heating.

Development of a SQUID-amplified low noise torque magnetometer (collaboration with Mackenzie)

www.cpfs.mpg.de/has/squid

Since the start of our group we have successfully installed a new powerful dilution refrigerator with a 15/17T magnet. In this cryostat, we have set up a SQUID-based low noise torque magnetometer [8]. The main achievement was to make use of the SQUID as a low temperature amplifier for measurements up to magnetic fields of 15 T. With this technique, we were able to improve the experimental resolution for the detection of quantum oscillations via magnetic torque by one order of magnitude at temperatures below 1 K.

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MPRG: Microstructured Quantum Matter

Group leader: Philip J.W. Moll

Our group's main research interest is to experimentally probe exotic electronic phenomena in quantum materials and to understand how quantum mechanics can give rise to new electron behavior far from that of free electrons that so successfully describe the band structure of copper or silicon. Examples could be metals with strong electronic correlations, unconventional super-conductors, and topologically non-trivial semi-metals. We employ Focused Ion Beams (FIB) to fabricate crystalline microstructures from high quality crystals or powders of these quantum materials. Our ultimate goal is total control over the shape of highest quality crystals on the sub-micron-scale. We aim to explore theoretical predictions of new electronic behavior in innovative ways, and we can also test a material's performance in electronic applications in prototype devices, mimicking their potential future use in electronic circuits.

In the following, we highlight three ongoing research projects; others are described at www.cpfs.mpg.de/mol/CeIrIn5, www.cpfs.mpg.de/mol/gate and www.cpfs.mpg.de/mol/weyl-fermion-extreme.

Unidirectional superconductivity in $CeIrIn_5$

Since its discovery two decades ago, the heavy-fermion superconductor $CeIrIn_5$ has harbored a mystery: while thermodynamic probes such as specific heat detect a superconducting transition at T_c~0.4K, all crystals exhibit a zero resistance state starting at temperatures as high as T_c*~1.2K~3T_c. Different mechanisms for the origin of the so-called "1K-phase" have been discussed in the field, involving, for example, structural defects, surface effects, internal strain, or strong superconducting fluctuations.

In collaboration with the Los Alamos National Laboratory, we have investigated the transport properties of $CeIrIn_5$ on the micron-scale by FIB-sculpting highest quality microstructures from single crystals grown using standard methods. This technology enables us to access transport properties along different crystallographic directions. Surprisingly, in dozens of experiments we have observed a unique, so far not understood phenomenon: The resistance in the "1K" phase is zero only for currents along the crystallographic c-direction of the tetragonal $CeIrIn_5$, while the transport along the Ce-layers remains metallic (Fig. 1) [1].

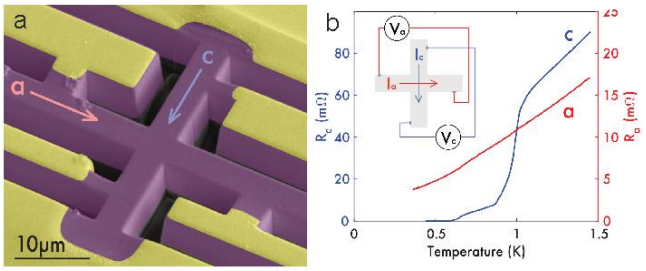

Fig. 1: A) Single crystal microstructure of $CeIrIn_5$. The cross-arrangement allows to microscopically probe for zero resistance along both a and c directions simultaneously. B) The resistance clearly shows a drop to zero at much higher temperatures for the c-direction compared to a.

This unexpected result defies the usual understanding of superconductivity and is a central topic of multiple ongoing collaborations. With Dr. Tobias Meng at TU Dresden, we explore theoretical models based on anisotropic hybridization of the Ce-4f1 state with an isotropic Fermi liquid as a possible origin of directional superconducting pairing and its relationship to the high field electronic nematic state that we have observed in the related compound $CeRhIn_5$ [2]. Together with Prof. Katja Nowack and Prof. Brad Ramshaw at Cornell University, we explore the microscopic evolution of the superconducting order parameter by combining our microfabrication technology with state-of-the-art scanning SQUID measurements. Furthermore, we aim to investigate the anisotropic sound velocity in $CeIrIn_5$ by pulse echo measurements, thus potentially providing evidence for a thermodynamic character of this phase.

Our research is also motivated by technological applications. Despite the microscopic mechanisms not being understood yet, the remarkable materials property discovered here is of strong interest for applications in quantum technology. A material with "quasi-one-dimensional" phase coherence may be used as a polarization filter, or tunable non-linearities. The latter we explore in a project with Prof. Ian Pop at KIT,

fabricating the first operating qbits from heavy fermion matter which exploit this unidirectionality.

Resonant torsion magnetometry

Our main motivation is to gain a complete understanding of quantum materials on the micron-scale. We are pioneering transport experiments based on Focused Ion Beam machining, however in many cases the complex nature of materials cannot be deciphered by resistance measurements alone. To close this gap, our group works actively on the development of novel experimental techniques to provide complementary, thermodynamic information about micron-sized samples.

In a recent project, we have developed a new method we call "resonant torsion magnetometry". This technique is the dynamic analogue of static torque magnetometry, and their relation is akin to that of static magnetization and ac-susceptibility measurements. A standard magnetometer probes $M = \partial F/\partial H$, while susceptibility measurements detect the derivative $\chi = \partial^2 F/\partial H^2$, where F denotes the free energy. Similarly to the magnetometer, standard magnetic torque detects the torque exerted onto an anisotropic single crystal when a magnetic field H is applied at an angle θ off a direction of symmetry. Accordingly, the torque is given by $\tau = \partial F/\partial\theta$. The associated torque susceptibility $k = \partial^2 F/\partial\theta^2$, however, has not been observed.

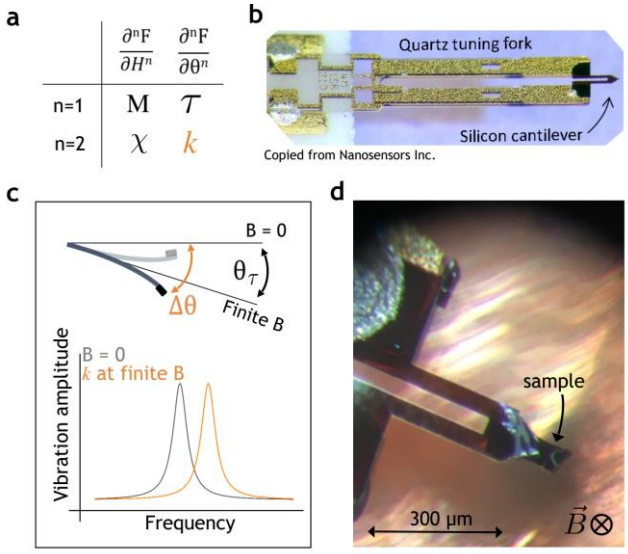

Fig. 2: A) The thermodynamic meaning of the magnetotropic coefficient k. B) Image of the coupled Si cantilever and the quartz tuning fork. C) Sketch of a typical resonant torsion experiment. D) Image of a microcrystal of a Weyl Semi-metal loaded onto the cantilever.

In our approach, a micron-sized single crystal is mounted onto a silicon cantilever coupled to a quartz tuning fork. The oscillation of the cantilever leads to a dynamic modulation of the field angle, θ, and the coefficient k can be conveniently detected as a frequency shift of the electrical resonance [3].

This technology rivals the resolution of SQUID magnetometers, while the commercially available cantilevers are very cheap (60€). We collaborate with the National High Magnetic Field Laboratory in Tallahassee, USA, to combine this new technology with high static and pulsed magnetic fields.

Ballistic flow in hexagonal Fermi surfaces

In a collaboration with PQM (Andy Mackenzie) and David Goldhaber-Gordon (Stanford) we explore the intriguing features of ultra-clean metals with hexagonal Fermi surfaces, building on our existing collaboration on electron hydrodynamics [4]. Ballistic transport occurs when the mean-free-path of the electrons is much larger than the device dimensions, such that the dominant source of scattering occurs at the boundaries. The stringent requirements on material perfection to achieve this regime have thus far be realized in graphene and semiconductor-heterostructures, which both are characterized by isotropic Fermi surfaces (=circular).

We have discovered that $PdCoO_2$ single crystals can also be FIB-structured to reach the ballistic limit. Unlike all previous materials, it hosts a hexagonal Fermi surface. As the electron group velocity is perpendicular to the Fermi surface, this implies that there are three directions of predominant electron motion, set by the triangular arrangement of the Pd atoms. This strongly modifies the ballistic behavior, and introduces strong crystalline anisotropy into the ballistic regime for the first time.

We study the fundamental physics of this unexplored transport matter, and work on potential applications. In particular, the preferential orientation is expected to lead to highly collimated electron beams which is an essential prerequisite for free-electron optics in a solid.

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Emeritus research group Inorganic Chemistry

Director Emeritus: Rüdiger Kniep[#]

Otoconia: A personal conclusion

The emeritus position at our institute was finished in May 2016. Then, a number of experimental data was still available, opening the chance to broaden the view on otoconia and their function.

The topic "otoconia" came up more or less accidentally, when calcite-based nanocomposite particles (µm-sized) were obtained by double-diffusion techniques in gelatine-gel matrices: An unexpected result in the course of our running activities in biomimetic apatite-gelatine-nanocomposite superstructures, ten years ago from now.

The outer shape of the calcite-based composite particles already indicated a significant relationship to a biomineral which is present as an array of thousands of tiny specimens in the inner ear of vertebrates (called otoconia; Greek: ear-dust; µm-sized), and which is considered to act as gravity receptor system responding to linear accelerations (control of balance). Detailed investigations in biomimetic specimens and biogenic (human) otoconia finally revealed that biomimetic otoconia represent the very first example for successful imitation of a biomineral, not only in outer shape but also in composite structure and hierarchical inner architecture (new and unknown data also for human otoconia at that time!).

The inner architecture of otoconia is characterized by 3+3 dense rhombohedral (wedge-shaped) branches with plane end-faces and a rounded more porous belly area. X-ray diffraction patterns (Bragg-part) of otoconia are representative for calcite single crystals. The wedge-shaped branches meet at a common point close to the center of the specimen. The branches include protein-fibrils in parallel arrangement which leave the composite volume perpendicular to the end-faces and which enable interconnections of the otoconial array in the inner ear [1].

The overall symmetry of otoconia is close to -3m. Considerable differences between the sizes of the rhombohedral faces of otoconia, however, already indicate that the inner architecture is not consistent with point-group -3m. In fact, otoconia are characterized by a non-centrosymmetric mass distribution within their volumes, as impressively demonstrated by rotational movements of single otoconia under gravitational influence within a viscous liquid medium. Moreover, the response of otoconia to linear acceleration forces was investigated by particle dynamics simulations, revealing that the dislocation of non-centrosymmetric otoconia includes significant tilting (rotation) which is not the case for centrosymmetric specimen. Thus, non-centrosymmetry leads to increased signal strength which is directly transmitted within the sensory system (balance) [2].

A final point concerns the question, whether magnesium is an intrinsic component of human otoconia, a subject which is not trivial. The biomineral can hardly be prepared in an absolutely pure form which allows to specify minor- and/or trace-elements as intrinsic components belonging to the complex otoconial composite system. We were lucky to solve the problem, not least because of our detailed knowledge on the growth conditions of "artificial" otoconia and, in addition, because of our crystal structure determinations of human (containing Mg?) and biomimetic (e. g. zero Mg!) otoconia. To make a long story short, our experimental data were consistent with substitutional effects on the Ca-site of calcite ($Ca_{1-x}Mg_x$) extending within the limits $0 \leq x \leq 0.05$. At the same time, we were able to grow biomimetic otoconia within this substitutional limit which were more elongated than the bulbous specimens ($x = 0$; aspect ratio length/diameter ~1.3), and which reached the aspect ratio of ~1.8 which is close to that of human otoconia (aspect ratio 1.8 - 2.2) [3]. This kind of "morphological stretching" is connected with separation of the density distribution along the "trigonal" axis of otoconia, and is assumed to be responsible for even stronger tilting (rotation) of otoconia by linear acceleration forces (see [2]).

It was great fun to learn about steps and principles of evolution. Sincere thanks to the Max Planck Society and the MPI-CPfS in Dresden.

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Emeritus research group Solid State Physics

Director Emeritus: F. Steglich

Within the last period, two review articles with S. Wirth were published on "Exploring heavy fermions from macroscopic to microscopic length scales" [1] and "Foundations of heavy-fermion superconductivity: lattice Kondo effect and Mott physics" [2]. Another article, coauthored by P. Gegenwart (EKM, U. Augsburg), C. Geibel and M. Brando [3], reviewed quantum criticality. In fact, a substantial part of our research was related to the interplay between unconventional superconductivity (SC) and quantum criticality. According to the so-called quantum critical paradigm, antiferromagnetic (AF) quantum critical points (QCPs) in clean, stoichiometric heavy-fermion metals should give rise to unconventional SC. The validity of this paradigm was supported by the very recent observation, made together with the groups led by H.Q. Yuan (CCM, ZJU, Hangzhou, China) and Q. Si (RCQM, Rice U., Houston, USA), that below $T_c \simeq 0.6$ K $CeCu_2Si_2$ with a conventional itinerant (3D spin-density-wave) QCP is a fully gapped, two-band *d*-wave superconductor [4]. Two-band SC of this material was also concluded from STS measurements by P. Wahl's group from the University of St Andrews, UK, in collaboration with S. Wirth et al. [5]; see also the work by S. Kittaka and T. Sakakibara (ISSP, U. Tokyo, Japan) as well as H. Ikeda (U. Kyoto) and K. Machida (Okayama U.) et al. [6]. For the isostructural heavy-fermion compound $YbRh_2Si_2$ with AF order below $T_N = 70$ mK, no SC could be found down to 10 mK. Here, the AF QCP is located at a very small external field of 60 mT, when applied within the basal tetragonal, easy magnetic, plane. For signatures of phase transitions in the microwave response of this material, see the recent work by M. Scheffler and M. Dressel (U. Stuttgart), in collaboration with C. Krellner (U. Frankfurt) and C. Geibel [7,8]. $YbRh_2Si_2$ is the prototype material exhibiting an unconventional Kondo-destroying QCP. For an overview of this surprisingly "local" QCP, cf. the recent paper with S. Paschen (TU Vienna, Austria), S. Friedemann (U. Bristol, UK), S. Wirth, S. Kirchner (ZJU, Hangzhou, China) and Q. Si [9]. Ultra-low temperature measurements by E. Schuberth (WMI, TU Munich) were performed on $YbRh_2Si_2$ single crystals with the aid of a nuclear demagnetization fridge. The subsequent analysis of the field-cooled (fc) and zero-field-cooled (zfc) dc-magnetization as well as specific-heat results revealed the formation of a nuclear 4*f*-electronic hybrid AF order (dominated by the Yb nuclear spins) slightly above 2 mK. It strongly competes, and eventually suppresses, the primary 4*f*-electronic order, i.e., pushes the system very close to, or even at, it's (Mott-type) QCP. This way, heavy-fermion, i.e., unconventional, SC can develop at $T_c = 2$ mK, as displayed by large diamagnetic jumps in the *T*-dependence of both ac-susceptibility and zfc dc-magnetization measurements [10,11]. These findings lend further support to the validity of the quantum critical paradigm.

In collaboration with S. Wirth, S. Rößler and H.L. Tjeng a new kind of density-wave order was found for the crystallographically simplest Fe-based superconductor FeSe [12]. A joint project with M. Nicklas, H. Pfau and the groups of Yu. Grin and H.Q. Yuan was devoted to the very weak multiband behavior of the *s*-wave skutterudite superconductor $LaPt_4Ge_{12}$, which was studied via penetration-depth, transverse-field μSR, specific-heat and thermal-conductivity measurements [13]. In addition, for both (centrosymmetric) $LaNiGa_2$ and (non-centrosymmetric) $LaNiC_2$, time-reversal symmetry (TRS) breaking below $T_c = 8.3$ K was observed in zero-field μSR, as contrasted to a fully developed gap concluded from thermodynamic probes. This seeming contradiction could be resolved, in close collaboration with H.Q. Yuan's group, M. Nicklas and theoreticians J. Quintanilla (Kent U., UK) and J.F. Annett (U. Bristol, UK), by analyzing results of low-*T* penetration-depth and specific-heat as well as upper-critical-field experiments, which revealed two-gap SC with a non-unitary spin-triplet state and even-parity gap symmetry. This suggests the possibility of TRS breaking SC mediated by phonons [14].

Bose-glass behavior in the randomly diluted quantum spin-1/2 system $(YB_{1-x}Lu_x)_4As_3$ [15], disorder-avoided QCPs of ferromagnetic nature in the 3*d*-electron material $Fe(Ga_{3-x}Ge_x)$ [16] and the 4*f*-electron compound $Ce(Pd_{1-x}Rh_x)$ [17], frustration-derived localization of the 4*f*-electrons in CePdAl [18], studies of the Nernst effect for the intermediate-valence compound YbA_{l3} [19] as well as the interplay of electronic correlations and topological effects in the low-carrier density, Kondo-like system CeSb [20], the rare-earth-based

monobismuthites [21] and the potential topological Kondo insulator SmB_6 [22,23] as well as the nodal Kondo insulator CeNiSn [24] have been in the focus of various multilateral activities. They include coauthors G. Kamieniarz (U. Poznań, Poland), P. Gegenwart, M. Baenitz, Yu. Grin and his team members, U. Stockert, C. Geibel, Y. Isikawa (U. Toyama, Japan), J.L. Luo, P. Sun and his students (IOP, CAS, Beijing, China), H.Q. Yuan, Y. Liu and their collaborators, F.C. Zhang (Kavli Institute for Theoretical Sciences; Beijing, China), C. Cao (Hangzhou Normal U., Hangzhou, China) L. Jiao, S. Wirth, U. Stockert, T. Takabatake (Hiroshima U., Japan), P. Coleman (Rutgers U., USA) and S. Paschen.

Last but not least, the continuing synergistic efforts between chemistry and physics at the MPI CPfS led to further joint works on cage compounds, i.e., the clathrates $Ba_8Ni_xGe_{46-x-y}\square_y$ [25] and $BaGe_5$ [26] together with Yu.Grin and his group members. An anomalous magnetic-field-independent term, $\sim (-A\sqrt{T})$, in the low-T electrical resistivity of the ternary intermetallic compound $ZrAs_{1.58}Se_{0.39}$ with PbFCl structure, synthesized and characterized by M. Schmidt, A. Czulucki, G. Auffermann and R. Kniep in collaboration with R. Niewa (U. Stuttgart), was detected by T. Cichorek and L. Bochenek (INTiBS, PAN, Wrocław, Poland). This could be ascribed, with the essential help by S. Kirchner (at that time at MPIs PKS & CPfS), to a non-magnetic two-channel Kondo effect which has never been observed in bulk materials before [27]. The excitations of the involved "quantum impurities" are especially strong pair breakers, cf. an investigation of homologous zirconium pnictide chalcogenide single crystals by M. Baenitz and K. Lüders (Free U., Berlin) in collaboration with R. Kniep and M. Schmidt [28].

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Quantum Devices

Max Planck Fellow Group

Laurens Molenkamp[#]

Professor Laurens Molenkamp joined the Institute as a Max Planck Fellow on 1 January 2018. Our collaborative work is therefore still at the planning stage, but good initial progress has been made. One of the major areas of overlap will be with the Solid State Chemistry department, and a post-doctoral scientist will be appointed to set up molecular beam epitaxy in Dresden under the joint supervision of Molenkamp and Felser.

Joint work is also planned with the Physics of Quantum Materials department. Two graduate students, Abu Alex Aravindnath and Arya Thenapparambil, have been recruited to work on joint projects on electronic hydrodynamics (with the Mackenzie group) and strain tuning of semiconductor heterostructures (with the Hicks group). Both will arrive in late summer 2018, and will split their PhD research time between Würzburg and Dresden. We hope that on both joint projects, we can bring together shared interests and complementary technical expertise. We have held several productive and enjoyable all-day meetings discussing an adventurous programme of future experiments, the implementation of some of which has already begun.

Chemistry of Metal-Rich Compounds and Topological Insulators

Max Planck Fellow Group

Michael Ruck[#]

Our group has its main affiliation at the TU Dresden and comprises besides the author of these lines the independent researchers Alexey Baranov, Thomas Doert, Kati Finzel, Anna Isaeva, and Maria Roslova. We are convinced that the synthesis of new compounds and the growth of high-quality samples is indispensable for innovation in fundamental materials research. For these purposes we on one hand optimize conventional high-temperature syntheses[1], such as crystallization from the melt or chemical gas-phase transport reactions, and, on the other hand, explore the potential and the mechanisms of alternative approaches to access inorganic materials at moderate temperatures between 20 and 250 °C. Among the latter are reactions in ionic liquids[2-5], the microwave-assisted polyol process[6-8], hydroflux syntheses, and post-synthetic topotactic transformations. We then characterize the obtained samples chemically and structurally before we explore their physical properties in close collaboration with colleagues from physics. The experiments are rounded off with calculations of the electronic structure and analyses of chemical bonding[9,10], to which we also contribute with methodical developments[11,12].

On the materials side we have special interest on metal-rich compounds that exemplify the continuous transition from localized to delocalized chemical bonding, or in other words, from the semiconducting to the metallic state. We thereby focus on compounds formed by the electron-rich heavy elements from the sixth period of the periodic table, because their protruding orbitals make multi-center bonding an attractive alternative to two-center bonding. To further influence the degree of electronic localization we introduce heteropolarity (ionicity) by adding highly electronegative elements (halogens or chalcogens)[13].

Many of the intermetallic and subvalent compounds that we made proved to be quantum materials, for example superconductors[14] or topological insulators (TIs)[15-20]. Among the currently discussed topological materials TIs have the most obvious potential for application in spintronics and quantum computing. Electrons in their topological surface states are protected against backscattering and the spin is locked to the propagation direction. Unfortunately, the number of known TIs is rather limited, in particular when going beyond theoretical predictions. The rareness arises from the fact that a proper TI material has to fulfill several criteria simultaneously, among which are a sizeable non-trivial band-gap at the Fermi level opened by strong spin-orbit coupling, chemical and thermal stability, non-toxicity, and the availability of larger quantities. We are happy that most of our TIs possess all these qualities. In total, we contributed to five families of TIs: (A) $Bi_{14}Rh_3I_9$ and variants thereof [15, 16], (B) Bi_nTeX (n = 1, 2, 3; X = Br, I) [17, 18], (C) $Bi_{2n}MnTe_{3n+1}$ (n = 1, 2, 3), (D) $QXTe$ (Q = Ga, In; X = Ge, Sn) [19], and (E) Bi_4X_4 (X = Br, I) [20]. The families A to D have layered crystal structures (Fig. 1), which opens the opportunity to delaminate them into thin layers that are required for technological application. Hence the development of appropriate wet-chemical exfoliation procedures is a new aspect in our research.

Moreover, we contributed to diverse fields of materials and inorganic chemistry, for example by providing

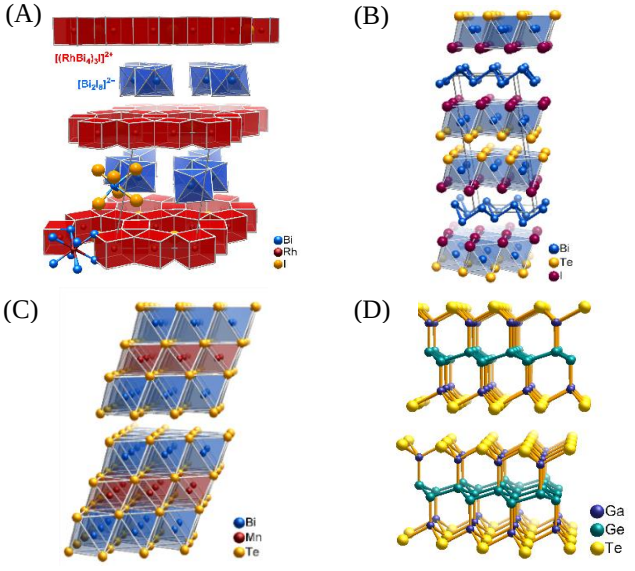

Fig. 1: Crystal structures of our layered TIs: (A) $Bi_{14}Rh_3I_9$ with intermetallic honeycomb nets of $[MBi_{8/2}]$ cubes (2D TIs) and iodidobismuthate chains (trivial spacer), (B) Bi_2TeI with alternating bismuth and [TeBiI] layers (both 2D TIs), (C) two of the seven-atomic magnetic TI layers in Bi_2MnTe_4 and (D) two of the six-atomic TI lavers in GaGeTe.

high-quality samples for the investigation of the frustrated magnetism of the Kitaev-Heisenberg magnet α-$RuCl_3$ [21], or by the discovery and characterization of the triply deprotonated acetonitrilide anion CCN^{3-} (in cooperation with Peter Höhn) [22].

Our group is participating in the collaborative research center SFB 1143 "Correlated Magnetism: From Frustration to Topology", in the research training group GRK 1621 "Itinerant Magnetism and Superconductivity in Intermetallic Compounds", in the priority programs SPP 1666 "Topological Insulators: Materials – Fundamental Properties - Devices" and SPP 1708 "Material Synthesis near Room Temperature", as well as in the International Max Planck Research School for Chemistry and Physics of Quantum Materials (IMPRS-CPQM). In the past three years we celebrated nine successful doctoral examinations and one habilitation. From 2015 to 2017 the author has served as vice-rector for structure and development of TU Dresden.

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Collaborative (inter-departmental/group) research activities

In the years 2015 (from May 1), 2016, 2017, and 2018 (until April 30) we have 844 peer reviewed publications, of which 157 involve authors from two or more different departments/research groups, i.e. about 20% percent of our publications are based on collaborations between scientists from different departments/research groups. Joint projects benefiting from cross-disciplinary expertise are part of our Institute's strategy and mission, so we give some prominent examples in this section of our report, highlighting their collaborative nature.

1.11.1. Superconducting and magnetic properties of Fe-chalcogenide materials (Physics of Correlated Matter, Chemical Metals Science, Physics of Quantum Materials)

In recent years, we perfected the growth of Fe-based chalcogenide materials. The excellent quality of the so-obtained single crystals allowed us to study the superconducting properties of FeSe in detail [see, e.g. 1, 2]. The structure of the superconducting gap, and hence the underlying detailed mechanism for superconductivity in FeSe, is still controversially discussed. Our scanning tunneling spectroscopy (STS) results clearly indicate the exsistence of at least two superconducting gaps and can be represented by a phenomenological two-band model. The "U"-shaped tunneling gap favors anisotropic nodeless models for describing superconductivity in FeSe [1]. We also observed a pair-breaking effect induced by non-magnetic impurities which is a hallmark of a sign-changing pairing state, likely of $s^{\pm}$ symmetry, in this material. Our STS results, along with magnetotransport measurements at temperatures above the superconducting transition (T_c ~ 8.5 – 9 K), reveal an incipient order setting in at around 25 K that appears to be associated with enhanced spin fluctuations resulting from a coupling between charge, orbital or pocket degrees of freedom [2]. These fluctuations commence at ~75 K. Both temperature scales can only be observed in samples of sufficiently high quality.

Although bulk $Fe_{1+y}Te$ does not exhibit superconductivity, it features a rich interplay of localized and itinerant magnetism and is expected to help understanding the relationship between magnetism and superconductivity in FeSe. Indeed, we observed magnetostructural phase transitions upon variation of temperature, composition or pressure in $Fe_{1+y}Te$. Based on a phenomenological Landau theory, we predicted the presence of liquid-like mesophases as precursors in $Fe_{1+y}Te$ with $y \geq 0.11$ [3]. Evidence for such magnetic precursors was found in Mössbauer spectroscopy [3]. Interestingly, upon applying pressures of 2.29 GPa and higher to $Fe_{1.08}Te$, a symmetry-conserving tetragonal–tetragonal phase transition was found [4]. Electronic-structure calculations indicate this symmetry-conserving transition from paramagnetic to ferromagnetic state to be a rare example of an electronic topological transition under pressure in a 3*d* system.

www.cpfs.mpg.de/pcm/FeSe-Wirth-Schwarz

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1.11.2. Heavy fermion materials (Physics of Correlated Matter, Physics of Quantum Materials, Solid State Physics)

Heavy fermion quantum criticality and superconductivity is at the focus of our research. Two extensive review articles have been published in renowned journals discussing the foundations of heavy fermion physics [5] and heavy fermion superconductivity [6].

Scanning tunneling spectroscopy on the first heavy fermion superconductor $CeCu_2Si_2$ [7] revealed a superconducting gap which is not completely formed and is indicative of a multigap order parameter. Moreover, in magnetic fields the vortex lattice could be visualized which allowed to unambiguously link the observed conductance spectra to superconductivity.

www.cpfs.mpg.de/pcm/HF-Wirth-Steglich

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1.11.3. Novel osmates and other transition metal oxides (Solid State Chemistry, Physics of Correlated Matter)

In recent years there has been an explosion of interest in the properties of Ir containing oxides, but much less work has been done on osmates which are harder to synthesis but reveal equally fascinating properties, e.g.

superconductivity in AOs_2O_7 (A = Cs, Rb,and K), metal-insulator transitions in $NaOsO_3$ and $Cd_2Os_2O_7$, and ferrimagnetism with very high T_C in Sr_2CrOsO_6.

We decided to develop a programme of synthesis of novel osmates. The Os valence can be 4+, 5+ and 6+, thereby giving possibilities for singlet magnetism ($5d^4$- $J_{eff}=0$), spin-only magnetism ($5d^3$ - $S=3/2$), and magnetism with orbital degrees of freedom ($5d^2$ - $S/J_{eff}=1$; $5d^1$ - $S/J_{eff}=1/2$), assuming an octahedral-like coordination of the Os ions in an insulating compound.

We started our project with preparing and studying the osmates in the double perovskite structure. This allows for a systematic investigation of the relative importance of the various interactions involved, as the double perovskite matrix $AA'BB'O_6$ enables us to probe a wide range of compositional modifications with corresponding structural variations. The results for Os^{5+} $5d^3$ containing double perovskites [8] revealed, among other things, that details of the distortions in the crystal structure do matter for the balance between the relative strengths of the various superexchange interactions and, enhanced by the presence magnetic frustration due to the crystal structure, ultimaltely for the emerging magnetic behavior.

We have also investigated the synthesis of Os oxides with other crystal structures. We found high temperature ferrimagnetism in a hexagonal perovskite $Ba_2Fe_{1.12}Os_{0.88}O_6$, [9] and the presence of frustrated magnetism between Os-Os dimers in $Ba_3Os_2O_9$ and also in $Ba_3CuOs_2O_9$/ $Ba_3ZnOs_2O_9$.

Recently, it has been proposed experimentally and theoretically that Ir^{5+} systems may host unconventional excitonic magnetism. We have therefore synthesized and investigated the magnetic properties of the double perovskite $SrLaBIrO_6$ (*B* = Ni, Mg, Zn) [10]. They crystallize isotypically in the monoclinic space group and the polycrystalline samples show semiconducting behavior. $SrLaNiIrO_6$ turned out to be an antiferromagnet with a Neel temperature of 74 K. The remaining two compounds containing the closed shell ions Mg^{2+} and Zn^{2+} show a weakly paramagnetic behavior. All compounds exhibit a large, temperature-independent susceptibility contribution, which can be ascribed to the van-Vleck type paramagnetism expected for octahedrally coordinated Ir^{5+} ions having the singlet ground state with $J_{eff} = 0$. Our study thus showed that the local electron-electron and spin-orbit interactions are stronger than the inter-Ir hopping in these compounds, and that it would be interesting to look for other crystal structures where the inter-Ir hopping can be made substantialy larger.

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1.11.4. Single crystal growth (Chemical Metals Science, Solid State Chemistry, Physics of Correlated Matter, Physics of Quantum Materials)

One of the most prolific areas of our joint research is on the single crystal growth and characterisation that drives so much of what we do. Chemical Metals Science and Solid State Chemistry have long-standing expertise in chemical vapour transport (indeed CM staff scientist Marcus Schmidt is a co-author of the authoritative text book in the field), Bridgman growth, flux growth, hydrothermal growth and floating zone techniques, some of which are also employed on focused projects by the two physics departments, along with radio-frequency, and arc melting techniques. Considerable exchange of ideas and expertise takes place between departments, with the result that the Institute has broadly achieved autonomy over the crystals on which it works. This is a vital aspect of our ability to lead in new fields, both because we can perform experiments without the restrictions that are often imposed by collaborations with external crystal growers, and because we can set our own goals regarding the necessary crystal quality.

Fig. 1 Crystals of the Weyl semimetal NbP grown by chemical vapour transport, and the Heusler compound $Mn_{1.4}PtSn$ grown by a floating zone method.

Particular highlights over the assessment period have been the chemical vapour transport growth of the phosphide and arsenides that display Weyl semimetal physics, but the vapour transport methods have also allowed us to build up 'libraries' of crystals of antimonides, sulphides, selenides, tellurides and halides (notably the spin liquid candidate $RuCl_3$), and to access large single crystals of oxides that could not be grown by other means. Bridgman techniques have been employed to grow a wide range of Heusler alloys, non-collinear antiferromagnets, chiral metals, pnictides and even crystals of elements such as Bi whose properties are stimulating a renaissance of research. Other Heusler and half-Heusler compounds as well as many chalcogenides and pnictides can be grown using flux methods, while hybrid flux / vapour methods (so-called 'mineralisation' reactions have been combined with traditional chemical vapour transport to grow a series of delafossite metals. Floating zone methods are usually applied to oxides, and have indeed been the key method for the growth of cobalates and ruthenates, but we have also shown that certain Heusler compounds can also be grown using these methods.

For further reading see for example:
www.cpfs.mpg.de/ssc/crystal-growth
www.cpfs.mpg.de/pqm/delafossites and
www.cpfs.mpg.de/pcm/high-ox-materials

1.11.5. Weyl fermion monopnictides: spectroscopy and magnetothermal transport (Physics of Quantum Materials, Solid State Chemistry and Physics of Correlated Materials)

The realisation that monopnictides and monoarsenides hosted potential Weyl metal candidates, combined with our ability to grow excellent crystals in-house (see 1.6.4 above) led to opportunities to perform detailed spectroscopic and magnetotransport studies. We performed a successful nuclear quadrupole resonance study on TaP [11], obtaining evidence for the expected linear quasiparticle dispersion, something confirmed by optical spectroscopy studies on TaP and TaAs [12]. Both optical spectroscopy and de Haas – van Alphen measurements provide experimental means of probing one of the most important issues surrounding Weyl metal physics, namely the proximity of the Weyl points to the Fermi level. In TaP they are too far away to give a well-defined chirality at the Fermi surface [13]; TaAs looks more immediately promising in this regard [14]. The case of NbP is very interesting because although the so-called W1 Weyl points lie far below the Fermi level the W2 points lie only a few meV above it [15], stimulating high pressure work that we have already begun [16], along with studies of magneto-thermal transport [17].

A key realisation stimulated by the discovery that the Weyl point in TaP is far from the Fermi level is the fact

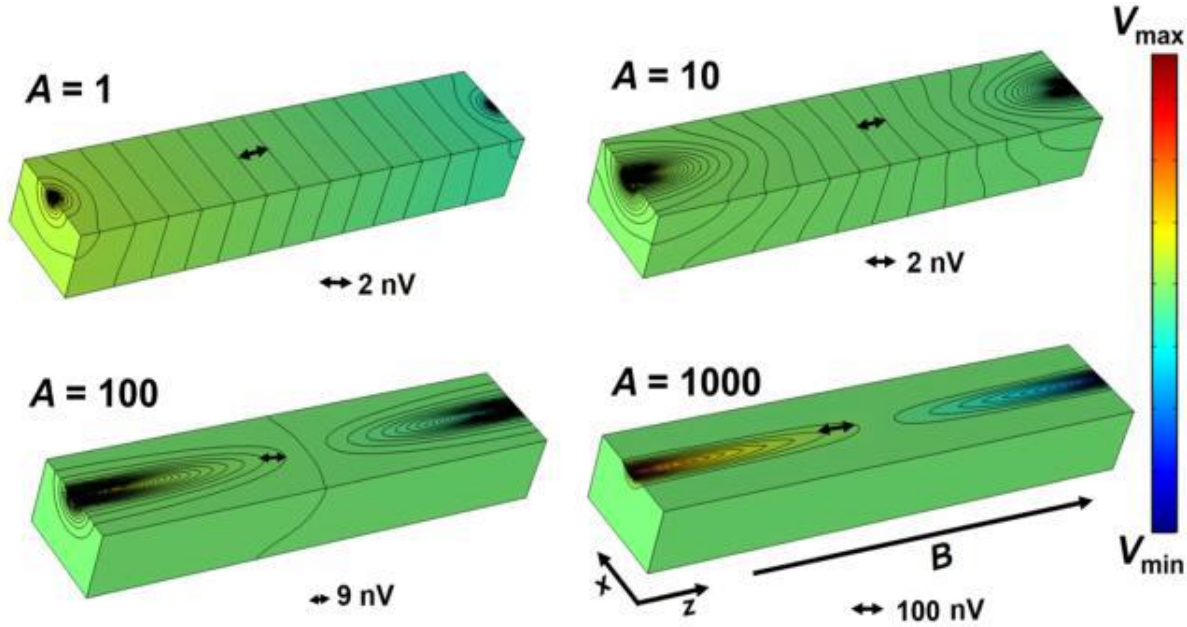


Fig. 2: Equipotentials for samples with different anisotropies with point injection of current. As the anisotropy (which is strongly field-dependent in typical Weyl semimetals for fields applied along the bar) increases, the current is seen to 'jet' across the sample. If careful multi-contact voltage measurements are not performed, this can lead to the impression of a negative longitudinal magnetoresistance [18].

that observation of negative longitudinal magnetoresistance in these high-mobility metals can result from an experimental artefact known as 'current jetting', and not from fundamental physics associated with the chiral anomaly [13,18]. Our work on this topic serves as a warning about the over-interpretation of data in this fast-moving field, as well as providing guidance on the checks that are required to give full confidence in the results of next-generation experiments on this topic.

For further reading see for example
www.cpfs.mpg.de/pqm/weyl-fermions,
www.cpfs.mpg.de/has/weyl-FS and
www.cpfs.mpg.de/ssc/TM-transport

[11] *H. Yasuoka et al*., Phys. Rev. Lett. **118** (2017) 236403
[12] *S. Kimura et al*., Phys. Rev. B. **96** (2017) 075119
[13] *F. Arnold et al*., Nat. Commun. **7**, 11615 (2016).
[14] *F. Arnold et al*., Phys. Rev. Lett. **117**, 146401 (2016)
[15] *J. Klotz et al*., Phys. Rev. B **93** (2016) 121105(R)
[16] *R.D. dos Reis et al*., Phys. Rev. B **93** (2016) 205102
[17] *U. Stockert et al*., J. Phys.: Condens. Matter **29** (2017) 325701
[18] *R.D. Dos Reis et al*., New J. Phys. **18** (2016) 085006

1.11.6 Chemical bonding, thermoelectricity and quantum criticality in $FeGa_3$ and related compounds (Chemical Metals Science and Physics of Quantum Materials)

Optimising the thermoelectric performance of materials has been a long-standing goal of collaboration between the CM and PQM departments, and an ideal challenge to be taken up by our Institute because to do so requires an intimate link between chemistry and physics. $FeGa_3$ and related materials are excellent platforms for this research because they are semimetals which show strong *d-p* hybridisation with a strong gradient of the density of states near the Fermi level: key ingredients for the existence of a large Seebeck coefficient.

In the assessment period we have extended our understanding of this family of materials by performing bonding analysis of $FeGa_3$ and its isotypes [19]. Coupled with a highly precise structural refinement, we have established the possibility of iron rich crystals, $Fe_{1+x}Ga_3$, $0 \leq x \leq 0.018$, whose magnetic properties change as a function of x [20] The phase diagram can be further expanded by substitution of Ge on the Ga site to produce $FeGa_{3-y}Ge_y$, and metallise the samples. By performing nuclear quadrupole and electron spin resonance experiments [21,22], we see a change from dominantly local antiferromagnetic

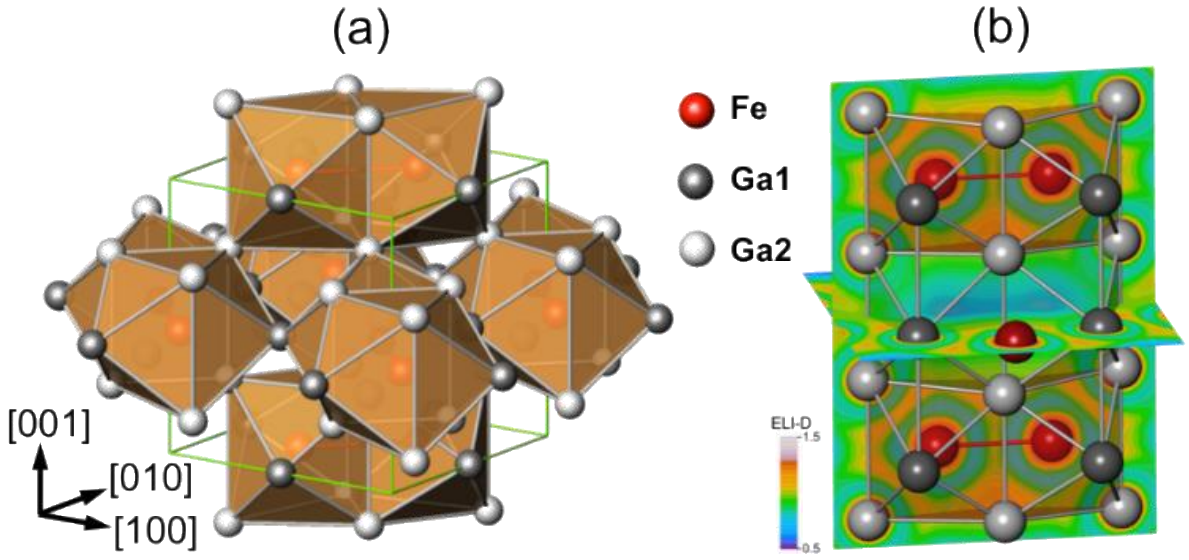


Fig. 3: The crystal structure of $FeGa_3$ with tetracapped trigonal double prisms as the main building block. b) Calculated electron localizability indicators in the (1-10) and (002) planes [ref].

flucutations to itinerant ferromagnetism, with magnetisation varying as $T^{-4/3}$ over a wide range of temperatures near the resultant quantum critical point. Our work highlights the potential of this class of compounds as hosts both of novel thermoelectric effects and quantum criticality, which we will pursue in future with extension to compounds in the $FeGa_3$ structure but with group six transition metals Cr, Mo and W on the iron site, combining with In as well as with Ga.

For further reading see
www.cpfs.mpg.de/cms/FeGa3

[19] *B. Boucher et al*., Inorg. Chem. **56** (2017) 4229
[20] *F.R. Wagner et al*., Inorg. Chem. submitted (2018)
[21] *M. Majumder et al*., Phys. Rev. B **93** (2016) 064410
[22] *B. Koo et al*., J. Phys.: Condens. Matter **30** (2018) 045601

2. Structure and Organization of the Institute

2.1 Structural Summary

The structure of our Institute, largely unchanged since the last review period except for the staffing developments outlined in the Executive Summary, can now be conveniently summarized in the diagram below.

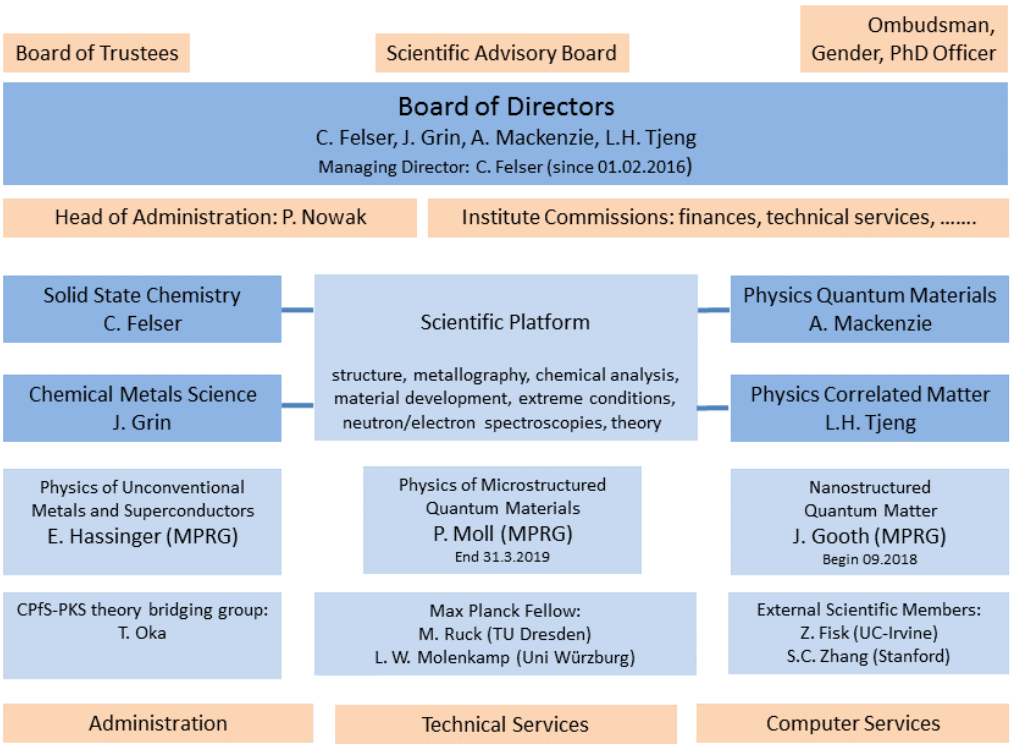
The scientific activities of the Institute are led by the Departments for Solid State Chemistry (SSC; Prof. Claudia Felser), Physics of Quantum Materials (PQM: Prof. Andy Mackenzie), Chemical Metal Science (CM; Prof. Juri Grin), and Physics of Correlated Matter (PCM; Prof. Liu Hao Tjeng), as well as by the Max Planck Research Groups (MPRG) for Physics of Unconventional Metals and Superconductors (Dr. Elena Hassinger), Physics of Microstructured Quantum Materials (Dr. Philip Moll) and Nanostructured Quantum Matter (Dr. Johannes Gooth).

The Board of Directors receives advice and recommendations from the Scientific Advisory Board, the Board of Trustees, the Ombudsman (Dr. Peter Höhn), the Gender Equality Officer (Dr. Gudrun Auffermann), the Officer for doctoral matters (Dr. Burkhard Schmidt) and the representatives of the scientists in the CPT section of the MPG (Dr. Ulrich Schwarz and Dr. Steffen Wirth).

The Board of Directors receives assistance in their decision making from the head of the Administration (Mrs. Petra Nowak) and Institute Commissions on finances, technical services, computer services, library, and safety issues.

The Scientific Platform, consisting of senior scientists from the four Departments, provides the long-term, stable expertise that we need in the fields of structure, metallography, chemical analysis, material development, extreme conditions, neutron/electron spectroscopies, and theory. Its flexible nature is demonstrated by the mutually beneficial inter-departmental moves during this review period of Dr. Oliver Stockert (a group leader who moved from PQM platform to PCM group), and Dr. Helge Rosner (a group leader who moved from PCM platform to PQM group). The departments hosting the other Scientific Platform members were judged to be appropriate choices and are unchanged since the last review period.

A close scientific collaboration with the Technical University Dresden is anchored by the Max Planck Fellowship of Prof. Michael Ruck from the Chemistry



Department. Our scientific collaboration with the German university sector has been further enhanced by the appointment of Prof. Laurens Molenkamp of the Julius-Maximilians-Universität (JMU) Würzburg as a second Max Planck Fellow, and we are in the process of setting up joint research projects with him. Common research activities with the neighboring Max Planck Institute for Physics of Complex Systems (PKS) are carried out by the CPfS-PKS bridging group headed by Dr. Takashi Oka who, following recommendations from the last report of the Advisory Board, has received greater assistance in these tasks from Prof. Moessner (MPI-PKS) and Prof. Mackenzie and Dr. Rosner from our Institute. Impulses for new scientific projects are provided by the External Scientific Members Prof. Zacharias Fisk (UC-Irvine) and Prof. Shoucheng Zhang (Stanford).

The Institute receives support from the groups for Administration (headed by Mrs. Petra Nowak), Technical Services (headed by Mr. Andreas Schwoboda) and Computer Services (headed by Mr. Jens Gerlach).

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Gruppenleiter "Catalysts for Syngas production and processing" BASF SE

2.2 Personnel Structure

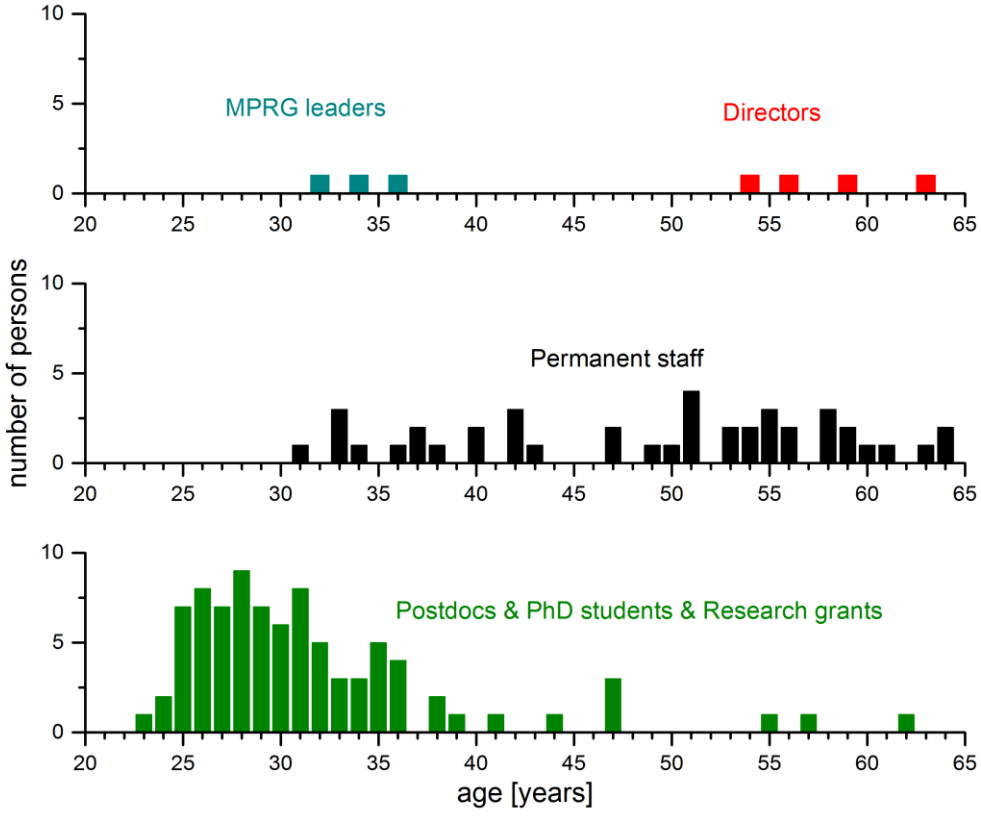
The overall structure of the scientific personnel of Institute is most compactly summarized in the following graph showing senior staff, permanent non-directorial staff scientists and those on temporary positions either as graduate students or as post-docs.

The permanent staff are each members of, or overseen by, one of our departments, Scientific Platform included. Physics of Quantum Materials has eight permanent staff members. Physics of Correlated Matter has six, Solid State Chemistry has six and Chemical Metals Science twelve members. Taking person-month totals and averaging over the assessment period, we had 45 graduate students inclusive IMPRS students (16 in Physics of Quantum Materials, 5 in Physics of Correlated Matter, 12 in Solid State Chemistry and 12 in Chemical Metals Science). Using the same procedure, the number of postdocs is 50 (10 in Physics of Quantum Materials, 10 in Physics of Correlated Matter, 23 in Solid State Chemistry and 7 in Chemical Metals Science). In addition, we have 6-10 international undergraduate interns from the Max Planck Centers with Korea/Taiwan and UBC Canada.

Of the three categories shown in the above graph, 33% of senior staff, (10%) of permanent staff scientists, and 30% of post-docs and students (17% of post-docs, 44% of students) are female.

The scientific work of the Institute is supported by 68 technical and engineering staff and 20.5 administrative staff.

Further details of all these statistics can be found in the Addendum and in the 'Data, Facts, and Figures' sheets which will be provided during the Scientific Advisory Board site visit in January 2016.



2.3 Structure of the Institute's Financing, Material Resources, Equipment and Spatial Arrangements

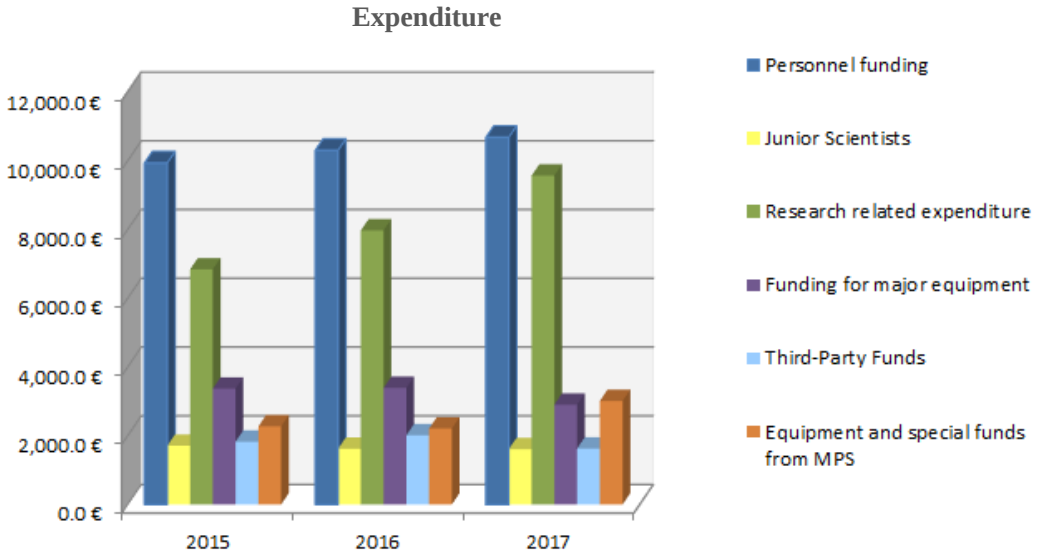
2.3.1 Institute financing

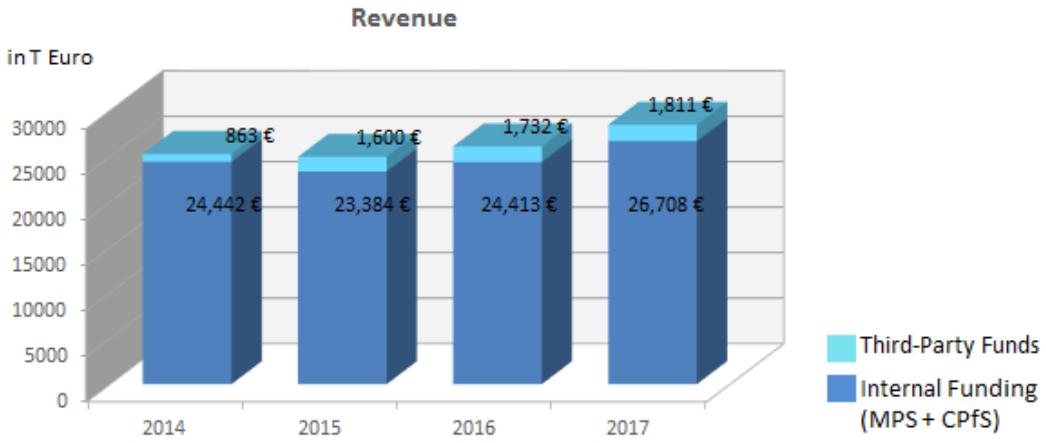
We summarise our budget structure in the enclosed graph, and provide extensive statistical details in the Addendum and in the 'Data, Facts, and Figures' sheets which will be provided during the Scientific Advisory Board site visit in November 2018.

2.3.2 Spatial arrangements

The main change in the physical infrastructure over the assessment period has been the welcome and necessary addition of substantial new office space following a space review and the building of a new office wing overseen by Marcus Schmidt and Juri Grin. In February 2018, the office extension with 50 work stations and a seminar room was completed.

The Max Planck Research Group of Philip Moll is on a phased wind-down due to Philip's appointment to a Professorship at EPFL (Lausanne) but will continue to receive core funding and oc-cupy its laboratory space until spring 2019. The new MPRG of Johannes Gooth will initially be housed in laboratory space from the Solid State Chemistry department and have access to the Physics of Quantum Materials department's clean room, and the Max Planck Fellowship group of Laurens Molenkamp will share the Solid State Chemistry department's thin film facilities and also use the clean room. We can already anticipate increasing pressure on our laboratory space as the Institute grows.





2.4 Junior and Guest Scientists and Career Development

Over the assessment period we have hosted approximately100 graduate students and post-doctoral research scientists on contracts or stipends at any given time. A particular focus of our activities, partly in response to comments from the Advisory Board, has been to harmonise our procedures for graduate student education and supervison

2.4.1 Graduate student education and supervision

January 2016 saw the establishment of our International Max Planck Research School for Chemistry and Physics of Quantum Materials (IMPRS-CPQM); see www.imprs-cpqm.mpg.de.

Entry to IMPRS-CPQM requires passing through a specific selection workshop, and the School contributes funding to the PhD costs of the successful candidates. However, this is not the only route to a funded PhD based at our Institute – students can also be paid from departmental funds or from external grant money. We decided, however, that there should be as little distinction as possible between the two classes of student. IMPRS-CPQM courses are available to everyone, and, importantly, the same guidelines for supervision and monitoring are also standard across the Institute. Each student has a Thesis Advisory Committee of three people including supervisor(s), and receives written guidelines about the schedule of formal meetings that are expected. More details can be found at http://imprs-cpqm.mpg.de/2991/Training.

The Institute PhD Officer, Dr. Burkhard Schmidt, is independent of IMPRS-CPQM and monitors the welfare and progress of all the students, holding regular meetings with PhD representatives, as well as individual interviews with each student, which include discussion of whether the pan-Institute harmonization policy is working properly. New systems take time to bed in fully, but we believe that all mechanisms have been put in place to ensure a smooth transition.

2.4.2 Graduate employability

We believe that the employability of our graduates is excellent: Of those 33 PhD students graduating from the groups of Institute staff in the 2015-2018 time period, 20 found employment in academic research science and 10 in industry (for three PhD students we have no entry about their job situation).

2.4.3 Academic career advancement

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

Ricardo Donizeth dos Reis: Group Leader, Brazilian Synchrotron Light Laboratory

Diego Franco: Staff scientist, Centro Atómico Bariloche, Argentina

Elena Hassinger: Professor (W2), TU München (with position at MPI-CPfS to continue to at least end 2019)

Maurits Haverkort: Professor (W3), Heidelberg

Julie Karel: Assistant Professor, Monash, Australia

Pallavi Kushwaha: Senior Scientist, National Physical Laboratory, Delhi India

Zhiwei Li: Associate Professor, Lanzhou, China

Wei Liu: Professor, Wuhan, China

Ajaya Nayak: Assistant Professor, NISER, Bhubaneswar, India

Philip Moll: SNSF Professor, EPFL Lausanne, Switzerland (with continued joint affiliation at MPI-CPfS to spring 2019)

Sanjay Singh: Assistant Professor, IIT Varanasi, India

Binghai Yan: Faculty position Weizmann Institute, Israel

Yanpeng Qi: Assistant Professor, School of Physical Science and Technology of Shanghaitech University, China

2.4.4 Security in Dresden

In our 2015 report we expressed concern about the situation in Dresden for foreign, particularly non-European, visitors. Things have eased over the past three years, and we have been active in a number of civic initiatives to help with the problems. We have joined the other Max Planck Institutes in the city in extensive discussions with the Integration Ministry and DVB, the organisation running public transport in the city, resulting in a number of positive steps regarding security and communication within the tram system. We also co-established Helpline Dresden, an English language service that can both aid the interface with the authorities in urgent situations and offer assistance with other issues faced by recent arrivals in a foreign

country. This last project is particularly satisfying because, with the help of the President, it was established by the Max Planck Institutes but has now become autonomous, with most of the required funds coming from a state government grant. Last but not least, we have developed an excellent relationship with the Dresden police, who have been helpful throughout. Our police liaison officer advises against complacency however; he says we should be thankful that the situation has improved, but should not rule out the possibility of a further outbreak of problems.

Note added: This assessment has been proven accurate by events taking place in the last days before printing this report. The serious civic disorder that broke out in Chemnitz has again resulted in adverse world-wide publicity, and highlighted the unusual challenges of maintaining an international research institute in Saxony.

2.5 Equal Opportunities

One of our foremost priorities is to strengthen the awareness of equal opportunity and to achieve good gender balance in our institute. Therefore, we attempt to provide gender-fair working conditions. We support our employees in their different career paths, ensuring work-life balance. In collaboration with our Gender Equality Officers Gudrun Auffermann and Renate Hempel-Weber, we have pursued our equal opportunity concept and fixed the most important items in our gender equality plan. The Gender Equality team takes care of gender fair language in our institute and has taken the following steps to improve the equal opportunities at the institute:

12th–13th August 2015: Workshop "Research Funding & Career Development" for junior female scientists. Coach Dr. Beate Scholz, CTC, Bonn/Trier, organization in cooperation with Anke Hübenthal (MPI for European Legal History, coordinator Minerva-FemmeNet).

3rd December 2015: Discussion dealing with the topic of gender equality.

4th February 2016: Informative meeting with a representative of the PME Family Service regarding support for parents and other family members (childcare and homecare/eldercare). Talk and discussion for all members of the institute.

26th August 2016: Workshop "Career development and third-party funding" for junior scientists. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

2nd-3rd November 2016: Intercultural training: "Intercultural Awareness, How do Germans tick? Intercultural Qualification: Successful Collaboration with Chinese and Indians". Open for all members of the institute.

11th November 2016: Intercultural training: "Intercultural qualification: Successful Collaboration with Chinese and Indians". Open for all members of the institute.

15th November 2016: Workshop "Career development and third-party funding" for junior scientists. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

1st December 2016: Reselection of the Gender Equality Team (12/2016-11/2020).

2017: Redesign of the gender equality plan of the institute and the web pages "Equal Opportunity" by mutual consent of the Collegium and the equal opportunity team.

12th April 2017: Discussion concerning equal opportunity. Open for all interested members of the institute.

22nd-23rd August 2017: Workshop "Developing your research brand" for junior scientists. Coach Dr. Beate Scholz, CTC, Bonn/Trier.

4th December 2017: Kathryn Arpino and Simone Altendorf were selected for the Sign Up! Career-Building 2018, which pursues the goal of supporting female postdocs and scientists in their career development and to prepare them for leadership roles. (The directors of the institute nominated six candidates).

21st December 2017: The gender equality plan of the institute (valid until 2020) was posted in the intranet in German and English.

31st January 2018: Visit of the Central Equal Opportunity Officer Dr. Ulla Weber for support of the Gender Equality Officer (Meeting with the Managing Director, Head of Administration and the Gender Equality Team).

8th-9th February 2018: Workshop "Exploring job opportunities on the non-academic job market" for PhD students (3rd year) and Postdocs, Coach Dr. Matthias Schwarzkopf, Jena.

18th-20th April 2018: The 22nd Annual Meeting of the Gender Equality Officers of the Max Planck Society

took place at the MPI CPfS in cooperation with the MPI PKS and the MPI CBG.

In July 2016, our institute hosted the Elisabeth-Schiemann-Kolleg, a mentoring networkby the CPT section of the Max Planck Society for women in natural sciences. 2015 the Kolleg selected our MPRG leader Elena Hassinger to participate in the network.

Gudrun Auffermann and Petra Nowak are the contact persons of our institute in the framework of the Career Steps Network of the MPG and continuously provide our scientists with information to support them at different steps of their career.

In addition to these in-house activities, Gudrun Auffermann was elected as deputy Gender Equality Officer of the CPT-Section for 2015-2017 and 2017-2019.

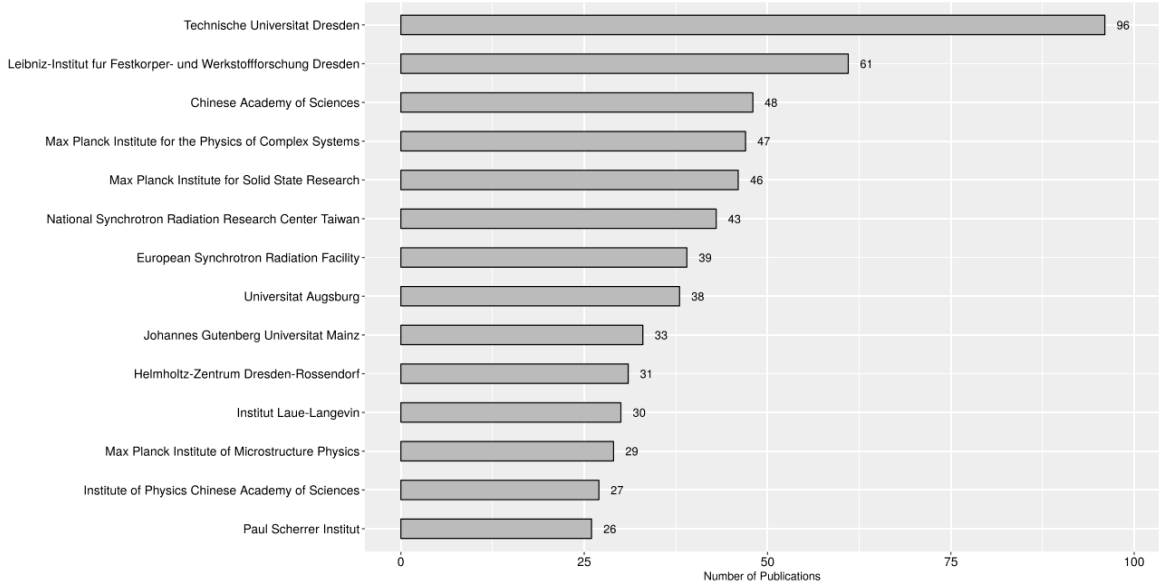
The current employment situation in our institute (31.12.2017, female in brackets) is well balanced for the PhD students (50%). The leaky pipeline obviously begins in the postdocs stage (19 %) and continues to exist at the level of permanent scientists (10%), W2 positions (20%) and W3 positions (25%).

2.6 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.

2.6.1 Major 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 in the successful extension in 2017 of the Max Planck Center of Complex Phase Materials with POSTECH (Korea) and NSRRC-NCTU-NHTU (Taiwan). Our Institut continues to be an active partner within the Max Planck Center with UBC (Canada) on Quantum Materials. This Center has also been extended recently as to include the University of Tokyo. Juri Grin leads the collaborations with the Max Planck Partner Groups at Moscow State University in Russia, at National University of Lviv in Ukraine, at NIMS Tsukuba in Japan and at Shanghai University in China. Claudia Felser leads the collaboration with a Max Planck Partner Group at Czech Academic and Max Planck Laboratory at Weizman. A formal agreement has also been made regarding the participation of TU Dresden and the University of St Andrews in IMPRS-CPQM. We will also participate with enthusiasm in the pan-German Graduate Centre in Quantum Materials headed by Prof. B. Keimer.

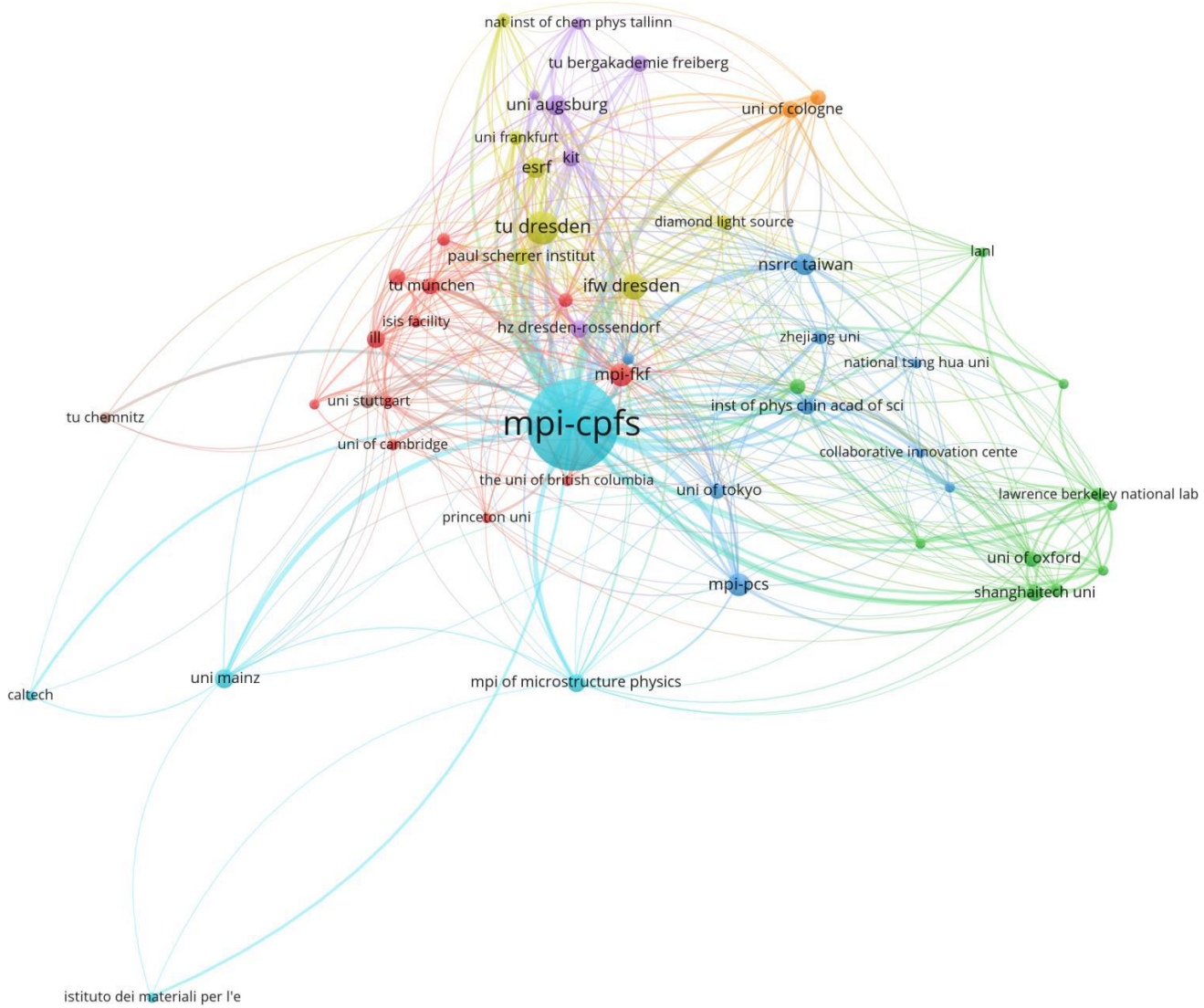


Bar chart of collaborating institutions with more than 25 common publications (database Scopus;mentioned in the 756 MPI-CPFS papers)

2.6.2. Scientific partners (from publications)

The most concrete evidence of our collaborative science comes from an analysis of our publications. During the assessment period, we jointly authored papers with more than 169 in situations elsewhere in Germany and beyond. The geographical spread of our major partners is illustrated below; a full list in alphabetical order can be found in the Addendum.

The network visualization in the Figure is a co-publication network. The distance between two institutions approximately indicates the relatedness of the institutions in terms of co-publications. In general, the closer two institutions are located to each other, the stronger their relatedness. The strongest links in terms of co-publications between institutions are also represented by lines. Items (here institutions) are represented by their label and by a circle. The sizes of the label and the circle of an item are determined by the number of co-publications of the corresponding institution with MPI-CPFS. The higher the number of co-publications of an institution, the larger the label and the circle of the corresponding item. The color of an item is determined by the cluster to which the item belongs. Lines between items represent links. All 289 links between items are displayed. For the purpose of optimal graphical presentation of the network the names of the institutions are abbreviated.



Visualization of the network of all collaborating institutions of the MPI-CPFS papers (articles, reviews, conference papers) between 2015 and 2017, using VOSviewer 1.6.7.

2.6.3 Industrial partners and patents

Our main industrial collaborations are with major international companies such as Western Digital (Felser), Intel (Felser), and BASF (Grin), but we also have links with smaller companies spawned from research by Institute members such as Razorbill and Innovative Measurement Technology.

In the census period we have applied for four patents and received one patent. The inventors and the working titles are:

(i) PD PhD Martin Valldor, Dr. Iryna Antonyshyn, Dr. Kwing To Lai
Novel chargeable crystalline materials, in particular for use as electrode materials in electrochemical storage devices

(ii) Mark Barber, Dr. Clifford Hicks, Dr. Alexander Steppke, Dr. Jack Barraclough, Dr. Alex Ward
Piezoelectric-driven uniaxial pressure cell with a capacitive force sensor and low torque transfer to the sample

(iii) Prof. Dr. Claudia Felser, Catherine Ranjitha Rajamathi, Dr. Nitesh Kumar, Prof. C.N.R Rao, Uttam Gupta
Increase in the photocatalytic water splitting of Weyl I Semimetals under the influence of an external magnetic field

(iv) Prof. Dr. Claudia Felser, Dr. S. Hossein Mir Hosseini, Dr. Sergiy Medvediev, B. Sc. Vicky Süß
Utilizing palladium diselenide ($PdSe_2$) insulator-metal transition induced by external stimulus in fast and low-energy consumption switches and memories

(v) Prof. Dr. Marc Armbrüster, Prof. Dr. Kryill Kovner, Prof. Dr. Juri Grin, Prof. Dr. Robert Schlögl, Prof. Dr. Peter Gille, Dr. Marc Heggen, Dr. Michael Feuerbacher
Hydrogenation process using ordered Cobalt-Aluminium and Iron-Aluminium intermetallic compounds as hydrogenation catalyst (European patent No. 2004577)

2.6.4 Research grants

Our members are partners in one DFG Collaborative Research Center (with TU Dresden), one Research Training Group (with TU Dresden), two DFG Research Units, seven DFG Priority Programmes, fifteen DFG Individual Grants, and one BMBF project.

In addition, we are partners in five EU and international grants including two ERC Advanced Grants (both held by Claudia Felser), and in two Excellence Cluster proposals that have been shortlisted in the 2018 Excellence Initiative round.

2.7 Statistical Summary of Publications and Invited Talks; Open Access and Archiving Policy

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. 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.

2.7.1 Publication statistics

In Section 1 of this Status Report and the related web-based research summaries we discussed research highlights and associated publications. In the table below, we provide statistics on our volume of publication from May 2015 to April 2018, 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 and the collaborative work within the institute are specified in detail.

2.7.2 Conference talks

During the assessment period, Directors and Emeritus Directors gave approximately 100 and 20 plenary, keynote and invited talks, respectively, at international conferences and workshops. About the same number of talks (115) were given at individual institutions. The MPRG leaders held about 40 talks, 25 of them on international conferences and workshops. Non-directorial staff (staff scientists, post-docs and PhD students) gave approximately 160 conference talks and 110 talks at individual institutions. Extensive further details of our invited talks and publications can be found in the Addendum.

Year	***2015***	***2016***	***2017***	***2018***	
Months	*05-12*	*01-12*	*01-12*	*01-04*	
					Sum
publications total	**137**	**277**	**315**	**115**	**844**
CMS	21	43	62	28	154
PCM	25	39	41	19	124
PQM	22	48	54	18	142
SSC	36	64	87	33	220
CMS/PCM	5	6	8	2	21
CMS/PQM	2	9	4	3	18
CMS/SSC	8	17	10	3	38
PCM/PQM	2	10	8	0	20
PCM/SSC	1	8	7	1	17
PQM/SSC	1	2	1	1	5
CMS/PCM/PQM	3	1	1	0	5
CMS/PCM/SSC	3	3	2	0	8
CMS/PQM/SSC	3	10	5	1	19
PCM/PQM/SSC	0	0	2	0	2
CMS/PCM/PQM/SSC	0	1	2	0	3
with HAS	1	3	3	1	8
with MOL	0	3	8	5	16
with RUC	6	13	14	2	35

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 from the individual departments and collaborations of two, three or all departments. In addition, the contribution of the MPRG's and the fellows are given. Since there are common publications with the departments as well, a small double counting of about 10 papers occurs. The departments, MPRG's and fellows are labeled as follows: CMS: Chemical Metal Science (Grin), PCM: Physics of Correlated Matter (Tjeng), PQM: Physics of Quantum Materials (Mackenzie), SSC: Solid State Chemistry (Felser), HAS: Max Planck Research Group (Hassinger), MOL: Max Planck Research Group (Moll), RUC: Max Planck Fellow (Ruck)

2.7.3 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. Andy Mackenzie sits on the Editorial Board of SciPost, a community-organised Open Access, Open Refereeing initiative that has also received financial Max Planck Society support since 2017.

2.7.4 Long-term archiving of research findings

We comply with the "Rules of Good Scientific Practice" - adopted by the senate of the Max Planck Society on November 24, 2000, amended on March 20, 2009; article 4:

2.8 Recognition: Scientific Awards, Fellowships and Memberships

The assessment period has seen a number of awards for our Directors, Emeritus Directors and, pleasingly, our junior staff and graduate students:

Claudia Felser: Fellowship of the IEEE**;** Election to the Leopoldina

Juri Grin: D. Phil. h.c., Ukrainian Academy of Sciences

Andy Mackenzie: Fellowship of the Royal Society of London

Frank Steglich: Fellowship of the American Physical Society (Condensed Matter Physics)

Clifford Hicks: International Union of Pure and Applied Physics Young Scientist in Low Temperature Physics Prize

Philip Moll: Nicolas Kurti Science Prize for Europe

Steffen Wirth: Fellowship of the American Physical Society (Condensed Matter Physics)

Alexander Steppke: Otto Hahn Medal - Max Planck Society; Richard L. Greene Dissertation Award of the American Physical Society

Heike Pfau: Otto Hahn Medal - Max Planck Society

Mark Barber: Otto Hahn Medal - Max Planck Society; Springer Thesis Award for Outstanding Doctoral Research

Stephen Edkins: Springer Thesis Award for Outstanding Doctoral Research; UK Institute of Physics prize for the Outstanding Doctoral Thesis in Superconductivity.

2.9 Service: Scientific Members' Committee Work and Institute Members' 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.

2.9.1. 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.

2.9.2. 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, 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 April 2015 – March 2018 period (semesters at TU Dresden start in April and October), Institute members have given more than 30 lecture courses and seminars with a total teaching load of more than 60 SWS (Semester Wochen Stunde = hours per week per semester). This converts approximately to 5 different lectures per semester with 2 SWS per lecture on average (as a reference: a full university professor has a teaching duty of 6-9 SWS).

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 the TU Dresden.

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

2.10 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 120 people 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.

2.10.1. Conferences, Workshops

In the May 2015 – April 2018 period, our Institute has hosted more than 25 workshops and meetings, varying in length between 2 and 5 days and with 30 to 120 participants. A list is given in the Addendum. In summer 2015, the MPI CPfS was the main organizer of the joined International Conference on Thermoelectrics (ICT) and the European Conference on Thermoelectrics (ECT) in Dresden with more than 700 participants.

2.10.2. Seminars

Our Institute has hosted about 116 seminars and colloquia from external scientists in the assessment period. A list can be found in the Addendum.

2.11 Public Relations Work

Our public relations team tries to reach out to the community and keep them up to date with our work – in a vivid and attention-grabbing way.

One of our highlights is the Long Night of Science – "Lange Nacht der Wissenschaften" (LNW). The LNW is a local science event in which the major research institutions of the city present their work to the curious and show them the fascination behind researching. It is now a well-established cultural event in the city, and our Institute's contribution typically attracts several thousand visitors.

In addition to that, we host events, workshops and lab tours and try to reach out to the public by news on our website, press releases, and image films.

We also participate in public life in Dresden through our membership of the networks "Dresden Stadt der Wissenschaften" and "DRESDEN-concept". We participated in the W.I.R. (World Identity Relations), a photo project featuring scientists with their individual story from Technische Universität Dresden and research institutions. For the HOPE online exhibition, our labs and the cellar were the stage.

In October 2016, we presented our research fields downtown on the Neumarkt on the occasion of the German National holiday. Last year, we started a design project together with design students that will help us to get an attractive institute's brochure and graphic elements to be used in poster presentations or exhibitions. This year we were very pleased to develop

a new image film, which was displayed at the MRS Spring Meeting.

Besides presenting our science, we have sought to express our societal commitment in supporting various refugee initiatives while hosting German language courses and offering free tickets for public transport to enable refugees to attend these courses. The latter was funded by a Max Planck donation. Our head of technical services, Mr Schwoboda, has also given very well-received follow-up tours of our technical facilities to participants in more advanced German classes, to help with their assimilation.

In 2015, we were happy to host the award of the Saxon Award for Democracy. Since then, two members of our institute Andy Mackenzie and Ingrid Rothe have been

members of the jury looking for awardable initiatives against racism, discrimination and for a better understanding of people for these annual awards.

http://www.wissenschaftsnacht-dresden.de/

https://wissenschaftliche-sammlungen.de/de/nachrichten/aktuelles/wir-world-identity-relations

http://newscenario.net/hope/

https://www.mpg.de/fluechtlingshilfe

http://www.demokratiepreis-sachsen.de/der-foerderpreis-2015/