# Max Planck Institute for Chemical Physics of Solids

Nöthnitzer Str. 40, 01187 Dresden, Germany

# Status Report

September 2012 – September 2015

## 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.

## Executive summary

The period September 2012 – September 2015 has seen considerable development of our Institute. In the following section we summarise the most important changes, and provide some overall performance statistics.

***New senior staff and independent research groups:*** We have recruited one new Director (Andy Mackenzie), two Max Planck Research Group leaders (Elena Hassinger and Philip Moll) and a leader for the group bridging between our activities and those of the neighbouring Max Planck Institute for Physics of Complex Systems (Takashi Oka). Our two Emeritus Directors, Frank Steglich and Rüdiger Kniep, have remained active contributors to our research through their leadership of their respective Emeritus Research Groups. The Max Planck Fellowship of Michael Ruck (TU Dresden) has been successfully extended.

***Summary of overall publication statistics:*** Over the three-year period covered by this report, Institute members have published 680 papers in Web of Science recognized journals. Many of our papers were published too recently for citation statistics to be a particularly useful guide, but by end October 2015 they had received nearly 3000 citations, with 67 papers cited 10 or more times and an *h*-index of 20. Many of our papers appeared in leading journals, e.g. 39 in Physical Review Letters, 24 in Science or Nature group journals, 15 in Applied Physics Letters, 13 in the Angewandte Chemie, 4 in Proceedings of the US National Academy of Sciences and 4 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 over 400 talks at international conferences, workshops and individual institutions. Just under half of these were delivered by Directors, with over 200 delivered by group leaders and more junior staff.

***Structural change:*** Since the last Scientific Advisory Board meeting in 2012 we have conducted an ongoing review of our administrative, scientific and technical structures. Scientifically, we have clarified the roles of the staff scientists and groups that form the Scientific Platform that is vital to our long-term success. Administratively, we have reorganized and streamlined our Technical Services, appointed a new Ombudsman and Gender Officer, updated the Institute Commissions that allow non-Directorial staff to feed into the decisions taken by the Board of Directors and conducted a comprehensive overhaul of our web site.

***Summary of Institute Scientific Staff:*** Following the restructuring, we comprise four departments in which, in addition to the Directors, are 32 staff scientists with permanent posts, 20 of whom are responsible for our Scientific Platform. We have approximately 60 Postdocs and 50 PhD students at any given time in our Institute. 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 post-docs plus PhD students is given in Section 2.2.

***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. We also strive to better the average of our field in the proportion of female post-docs and students, with 26% female post-docs and 47% female PhD students over the assessment period. Details are given in Section 2.4.

***Career development:*** One of our targets is to provide a good platform for the scientific careers of our junior staff. In the assessment period nine of them (Binghai Yan, Maurits Haverkort, Mark Armbrüster, Roman Gumeniuk, Stephan Kirchner, Sven Friedemann, Silvia Seiro, Raul Cardoso-Gil and Steffen Wirth) have been offered senior and junior Professor/Lectureships at universities in Germany, Austria, the UK, China, Chile and the USA, while Ambrüster and Alexey Baranov completed their Habilitations in the Institute. See Section 2.3.

***PhD training:*** Over the assessment period we have had around 50 PhD students in-house at any time, and graduated 46. To improve the monitoring of their training we appointed a PhD Officer in 2015. After several years of participation at the IMPRS for Dynamical Processes in Atoms, Molecules and Solids, we will lead from 2016 the IMPRS for Chemistry and Physics of Quantum Materials, a three-way joint venture with TU Dresden and the University of St Andrews, enhancing the prominence of PhD training among our activities.

***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 on the Excellence Initiative.

## 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 MPRG of E. Hassinger, the work of the emeritus directors F. Steglich and R. Kniep, and the Max Planck Fellowship group of M. Ruck are described in separate sections. Collaborative (inter-departmental/group) research is strongly encouraged in our Institute, so we highlight selected joint ventures in section 1.6. The research activities of the MPRG of P. Moll and the bridging group of T. Oka are not included since they only arrived at the Institute in autumn 2015.

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.

The report is organized as follows:


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

1.1. Department for Physics of Quantum Materials (A.P. Mackenzie)
1.2. Department for Physics of Correlated Matter (L.H. Tjeng)
1.3. Department for Solid State Chemistry (C. Felser)
1.4. Department for Chemical Metals Science (J. Grin)
1.5. Max Planck Research Group for Physics of Unconventional Metals and Superconductors (E. Hassinger)
1.6. Collaborative (inter-departmental/group) research activities
1.7. Emeritus Research Group Solid State Physics (F. Steglich)
1.8. Emeritus Research Group Inorganic Chemistry (R. Kniep)
1.9. Max Planck Fellow Research Group (M. Ruck)

**2. Structure and Organization of the Institute**

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2.2. Personnel Structure
2.3. Junior and Guest Scientists and Career Development
2.4. Equal Opportunities
2.5. Structure of the Budget, Material Resources, Equipment and Spatial Arrangements
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2.7. Statistical summary of publications and invited talks; open access and archiving policy
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2.10. Conferences, Workshops, and Seminars
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# 1. Institute's Research Program and Departments' Research Areas

## 1.1. Department for Physics of Quantum Materials (A.P. Mackenzie)

### 1.1.1. Introduction

***Background:*** The period September 2012 – September 2015 has been one of transition for the Department of Physics of Quantum Materials (PQM). It has changed its Director, its name (formerly Department of Solid State Physics) and its structure. It now runs as a set of seven independent but collaborative research groups, led by Dr. Michael Baenitz, Dr. Manuel Brando, Dr. Christoph Geibel, Dr. Clifford Hicks, Prof. Andy Mackenzie (Director), Dr. Michael Nicklas and Dr. Oliver Stockert. Four of these groups are part of the Institute's Scientific Platform, but now operate within PQM, and are cross-subsidised from its funds.

***Department Strategy:*** The core research strategy of PQM is to select projects of fundamental interest, maintaining a mix between high-impact, medium term work and work with longer term goals, and carry those projects out with internal and external collaboration as appropriate. We also aim to devote a significant fraction of our work to the development of new experimental apparatus and techniques, particularly those relevant to work at the chemistry/physics interface, something that would be harder to achieve in a university environment. Another goal is to reach a sensible gender balance for our field, and to vigorously promote the careers of our younger members.

***Distributed structure:*** One of our goals is to operate as a department of individual internationally visible groups, collaborating where appropriate but also performing high quality independent work. Evidence of progress in this direction comes from a breakdown of the above-mentioned statistics. Of the department's papers, fewer than 15% were co-authored by Mackenzie. Of the invited talks, just over one quarter were given by Mackenzie, and just over half by the department's other group leaders. The remaining 20% were given by junior staff members and post-docs.

### 1.1.2. Selected research highlights

In this section we provide a brief summary, with bibliography, of some of our highlight research themes from the past three years. The work is attributed to group leaders, staff scientists and Institute research fellows; the contributions of post-doctoral scientists and graduate students are shown in the author lists of the publications. Given the 'publication time lag' during a period of transition, many of the reported papers are the result of projects inspired and led by Frank Steglich as described in more detail in his contribution in section 1.7. Many of our projects involve collaboration with other groups in the Institute; the most directly collaborative are described in section 1.6.

***Ferromagnetic quantum criticality (Brando, Geibel, Nicklas):*** The general concept of quantum criticality has become one of the foundations for the study of strongly correlated electron physics. In antiferromagnets the situation has been clear and consistent; many antiferromagnetic quantum critical systems, both localized and itinerant, have been identified. For ferromagnetic systems the path to understanding has been more challenging. At first, no theoretical barriers to ferromagnetic quantum criticality were foreseen, but first order transitions rather than critical points were seen in real systems. Then, just over ten years ago, seminal work by Belitz and Kirkpatrick showed why this was the case, and led to speculation that ferromagnetic criticality would never be observable. Using thermodynamic techniques for investigating quantum criticality that were invented in this Institute, and materials grown here, we first demonstrated close proximity to ferromagnetic quantum criticality in some example systems [1, 2], and then the existence of the first known metallic ferromagnetic quantum critical point in $YbNi_4(P_{1-x}As_x)_2$ [3]. One of us (Brando) has since led the writing of a major review on the subject [4]. Furthermore, this project has led to the discovery of an unconventional pressure phase diagram in the compound CeCoSi, establishing the foundations for a new area of future research [5].

www.cpfs.mpg.de/pqm/FM-QC-Brando-Geibel-Nicklas


[1] *Avoided Ferromagnetic Quantum Critical Point: Unusual Short-Range Ordered State in CeFePO*,
S. Lausberg, J. Spehling, A. Steppke, A. Jesche, H. Luetkens, A. Amato, C. Baines, C. Krellner, M. Brando, C. Geibel, H.H. Klauss, and F. Steglich, Phys. Rev. Lett. **109**, 216402 (2012).

[2] *Doped $YbRh_2Si_2$: Not Only Ferromagnetic Correlations but Ferromagnetic Order*
S. Lausberg, A. Hannaske, A. Steppke, L. Steinke, T. Gruner, L. Pedrero, C. Krellner, C. Klingner, M. Brando, C. Geibel, and F. Steglich, Phys. Rev. Lett. **110**, 256402 (2013).

[3] *Ferromagnetic Quantum Critical Point in the Heavy-Fermion Metal $YbNi_4(P_{1-x}As_x)_2$*
A. Steppke, R. Küchler, S. Lausberg, E. Lengyel, L. Steinke, R. Borth, T. Lühmann, C. Krellner, M. Nicklas, C. Geibel, F. Steglich and M. Brando, Science **339**, 933 (2013).

[4] *Metallic Quantum Ferromagnets*

M. Brando, D. Belitz, F. M. Grosche, T. R. Kirkpatrick, arXiv:1502.02898 (to appear in Reviews of Modern Physics).

[5] *Temperature-pressure phase diagram of CeCoSi: Pressure-induced high-temperature phase*
E. Lengyel, M. Nicklas, N. Caroca-Canales, C. Geibel, Phys. Rev B. **88**, 155137 (2013).

***Uniaxial strain and dilatometry as new ways of controlling solids (Hicks, Brando, Mackenzie):*** Although uniaxial pressure has been applied to solids for many decades, traditional techniques made it extremely difficult to obtain homogeneous strain fields. We have developed an entirely new piezoelectric-driven approach to the problem, demonstrating levels of homogeneity and achieved strain that are approximately an order of magnitude better than those shown in previous work [6]. We are able, under computer control from room temperature, to make energetic changes to electronic structure that are equivalent to Zeeman energies of hundreds of tesla. The first application of the new technique was to the unconventional superconductor $Sr_2RuO_4$ [7], but the technology will be useful for the study of a wide range of strongly correlated and topological materials. In a complementary experimental development, we have designed and patented (patent filed by R. Küchler) novel apparatus for measuring magnetostriction and thermal expansion, and demonstrated its effectiveness in a project on bismuth [8]. Collaborations to profit from our new techniques have been set up groups across our Institute, with MPI-FKF (Stuttgart), and with colleagues in Paris, Tokyo and Kyoto.

www.cpfs.mpg.de/pqm/Strain-dilatometry-Hicks-Brando

[6] *Piezoelectric-based apparatus for strain tuning*
C.W. Hicks, M.E. Barber, S.D. Edkins, D.O. Brodsky and A.P. Mackenzie, Rev. Sci. Inst. **65**, 65003 (2014).

[7] *Strong increase of $T_c$ of $Sr_2RuO_4$ under both tensile and compressive strain*
C.W. Hicks, D.O. Brodsky, E.A. Yelland, A.S. Gibbs, J.A.N. Bruin, M.E. Barber, S.D. Edkins, K. Nishimura, S. Yonezawa, Y. Maeno and A.P. Mackenzie, Science **344**, 283 (2014).

[8] *Thermodynamic evidence for valley-dependent density of states in bulk bismuth*
R. Küchler, L. Steinke, R. Daou, M. Brando, K. Behnia, and F. Steglich, Nature Materials **13**, 461 (2014).

***Nuclear magnetic resonance (NMR) of correlated metals, thermoelectrics and quantum magnets (Baenitz, Geibel):*** Highlights of our NMR research have come in the fields of ferromagnetic criticality, correlated metals and new quantum magnets with strong spin orbit coupling. NMR is a microscopic tool for study of the correlated (renormalized) density of states, magnetic fluctuations at the verge of magnetic order and local fields in the magnetically ordered state. Over the review period 4*f* -aluminides were studied in depth, and unique and unexpected Kondo-lattice behavior was seen in the Fe 3*d* moments of $YbFe_2Al_{10}$ [9], see section 1.6.7. Furthermore, neutron scattering evidence for Skyrmion lattice formation resulted from our long-standing work on the chiral magnet FeGe [10]. Unconventional multi-valent charge ordering in $YbPtGe_2$ was evidenced from on site Yb-NMR [11]. Finally, local NMR fields supported a model for the giant exchange bias in Mn-Pt-Ga Heusler alloys (section 1.6.5). Many of the advances made in our NMR work result from long-standing interdisciplinary collaboration with both the Chemical Metals Science and Solid State Chemistry departments of Yuri Grin and Claudia Felser.

www.cpfs.mpg.de/pqm/NMR-chiral-Baenitz

[9] *Contiguous 3d and 4f Magnetism: Strongly Correlated 3d Electrons in $YbFe_2Al_{10}$*
P. Khuntia, P. Peratheepan, A.M. Strydom, Y. Utsumi, K.T. Ko, K.D. Tsuei, L.H. Tjeng, F. Steglich, and M. Baenitz, Phys. Rev. Lett. **113**, 216403 (2014).

[10] *Complex Chiral Modulations in FeGe Close to Magnetic Ordering*
E. Moskvin, S. Grigoriev, V. Dyadkin, H. Eckerlebe, M. Baenitz, M. Schmidt and H. Wilhelm, Phys. Rev. Lett. **110**, 077207 (2013).

[11] *Unconventional magnetism in multivalent charge-ordered $YbPtGe_2$ probed by 195Pt- and 171Yb-NMR*
R.Sarkar, R. Gumeniuk, A. Leithe-Jasper, W. Schnelle, Y. Grin, C. Geibel, M. Baenitz, Phys. Rev. B **88**, 201101 (2013).

***Spectroscopic investigation of the heavy fermion problem (Stockert, Geibel, Steglich, Mackenzie)*:** The heavy fermion problem, which was the main focus of the Solid State Physics department under the leadership of Frank Steglich, remains a key exemplar of the challenges of correlated electron physics. In the new PQM department, we have extended our study of heavy fermion physics, concentrating on techniques and probes that have not previously been widely applied to this class of material, and on high-profile external collaboration and use of external facilities. Angle-resolved photoemission [12], elastic neutron scattering [13] and spectroscopic scanning tunneling microscopy [14] have led to new insight on the temperature-dependent formation of the heavy fermion state and the mechanisms of heavy fermion superconductivity. Our world lead in the preparation of heavy fermion materials means that we anticipate a continued high-impact presence in this field.

www.cpfs.mpg.de/pqm/Heavy_fermion_spectroscopy

[12] *Temperature independent Fermi-Surface in the Kondo lattice $YbRh_2Si_2$*
K. Kummer, S. Patil, A. Chikina, M. Güttler, M. Höppner, A. Generalov, S. Danzenbächer, S. Seiro, A. Hannaske, C. Krellner, Y. Kucherenko, M. Shi, M. Radovic, E. Rienks, G. Zwicknagl, K. Matho, J.W. Allen, C. Laubschat, C. Geibel, and D. Vyalikh, Phys. Rev. X **5**, 011028 (2015).

[13] *Evolution of the Magnetic Structure in $CeCu_{5.5}Au_{0.5}$ under Pressure towards Quantum Criticality*
A. Hamann, O. Stockert, V. Fritsch, K. Grube, A. Schneidewind and H. von Löhneysen, Phys. Rev. Lett. **110**, 096404 (2013).

[14] *Imaging Cooper pairing of heavy fermions in $CeCoIn_5$*
M.P. Allan, F. Massee, D.K. Morr, J. van Dyke, A.W. Rost, A.P. Mackenzie, C. Petrovic and J.C. Davis, Nature Physics **9**, 468 (2013).

***Physics of valence fluctuation as exemplified by Eu-based materials (Geibel, Seiro):*** Another major challenge in strongly correlated physics is obtaining a broad-based understanding of the electronic states and their excitations. Several years ago we initiated a project to study those properties in Eu-based valence fluctuating compounds, which are prototype systems dominated by charge fluctuations. Meanwhile, interest in this topic has increased because of the possibility of unconventional superconductivity induced by quantum critical valence fluctuations. Based on a successful growth of high quality $EuIr_2Si_2$ and $EuNi_2P_2$ single crystals we were able to present the first study of the optical conductivity in such systems [15]. These results provide a basis for developing and testing appropriate theoretical models, and this project also led to the discovery of a surface state with an unexpected strong ferromagnetic polarization in $EuRh_2Si_2$. Our ARPES data (in collaboration with TU Dresden) revealed the exchange and spin-orbit induced splitting of this surface state with unprecedented resolution, allowing a very precise study of these interactions [16].

www.cpfs.mpg.de/pqm/valence-Seiro-Geibel

[15] *Optical Study of Archetypical Valence Fluctuating Eu Systems*
V. Guritanu, S. Seiro, J. Sichelschmidt, N. Caroca-Canales, T. Iizuka, S. Kimura, C. Geibel, and F. Steglich, Phys. Rev. Lett. **109**, 247207 (2012).

[16] *Strong ferromagnetism at the surface of an antiferromagnet caused by buried magnetic moments*
A. Chikina, M. Höppner, S. Seiro, K. Kummer, S. Danzenbächer, S. Patil, A. Generalov, M. Güttler, Yu. Kucherenko, E. V. Chulkov, Yu. M. Koroteev, K. Koepernik, C. Geibel, M. Shi, M. Radovic, C. Laubschat, D. V. Vyalikh, Nature Communications **5**, 3171 (2014).

***Ultra-high purity delafossite metals (Mackenzie, Hicks):*** The delafossite structural series of general formula $ABO_2$ features a wide range of physical properties including transparent conductors, candidate magneto- and thermoelectrics and magnetic insulators. Arguably less well-known are an astonishing series of metals such as $PdCoO_2$, $PtCoO_2$ and $PdCrO_2$. Quasi-two-dimensional and with conduction taking place in planes of triangular lattice noble metals, they have both the highest known conductivity of any oxide and in some cases higher room temperature conductivity than elemental copper. Our work has established that, at low temperatures, resisitivities of only a few nΩcm, corresponding to mean free paths as high as 50 μm, can be obtained in $PdCoO_2$. The microscopic origins of these record-breaking electrical properties are not well understood. Building on work begun before coming to Dresden [17], we have grown single crystals of the above materials and $PdRhO_2$ and $PdIrO_2$ and are investigating the origins [18] and consequences of the ultra-high conductivity. This project has benefited from collaboration with Markus Schmidt and Horst Bormann (Chemical Metals Science) and Helge Rosner (Physics of Correlated Matter) and will be a focus of collaborative work between our department and the new Max Planck Research Groups of Elena Hassinger and Philip Moll. In the long term, the delafossites have the potential for epitaxial growth, so this programme offers the promise of technological relevance as well as fundamental science.

www.cpfs.mpg.de/pqm/delafossites-Kushwaha-Hicks-Mackenzie

[17] *Quantum oscillations and high carrier mobility in the delafossite $PdCoO_2$*
C.W. Hicks, A.S. Gibbs, A.P. Mackenzie, H. Takatsu, Y. Maeno and E.A. Yelland, Phys. Rev. Lett. **109**, 116401 (2012).

[18] *Nearly-free electrons in a 5d delafossite oxide metal*
P. Kushwaha, V. Sunko, P. J. W. Moll, L. Bawden, J. M. Riley, N. Nandi, H. Rosner, F. Arnold, E. Hassinger, T. K. Kim, M. Hoesch, A. P. Mackenzie and P. D. C. King, Science Advances **1**, 1500692 (2015).

### 1.1.3. Major collaborative projects with other departments

In addition to work conducted mainly in our own department, we actively seek to collaborate inter-departmentally on topics of particular joint interest. Highlights from this collaborative work will be described in section 1.6. Project titles and the leaders of the Physics of Quantum Materials groups involved are:

***Fe-chalcogenide (11-type) based superconductors (Stockert):*** This project is in collaboration with the PCM, CMS and SSC departments, see section 1.6.1.
http://www.cpfs.mpg.de/pcm/FeSe-Wirth-Schwarz

***Heavy fermion materials (Geibel, Brando, Stockert):*** This project is in collaboration with the PCM, CMS and SSC departments, see section 1.6.2.
http://www.cpfs.mpg.de/pcm/HF-Wirth-Steglich

***High-field investigation of Heusler compounds for magnetoelectronics and magnetocalorics (Nicklas):*** This project is in collaboration with the SSC department, see section 1.6.5.
http://www.cpfs.mpg.de/pqm/Heuslers-Nicklas

***Topological Weyl Semimetals (Baenitz):*** This project is in collaboration with the SSC and CMS departments and the MPRG PMS, see section 1.6.6.
www.cpfs.mpg.de/yan
www.cpfs.mpg.de/Weyl_semi_metals_Hassinger

***NMR as a local probe for ferromagnetic quantum criticality in Fe-based systems (Baenitz):*** This project is in collaboration with the CMS and PQM departments, see section 1.6.7.
http://www.cpfs.mpg.de/pqm/Fe-crit-Baenitz

### 1.1.4. Future plans

The scientific goals that guide our future planning are the creation / discovery of new physics in quantum materials, the creation of new technology for the study of quantum materials and in some cases the development of quantum materials to enable new technology. In order to do this we aim to profit from the interdisciplinary strengths of our Institute, and to develop collaborative interfaces with other top-level institutions in Germany and beyond.

A major technological advance will be based on newly-commissioned infrastructure for ion-beam lithography and complementary fabrication techniques that will enable us to perform micro/meso scale experiments on complex quantum materials *(Mackenzie, Hicks, Koenig,* strong collaboration with *Moll*). Because of the microscopic nature of the final samples, the parent material will not necessarily have to be prepared as melt-grown single crystals. The goal here is to extend the range of novel materials to which the techniques of condensed matter physics can be applied, opening new frontiers at the chemistry/physics interface and new collaborations with the chemistry departments at the Institute. Further, novel phenomena inherent to the mesoscopic regime will become directly accessible in our experiments. Rapid improvements in the spatial resolution of angle-resolved photoemission spectroscopy (ARPES) mean that sample size is no longer a strong barrier, so some of the same materials used for mesoscopic work will also be studied as part of collaborations with the groups of Phil King (St Andrews) and Clemens Laubschat (TU Dresden). Such joint projects will play a major role in the development of the International Max Planck Research School for Chemistry and Physics of Quantum materials and can be viewed on its web site www.imprs-cpqm.mpg.de .

In addition to building on most of the highlight research avenues described above, we will focus attention on density wave systems and their proximity to superconductivity *(Geibel)*. We also anticipate a major programme of research on ultra-pure metals that we believe might allow observation of electronic hydrodynamic effects, which have been sought in bulk materials for over fifty years *(Mackenzie)*.

We will continue to devote considerable effort and resource to our development of new measurement techniques, because apparatus that benefits work at the interface between experimental physics and chemistry is core to the mission of the Institute. These will include uniaxial strain techniques *(Hicks)*, complementary measurement at high hydrostatic pressure *(Nicklas)* and SQUID NMR for work at ultra-low temperatures and fields *(Brando, Baenitz)*. Formal collaborations stimulated by our work in these areas include partnership in the TOPO-Q Grant for Global Networking based at Kyoto University and the University of Tokyo led programme “Topological Phenomena in Novel Quantum Materials”.

Our neutron spectroscopy activities *(Stockert, Sokolov)* will make use of unique facilities such as the high field magnet at the Helmholtz Center in Berlin, whose reactor will be operational until 2020.

Posters on these plans and the specific research on which they are based will be presented during the Advisory Board site visit in January 2016.

## 1.2. Department for Physics of Correlated Matter (L.H. Tjeng)

The activities of our department are centered around eight researchers with specific, complementary expertise. They are trained as theorists or experimentalists, as physicists or chemists. They lead groups and follow their own scientific interests both independently and as part of an overall team that carries out projects in a collaborative manner. They complement each other and share a common interest in various aspects of correlated materials. At present we have the following group leaders (in alphabetical order): Dr. Chun-Fu Chang, Dr. Maurits Haverkort, Dr. Zhiwei Hu, Dr. Alexander Komarek, Dr. Helge Rosner, Dr. Martin Valldor, Dr. Steffen Wirth, and Prof. Hao Tjeng (Director). Three of them (Chang, Hu, and Rosner) are also part of the Institute's Scientific Platform (for electron spectroscopy and theory, respectively), while Tjeng is serving as managing director of the CPfS from 01 Nov. 2011 until 31 Jan. 2016.

### 1.2.1. Interests and Objectives

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. From a theoretical viewpoint it is clear that the underlying many body problem cannot be solved exactly. Moreover, tiny changes in temperature, pressure or in the material composition can cause large changes of the properties, implying that many solutions exist which have very similar energies.

With exact solutions out of reach, the objective of our 'Physics of Correlated Matter' department is to find smart approximations by which we can capture the essential physics to describe the correlated motion of the electrons in such materials. It is likely that we need to develop and use different theoretical starting points for different materials. 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 combined experimental and theoretical work is essential to identify the most suitable working models. The experimental activities have also 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. 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

***Unravelling the charge-spin-orbital degrees of freedom using x-rays (Hu, Chang, Haverkort, 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. Using polarization dependent x-ray absorption spectroscopy (XAS), we were able to show that it is the anisotropy of the Ce 4f ground state wave function which correlates with the occurrence of unconventional superconductivity or long range magnetic order (and their coexistence) in the $CeMnIn_5$ compounds (M=Co,Rh,Ir) [1]. This implies that anisotropic hybridization must be considered for an appropriate description of Kondo lattice materials and the evolution of their properties as a function of non-thermal tuning parameters. We have also investigated the orbital orientation of the Ce 4f wave function in $CeCu_2Ge_2$ using non-resonant inelastic x-ray scattering (NRIXS) [2].

Using XAS we discovered that the $Co^{3+}$ ions in the complex metal oxide $SrCo_{0.5}Ru_{0.5}O_{3-\delta}$ possess a pure high-spin configuration at room temperature, which is quite unique for $Co^{3+}$ in an octahedral oxygen surrounding [3]. We were also able to induce a complete high-to-low spin state transition by applying high hydrostatic pressure. These results allow us to draw an energy diagram depicting relative stabilities of the high-, intermediate-, and low-spin states as a function of the metal−oxygen bond length for a $Co^{3+}$ ion in an octahedral coordination. Using XAS and x-ray photoelectron spectroscopy (XPS) we have also resolved the debate about the type of spin-state order/disorder, metal-insulator and valence-state transitions in other fascinating $Co^{3+}$ compounds [4,5]. X-ray magnetic circular dichroism (XMCD) has shown on the other hand that the claimed spin-state transition does not occur in $SrRuO_3$ thin films [6].

The extremely large orbital moment that we have observed in $\alpha$-$CoV_2O_6$ using XAS [7] is also surprising. We are able to trace this back to the unusual mixing of the Co 3d $t_{2g}$ and $e_g$ orbitals associated with the particular local distortions. X-ray magnetic linear dichroism (XMLD) is a very powerful and direct tool to determine the spin-orientation of the Fe ions in multiferroic $BiFeO_3$ thin films and alleged multiferroic $SmFeO_3$ [8,9].

Resonant x-ray diffraction is another variant of spectroscopy that can give new insights into the intricacies of the charge and orbital order in complex systems such as magnetite [10].

http://www.cpfs.mpg.de/pcm/x-ray-spectroscopies


[1] *Correlation between ground state and orbital anisotropy in heavy fermion materials*
T. Willers *et al.,* Proc. Natl. Acad. Sci. USA **112**, 2384 (2015).

[2] *Absence of orbital rotation in superconducting $CeCu_2Ge_2$*
J.-P. Rueff *et al.*, Phys. Rev. B **91**, 201108 (Rapid Com.) (2015).

[3] *A complete high-to-low spin state transition of trivalent cobalt ion in octahedral symmetry in $SrCo_{0.5}Ru_{0.5}O_{3-\delta}$*
J.-M. Chen *et al.*, J. Am. Chem. Soc. **136**, 1514 (2014).

[4] *Spin-state order/disorder and metal–insulator transition in GdBaCo2O5.5: experimental determination of the underlying electronic structure*
Z. Hu *et al.*, NJP **14,** 123025 (2012).

[5] *Coupled valence and spin state transition in $(Pr_{0.7}Sm_{0.3})_{0.7}Ca_{0.3}CoO_3$*
F. Guillou *et al.*, Phys. Rev. B **87**, 115114 (2013).

[6] *Electronic and spin states of $SrRuO_3$ thin films: An x-ray magnetic circular dichroism study*
S. Agrestini *et al.*, Phys. Rev. B **91**, 075127 (2015).

[7] *Spectroscopic evidence for exceptionally high orbital moment induced by local distortions in α-$CoV_2O_6$*
N. Hollmann *et al.*, Phys. Rev. B **89**, 201101 (Rapid Com) (2014).

[8] *Orthorhombic BiFeO3*
J.C. Yang, *et al.,* Phys. Rev. Lett. **109**, 247606 (2012)

[9] *k=0 magnetic structure and absence of ferroelectricity in $SmFeO_3$*
C.-Y. Kuo *et al.*, Phys. Rev. Lett. **113**, 217203 (2014)

[10] *Analysis of charge and orbital order in $Fe_3O_4$ by Fe $L_{2,3}$ resonant x-ray diffraction*
A. Tanaka *et al.,* Phys. Rev. B **88**, 195110 (2013)


***Hour-glass shaped magnetic excitations in non-cuprate oxides (Komarek):*** Magnetic excitation spectra shaped like an hour glass were found to be a universal property of high-temperature superconducting cuprate materials, and therefore became a major field of research in the neutron scattering community. Surprisingly, these types of spectra have also been observed recently in copper-free and insulating single layer perovskite cobaltates $La_{2-x}Sr_xCoO_4$, implying that their occurrence does not necessarily depend on Fermi surface effects. Hence, it was first assumed that charge stripe correlations are responsible. However, we were not able to detect the presence of charge stripes even when using 100 keV x-rays [11,12]. Instead, we observed broad peaks at commensurate half-integer positions in reciprocal space [11-13], indicative of checkerboard charge order correlations. From the doping dependence of the peak intensities and correlation lengths we inferred the presence of phase separation between hole-doped and undoped regions in the nanometer scale. The presence of the incommensurate magnetic peaks can then be attributed to frustration effects that arise in the magnetically disordered phases. Using simulations we were able to reproduce the experimental data, thereby revealing the origin of the magnetic hour glass spectra and the importance of the interplay between the hole doped and undoped regions on the nano-scale in the cuprates and beyond [12].

http://www.cpfs.mpg.de/pcm/hourglass-Komarek


[11] *Hour-glass magnetic spectrum in a stripeless insulating transition metal oxide*
Y. Drees, D. Lamago, A. Piovano, and A.C. Komarek, Nature Communications **4**, 2449 (2013)

[12] *Hour-glass magnetic excitations induced by nanoscopic phase separation in cobalt oxides*
Y. Drees, Z.W. Li, A. Ricci, M. Rotter, W. Schmidt, D. Lamago, O. Sobolev, U. Rütt, O. Gutowski, M. Sprung, A. Piovano, J.P. Castellan, and A.C. Komarek, Nature Communications **5**, 5731 (2014)

[13] *Charge correlations in cobaltates $La_{2-x}Sr_xCoO_4$*
H. Guo, W. Schmidt, L.H. Tjeng, and A.C. Komarek, Physica Status Solidi - RRL, 1–3 (2015)


***Correlated and non-correlated topological insulators (Rößler, Kasinathan, Höfer, Wirth, Haverkort, Thalmeier, Tjeng):*** $SmB_6$ has become of enormous topical interest because it is a candidate to be recognized as 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, namely being caused by the topologically protected surface states. In our scanning tunneling microscopy (STM) experiments we could detect 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, all types of surfaces, reconstructed and non-reconstructed, displayed a finite zero-bias conductance of considerable magnitude [14] which confirms the robustness of the metallic states and is in line with the proposal of $SmB_6$ being a topological insulator. We have also carried out a theoretical study to determine the conditions under which the strongly correlated SmO may host non-trivial topological properties [15].

In the field of non-correlated topological insulators, we can report that we have been able to prepare $Bi_2Te_3$ material which is insulating in the bulk and has a conductivity due to the topologically protected surface states only [16]. Highly stoichiometric and single crystalline thin films with mobilities as high as 4600 $Vs/cm^2$ were grown using molecular beam epitaxy (MBE) under Te distillation conditions. The preparation, the characterization with angle-resolved photoelectron spectroscopy (ARPES) and the four-point probe resistivity measurements were all carried out *in-situ* under ultra-high vacuum (UHV) conditions. We have discovered that the smallest amounts of contamination, e.g. by short exposure to air, have a dramatic effect on the conductivity of the film. This can be explained by the fact that the Fermi surface area of the topological surface states is only of order 1 percent of the surface Brillouin zone with the Dirac point being very close to the Fermi level. Very recently, we have also succeeded in putting a (removable) protective capping on the $Bi_2Te_3$ films such that the topological surface states remain unaffected (and undoped) [17], thereby opening possibilities to carry out experiments *ex-situ* (e.g. in high magnetic fields, devices).

http://www.cpfs.mpg.de/pcm/topological-insulators-correlated-non-correlated

[14] *Hybridization gap and Fano resonance in $SmB_6$*
S. Rößler T.-H. Jang, D. J. Kim, L. H. Tjeng, Z. Fisk, F. Steglich and S. Wirth, Proc. Natl. Acad. Sci. USA **111**, 4798 (2014).

[15] *SmO thin films: A flexible route to correlated flat bands with nontrivial topology*
D. Kasinathan, K. Koepernik, L.H. Tjeng, and M.W. Haverkort, Phys. Rev. B **91**, 195127 (2015).

[16] *Intrinsic conduction through topological surface states of insulating $Bi_2Te_3$ epitaxial thin films*
K. Hoefer, C. Becker, D. Rata, J. Swanson, P. Thalmeier, and L. H. Tjeng, Proc. Natl. Acad. Sci. USA **111**, 14979 (2014).

[17] *Protective capping of topological surface states of intrinsically insulating $Bi_2Te_3$*
K. Hoefer, C. Becker, S. Wirth, and L.H. Tjeng, AIP Advances **5**, 097139 (2015).

***New theoretical methods for correlated systems (Haverkort):*** We have developed a new method for the *ab-initio* description of the ground state, excitations, and dynamics of materials with a variable amount of correlation. One of the challenges in the calculation of correlated electron systems is the exponential scaling of the number of possible many body states (determinants) as a function of system size. This scaling is so bad that calculations with only a few atoms are already numerically intractable. We circumvent this problem by merging ideas from quantum chemistry and density matrix renormalization group theory. Not all determinants are equally important and our method, by iteratively optimizing the basis set, finds those $10^9$ determinants that are most important to represent the wave-function at any given point in time. Our method works well as an impurity solver for dynamical mean-field theory [18], with the advantage of working fully on the real-frequency axes and at the same time able to include arbitrary interactions. It also works well for time evolution and can thus handle spectroscopy and dynamics [19]. An important step forward is that we now can describe fully localized states (excitons) with multiplets, fully delocalized states (band-transitions) and their interactions (resonances) on equal footing in one method.

http://www.cpfs.mpg.de/pcm/solvers-Haverkort

[18] *Efficient real-frequency solver for dynamical mean-field theory*
Y. Lu, M. Höppner, O. Gunnarsson, and M.W. Haverkort, Phys. Rev. **B** 90, 085102 (2014).

[19] *Bands, resonances, edge singularities and excitons in core level spectroscopy investigated within the dynamical mean-field theory*
M.W. Haverkort, G. Sangiovanni, P. Hansmann, A. Toschi, Y. Lu, and S. Macke, Europhys. Letters **108**, 57004 (2014).

***The quantum nature of skyrmions in $Cu_2OSeO_3$ (Rosner):*** Skyrmions were observed in metallic helimagnets like MnSi and FeGe, forming nanoscale spin-textures. Extending over length scales much larger than the interatomic spacing, they behave as large, classical objects, yet deep inside they are of quantum nature. Penetrating into their microscopic roots requires a multi-scale approach, spanning the full quantum to classical domain. For the mentioned metallic systems such an approach is presently intractable due to the strong mixing of delocalized low energy electronic and magnetic degrees of freedom. However, since its band gap enforces a natural separation between electronic and magnetic energy scales, we achieved for the first time a complete multi-scale approach in the skyrmionic Mott insulator $Cu_2OSeO_3$ [20]. We have used density functional based (DFT) methods to estimate the Heisenberg exchange parameters and the Dzyaloshinskii-Moriya (DM) interactions and cross-check these with Quantum Monte Carlo (QMC) simulations of the experimental data. We then arrived at an effective model of weakly interacting $Cu_4$ tetrahedra in a spin-1 triplet state, and using a long wavelength approximation we extracted the two basic parameters which control the skyrmion physics, namely the exchange stiffness $A$ and the twisting parameter $D$. Micromagnetic simulations

then enabled a detailed investigation of the magnetic phase diagram, and in particular, the complex skyrmion formation in $Cu_2OSeO_3$.

http://www.cpfs.mpg.de/pcm/cu-skyrmions-Rosner

[20] *The quantum nature of skyrmions and half-skyrmions in $Cu_2OSeO_3$*
O. Janson, I. Rousochatzakis, A.A. Tsirlin, M. Belesi, A.A. Leonov, U.K. Rößler, J. van den Brink, and H. Rosner, Nature Communications **5**, 5376 (2014).

***Fe-chalcogenide (11-type) based superconductors (Wirth), Heavy fermion materials (Wirth), New materials with composite anionic lattices (Valldor), as well as Osmates and novel transition metal oxides*** are projects in collaboration with the other departments, see sections 1.6.1.-1.6.4.

http://www.cpfs.mpg.de/pcm/FeSe-Wirth-Schwarz
http://www.cpfs.mpg.de/pcm/HF-Wirth-Steglich
http://www.cpfs.mpg.de/pcm/CAL-Valldor
http://www.cpfs.mpg.de/pcm/Os-spin-orbit

### 1.2.3. Future directions

Electron and x-ray spectroscopies are at the heart of our research activities. This is, for example, documented by the 48 publications (7 PRL, 2 PNAS, 1 NatMater, 1 JACS. 1 EPL) from the Sep. 2012 – Sep. 2015 period that rely on information acquired from photoemission, x-ray absorption and x-ray inelastic scattering experiments. Since the start of the Physics of Correlated Matter department in 2009, most of the investments (3/4) were made for sample preparation (mirror furnaces) and characterization (SQUID, PPMS, XRD's) facilities, while for the spectroscopy we relied heavily on existing (but modern in 2009) instruments. It is now time to modernize and improve substantially our portfolio of spectroscopic methods.
---> µm-soft-x-ray beamline at NSRRC *(Chang, Tjeng):* A new undulator-based soft-x-ray beamline is being constructed at the brand new high-brilliance Taiwan Photon Source of the NSRRC in Hsinchu, Taiwan. With 1.5 MEuro investments from the PCM department (*Tjeng*) plus 0.5 MEuro from the SSC department (*Felser*), we will have a new facility to carry out x-ray absorption (XAS, XMCD) and photoelectron spectroscopy (XPS, ARPES) with a beam spot size of order 1 µm x 1 µm. This will give us the unique opportunity to investigate small samples. In particular, we expect to obtain single-crystalline quality data from even powder samples by searching for grains which have dimensions larger than several µm. This in turn will give us worldwide a major advantage in the study and characterization of new materials.
---> inelastic x-ray scattering beamline at PETRA-III Hamburg *(Tjeng):* We will spend about 1 MEuro to build up an end-station at the P01 beamline to carry out core-level resonant and non-resonant inelastic scattering using x-rays (5-18 keV). The objective is to obtain element specific information about the electronic structure of narrow band materials containing transition metal (3d, 4d, 5d), rare-earth (4f) and uranium (5f) atoms. The emphasis will be on the determination of the orientation or even charge density of the orbitals (wave functions) occupied, by making use of higher-than-dipole transitions. The project is very challenging, but the results will provide unique insight into the essential intricacies of the electronic structure of many correlated materials.

We are very much excited about our capability to prepare, characterize, and protect thin films under UHV conditions. We will continue with our projects to tune and optimize the properties of oxide thin films using doping and strain [21,22] *(Chang, Tjeng).* Also our achievements in the $Bi_2Te_3$ research provide the necessary conditions to start the project "Interfacing superconductors and ferromagnets with topological insulators using all in-situ/ultra high vacuum processes" *(Wirth, Tjeng).*

The topic of strongly correlated topological insulators is extremely exciting and intriguing at the same time. Theoretical issues need to be clarified, both on the band structure as well as on the many body level (*Kasinathan, Haverkort*). We will need to identify other strongly correlated materials with non-trivial topology, and the use of modern spectroscopies is indispensable here (*Tjeng*). The experimental work will be done collaboration with Dr. A. Severing from the University of Cologne.

The search for new materials is a key activity in our institute. Of particular interest for our department are materials with transition metal ions in unusual valences and crystal/ligand fields. For example, high oxidation state materials (*Komarek, Jansen*) may show spin-compensated states or self-doped states, with large consequences for the transport properties. It is interesting to study the doping dependence of these materials, i.e. the vicinity of metallic phases and (low-spin) magnetic phases may very well lead to unexpected phenomena.

[21] *Growth and characterization of Sc-doped EuO thin films*
S.G. Altendorf, A. Reisner, C.F. Chang, N. Hollmann, A.D. Rata, and L.H. Tjeng, Appl. Phys. Lett. **104**, 052403 (2014).
[22] *Verwey transition in $Fe_3O_4$ thin films: Influence of oxygen stoichiometry and substrate-induced microstructure*
X.H. Liu, A.D. Rata, C.F. Chang, A.C. Komarek, and L.H. Tjeng, Phys. Rev. B **90**, 125142 (2014).

Posters on these plans will be presented during the Scientific Advisory Board site visit in January 2016.

## 1.3. Department for Solid State Chemistry (C. Felser)

### 1.3.1. Introduction

The vision of the Institute of Chemical Physics of Solids: *designing new high quality materials with symmetries and topologies leading to a giant response* is strongly consistent with the scientific vision of the Solid State Chemistry (SSC) department. A part of the recent success is the close and fruitful collaboration with all the departments of the institute. The SSC department has had three main foci during the most recent three-year period: (i) Heusler compounds for energy applications and spintronics, (ii) Topological materials, and, (iii) Magnetic oxides. The common research philosophy of the department is the directed design of new multifunctional materials. Density functional theory at all levels including correlations and disorder and its predictive power plays an important role in identifying new materials and in giving insight into the bonding and magnetism in complex intermetallic compounds. These compounds are synthesised in various forms: as polycrystalline materials, as single crystals and as thin films. Physical characterization of the desired functionality of the materials is performed in the department and in collaboration with the other departments of the institute.

### 1.3.2. Scientific Highlights

The material systems under investigations have three main focus-areas:

***(i) Heusler compounds for spintronics and energy applications (Claudia Felser and co-workers)***

For more than 15 years the SSC team has worked on Heusler compounds with a unique world-wide recognized expertise [1a]. The story of success started with highly spin-polarized Heusler compounds for spintronics applications. In collaboration with Western Digital, Santa Clara, USA, $Co_2MnZ$ and related compounds were integrated into magnetic recording read-head prototypes for hard disks. $Co_2MnZ$ has been shown to be a half-metallic ferromagnet in tunnel devices (magneto resistance values of more than 2000 %) and via spin-polarized photoemission studies in collaboration with Jourdan in Mainz [1b]. However, the future of data storage for computers and smart devices is not clear: one potential candidate for data storage is Magnetic Random Access Memory based on the Spin Transfer Torque effect (STT-MRAM) or Spin Hall effect (SHE-MRAM). For new generations of extremely dense non-volatile STT-MRAM, the magnetic bits have to be switched by a small current: a material with a low magnetic moment, a high Curie temperature, a low Gilbert damping and a high spin polarization is needed. Heusler compounds with a tetragonal (along the 1 0 0) or a hexagonal (along the 1 1 1) distortion are one very promising option. Therefore, in the past three years the focus on magnetic Heusler compounds has changed from *ferro*magnetic $Co_2YZ$ (Y=transition metal, Z main group element) to *ferri*magnetic Mn2YZ Heusler compounds. Only a few members of manganese rich Heusler compounds are known. Guido Kreiner and his team are looking *for New Mn- and Ni-based Heusler compounds* [2]. A large crystalline anisotropy is also an important element for new permanent magnets: since Heusler compounds can be made from abundant elements, research activities have been started in cooperation with the Fraunhofer Institute and the Max Planck Institute in Halle. Note that already a joint patent has been submitted.

[1] www.cpfs.mpg.de/solid_state_chemistry
[1a] Graf, et al., Progress Solid State Chem. 39 (2011) 1
[1b] Jourdan, et al., Nature Com. **5** (2014) 3974

[2] www.cpfs.mpg.de/kreiner

The understanding of *magnetism in Manganese-based Heusler Compounds and compositional tuning of the functionalities* [3] are the primary research focus of the theory team of Stanislav Chadov. A basic understanding is necessary for the design of materials for MRAM devises and for new permanent magnets. Depending on the valence electron concentration and the spin-orbit coupling, $Mn_2YZ$ Heusler compounds can be designed with the desired properties [3a-c]. However, the interface and control over order and disorder [3d] in the devices remains a challenge and is the subject of future investigations. Until recently, only collinear magnetism was taken into account, without considering the broken symmetry of $Mn_2$-compounds (non-centro-symmetry) and the high spin-orbit coupling for Y = 4d and 5d elements [3d,f]. Compounds such as $Mn_2RhSn$ open the path to Dzyaloshinskii-Moriya exchange interactions, a pre-condition for Skyrmion instabilities and non-collinear magnetism [3d]. This new area is the subject of Ajaya Najak's team in collaboration with Michael Niklas (Physics of Quantum Materials), the theory group at the IFW (Ulrich Rössler) and the high-field team at Rossendorf [4]; the collaborative project is described in section 1.6.5. By rational design of the magnetic anisotropy, it should be possible to stabilize a skyrmion phase at room temperature. The future goal, in collaboration with Stuart Parkin (MPI-Halle), is the electric field induced motion of Skyrmions for its application in racetrack memory.

A second direction of Nayak's team is to search for large exchange bias effects in $Mn_2$-compounds, induced by controlled disorder of *ferro*magnetic nano-clusters in the *ferri*magnetic host compound [4a]. A giant exchange bias was achieved by tuning the two magnetic sublattices nearly to the compensation point [4b]. Localized moments on the manganese atoms allows for the design and realization even of spin gapless semiconductors in manganese based rich Heusler compounds [4c]. In theory ferromagnetic semiconductors with Curie temperatures even above 800°C should be possible. However, for the realization of these materials, well ordered compounds are necessary: this is one reason for us to have extended our thin film capabilities by the purchase of a molecular beam epitaxy thin film growth system. A systemic understanding of the first order phase transition between the cubic and the tetragonal Heusler compounds is important for the application of manganese compounds in novel multi-ferroic devices: these include, for example, the voltage control of magnetic orientation in magnetic memory devices and for magnetic cooling devices. Both of these are new directions of the SSC team led by Singh [5]. The transition temperature and magnetocaloric properties in Heusler alloys are highly composition dependent and therefore can be readily tuned. Our goal is to design a material with a 1st order transition at room temperature with a large change in magnetization but which is volume conserving to allow for many repeated cycles through the phase transformation. These materials would also be ideal for a new voltage-controlled multi-ferroic device. A huge change in the magnetic properties could be be achieved by sputtering magnetoelastic Heusler compounds onto ferroelectric substrates. A new concept that we have proposed is to take advantage of the completely reversible behaviour of a 2nd order phase transition by designing non-phase transforming Heusler compounds yet which show a large magnetic moment change and exhibit a ferromagnetic transition close to room temperature [5a].


[3] www.cpfs.mpg.de/chadov,
[3a] Wollmann, et al. Phys. Rev. **B90** (2014) 214420,
[3b] Wollmann et al. Phys. Rev**. B92** (2015) 064417,
[3c] Winterlik,et al., Advanced Materials **24** (2012) 6283,
[3d] Chadov, Kiss and Felser, Adv. Funct. Mater. **23**, (2013) 832
[3e] Meshcheriakova, et al., Phys. Rev. Lett. **113** (2014) 087203
[3f] Felser, Angewandte Chemie **52** (2013) 1631
[4] www.cpfs.mpg.de/nayak
[4a] Nayak, et al., Physical Review Lett. **110** (2013) 127204,
[4b] Nayak, et al., Nature Materials **14** (2015) 679
[4c] Ouardi, et al., Phys. Rev. Lett. **110** (2013) 100401
[5] www.cpfs.mpg.de/singh,
[5a] Singh, et al., arXiv:1505.07677 (2015).


Our thin film laboratory has been operational since 2014: thin film growth via two sputtering chambers and characterisation via in-situ Scanning Tunneling Microscopy (STM) is already available. A molecular beam epitaxy system (MBE) and in-situ angle resolved photoemission (ARPES) will be installed next spring [6]. For the next two years we will run the laboratory together with Stuart Parkin's group: our focus is on materials, whereas Parkin's group is focussed on devices. First thin films (topological insulators and tetragonal Heusler compounds [6a-e]) were successfully grown and characterized. Tetragonal Heuslers with compositions such as Mn-Ga, and Mn-Pt-Ga-Sn, that have zero or low magnetisation, are especially compelling for compensated ferrimagnets, exchange bias and STT-MRAM and SHE-MRAM. Tetragonal and hexagonal Heusler compounds based on our thin film studies with larger moments are under investigation for rare earth free hard magnets: two patents have been filed. The element specificity of L-edge X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) allows for the opportunity of probing the magnetic properties of these materials, including the individual magnetic sub-lattices [7]. Hard X-ray photoemission (HAXPES) [8] enables the investigation of the electronic and crystal structure of buried interfaces in devices [8a].


[6] www.cpfs.mpg.de/felser,
[6a] Ouardi, et al., Appl. Phys. Lett. **101** (2012) 242406,
[6b] Köhler, Knez, Ebke, Felser, Parkin, Appl. Phys. Lett. **103** (2013) 162406.
[6c] Jeong, Ferrante, Faleev, Samant, Felser, Parkin, Nature Com. accepted (2015)
[6d] Shan, et al., Appl. Phys. Lett. **101** (2012) 212102,
[6e] Shan, et al., Phys. Status Solidi RRL **7** (2013) 145.

[7] www.cpfs.mpg.de/karel

[8] www.cpfs.mpg.de/1862184/haxpes
[8a] ViolBarbosa, et al., Applied Phys. Lett. **106** (2015) 052402.


Most Heusler compounds with C1b symmetry, so called Half-Heusler compounds, are ternary semiconductors but are structurally and electronically strongly related to binary semiconductors. The band gap can be tuned from 4 eV to zero based on simple chemical rules [1a]. We have been working for more than 10 years in collaboration with IBM, Schott and the Helmholtzzentrum for Energy on ternary semiconductors for solar cells. Deep understanding of interfaces, grain boundary via density functional theory is necessary for high efficiencies [9]. The foci for semiconducting Heuslers XYZ are in two main areas: thermoelectric materials and

topological insulators. Semiconducting Heusler compounds are one of the most promising materials for thermoelectric applications since the materials are extremely stable. Moreover, cheap devices can be readily designed using p- and n-type Half Heusler compounds that are made from abundant elements [10]. The key to their excellent performance was the reduction of the thermal conductivity via the invention of phase separation on the micro- to nano-scale [10a]: this led to an international patent with Bosch GmbH. In recent years we have concentrated on the improvement of the p-type CoTiSb system and have tried to achieve a similar reduction of the thermal conductivity [10a-d]. The theoretical understanding of the phase separation of quaternary semiconducting Half-Heusler compounds via a miscibility gap, in collaboration with Thomas Gruhn (Bayreuth), will usher in new artificially nanostructured Heusler compounds with high figure of merits [10e].

[9] ] www.cpfs.mpg.de/kiss

[10] www.cpfs.mpg.de/ouardi,
[10a] Schwall, et al. Adv. Funct. Mater. **22** (2012) 1822.
[10b] Schmidt, Gibbs, Snyder, and Felser, Materials Horizont. **2** (2015) 68.
[10c] Rausch, et al., APL Materials **3** (2015) 041516.
[10d] Rausch, et al. Phys. Chem. Chem. Phys. **16** (2014) 25258
[10e] Mena, et al., Journal of Electronic Materials online (2015)

More than 50 zero band gap Half-Heusler compounds show a band inversion. In addition to the known applications for binary semiconductors, multifunctional properties are possible in this class of materials. Many of these ternary zero-band semiconductors contain rare earth elements, which can induce secondary properties, ranging from non-conventional superconductivity (e.g. LaPtBi) for Majorana quasiparticles to antiferromagnetism (e.g. GdPtBi) for devices with a Quantum Anomalous Hall effect and heavy fermion behaviour (e.g. YbPtBi) [11]. Ultra-high mobilities and large magnetoresistance effects were discovered in high quality single crystals of YPtBi and LuPtBi [11a,b]. Jointly with the group of Yulin Chen, Oxford, ARPES measurements have verified the band inversion in LuPtBi and YPtBi. However, the [1 1 1] surface has an additional surface state, which shows unconventional superconductivity (under investigation with A. Kapitulnik, Stanford). Single crystals were used to design nano-SQUIDs for the search for Majorana Fermions. This concept using cleaved single crystals as a basis for device fabrication will be extended in the future. The quality of the single crystals is better than compared to sputtered thin films. First thin films were successfully grown [6c,d] and, in analogy to the Quantum Spin Hall effect in CdTe/HgTe, quantum well structures with ultra-thin layers of YPtBi were predicted to lead to a semiconductor with band inversion. A Quantum Spin Hall (QSH) effect should be found in thin films of these topological Half-Heusler compounds, observable via robust edge states and in a quantization of the transport. Additionally, a large Spin Hall Effect (SHE) was predicted in devices with topological Half-Heusler compounds for a certain composition with a magnetic interface by the Chadov team [11c]. These could be the basis to design efficient SHE-MRAM for data storage. In the future, an important goal is the growth of topological Heusler compounds via MBE to achieve high quality samples for new quantum effects.

[11] www.cpfs.mpg.de/shekhar,
[11a] Shekhar, et al. Phys. Rev. B **86** (2012) 155314. Editors choice,
[11b] Shekhar, et al. arXiv:1501.00604;
[11c] Kiss, et al. arXiv:1510.06935

Based on our research on topological Heusler compounds our interdisciplinary team has started to investigate other material classes for topological effects.

***(ii) Topological materials and superconductors (Binghai Yan and co-workers)***

With the identification of the Heusler compounds - REPtBi, REPdBi und REAuPb (RE= rare earth metal) - as topological insulators, an intensive search for new materials, guided by theory, was started. Many new materials were predicted theoretically; a sub-group of them verified by experiment via ARPES or transport; many have to be synthesised in the future. The combination of excellent theoretical support by the Binghai Yan group [12], the availability of all kind of single crystal growth techniques the SSC group and in collaboration with Marcus Schmidt and Yuri Grin's team and high level physical characterization techniques in Andy Mackenzie's and Elena Hassinger's team has enabled us to compete at the same level with Princeton and Stanford. New materials such as layered variants of the Heusler compounds [12a], Actinide materials [12b], correlated Skutterudites [12c], and $BaBiO_3$ [12d] were identified. Among the layered materials (related to graphite with heavy elements), several compositions such as KHgSb were predicted to be the first weak topological insulator materials [12a]. There are two ways to approach topological compounds: one way is via Berry curvature, time reversal symmetry breaking and quantum field theory; the second is via band, bond, inert pair effect and spin orbital coupling, and how Roald Hoffman has taught chemists

[12e]. Many excellent thermoelectric compounds are topological insulators [12f]. The analogy with high energy physics and astrophysics concepts is what makes the field so exciting and truly transdisciplinary. Concepts such as Weyl, Dirac, Higgs and Majorana quasi particles, including magnetic monopoles, might be possible to be realized in condensed matter phases. One recent focus in our group are Weyl semimetals [12g-j], which was predicted in January 2015 by the Princeton group in the compounds, NbP, TaP, NbAs and TaAs. The (i) fast growth of high quality single crystals, (ii) Binghai Yan and his deep theoretical understanding, (iii) the strong and easy collaboration between chemistry and physics in the institute, (iv) excellent co-workers such as the high field laboratory members in Rossendorf and Nijmegen, and (v) the ARPES team in Oxford, enabled us to publish high level research only a few weeks after the first paper was published on arXiv. The most surprising invention in the area of topological matter concerns simple Gold metal. We recognized that the Gold surface state is due to a band inversion between the s and p-states, and this insight brings us back to chemistry. The predicted nontrivial features in the electronic structure of unoccupied states were detected by two-photon ARPES, in collaboration with Martin Aeschlimann's group in Kaiserslautern [12k]. The inert pair effect, the inversion of *s*- and *p*-states, that has been known for decades in chemistry, and the Gold surfaces, named after the inventor Shockley in physics, have to be reinterpreted in the light of this new insights.

However, despite the exciting physics observed in these materials, the question is raised whether topological states can have an impact for applications. It is not fully clear whether the good thermoelectric performance of all topological materials is correlated with their unique band structure. Other features, such as low band gaps, and ultra-high mobilities, including the violation of the Wiedemann-Franz law, might favour high figure of merits. Another potential application are spintronics devices based on spin momentum locking, and the stable spin polarized surface states. Surprisingly, the Spin Hall Effect in topological insulators are extremely high and therefore an interesting application is the SHE-MRAM. Thin films and devices (even made from single crystals) will be synthesised and the Spin Hall Effect for SHE-MRAM devices will be investigated in collaboration with Stuart Parkin and Günther Reiss, Bielefeld in the near future. High mobility and stable surface states play an important role in catalysis. This is an interesting hypothesis, which we have discussed over several years with our colleagues in Stanford and Bangalore. The prediction of Yan et al. that 1T'-$MoTe_2$ and relatives are Weyl semimetals [12l] and the fact that these materials exhibit superior electrocatalytic activity in the hydrogen evolution reaction ($MoTe_2$ is even better than 1T'-$MoS_2$, which is better than 2H-$MoS_2$ and Pt) can have an enormous impact in chemistry. However, further systematic investigations in collaboration with CNR Rao are necessary to confirm this hypothesis.


[12] www.cpfs.mpg.de/yan,
[12a] Yan, Müchler, Felser, Phys. Rev. Lett. **109** (2012) 116406,
[12b] Yan, Müchler, Qi, Zhang, Felser, Phys. Rev. B **85** (2012) 165125,
[12c] Zhang, et al. Science **335** (2012)1464,
[12d] Yan, Jansen, Felser, Nature Physics **9** (2013) 709.
[12e] Müchler, et al., Angewandte Chemie **51** (2012) 7221.
[12f] Müchler, et al., Phys. Status Solidi RRL 7 (2013) 91,
[12g] Shekhar, et al., Nature Physics **11** (2015) 645,
[12h] Yang, et al., Nature Physics **11** (2015) 728,
[12i] Shekhar, et al. arXiv: 1506.06577,
[12j] Liu, et al., Nature Mat. (2015), doi:10.1038/nmat4457
[12k] Yan, et al., Nature Com. accepted, arXiv: 1504.01971,
[12l] Yan Sun, et al., Phys. Rev. B 92 (2015) 61117(R).


High pressure is a powerful method to tune, in a controllable manner, the interatomic distances in elements and in compounds. In response to application of high pressure, condensed matter undergoes structural, electronic, magnetic and other phase transitions leading to unusual and sometimes unexpected properties of materials. The high pressure group of Medvedev [13] can measure transport properties and Raman spectroscopy up to 100 GPa, in-house, and structure, Mößbauer and XMCD under pressure at synchrotrons in Grenoble, France and Taiwan. The electronic transport properties of two polymorphic phases of $MoTe_2$ have been studied at high pressures up to 40 GPa. Semiconducting 2H-$MoTe_2$ undergoes an insulator to metal transition at a pressure of ≈16 GPa, but no superconductivity is observed up to 40 GPa. 1T'-$MoTe_2$ is metallic over the whole pressure range that we have explored and superconducting. The critical temperature of superconductivity is found to be extremely sensitive to pressure in the low pressure range [13a]. Further systems under investigation are $BaCr_2As_2$, FeSe-related compounds [13b] and other binary semiconductors.


[13] www.cpfs.mpg.de/medvediev,
[13a] Qi, et al., arXiv:1508.03502;
[13b] Ksenofontov, et al., Phys. Rev. B **85** (2012) 214519.

### *(iii) Magnetic oxides (Jansen and co-workers)*

The motivation for the invitation of Martin Jansen [14] as a guest scientist is based on the interest of the physics groups in oxides and Jansen's unique expertise in synthesizing new and not widely available oxide materials. Oxides have many interesting properties such as magnetic frustration, unique valence states, superconductivity, etc.. Double perovskites (DPs) $A_2BB'O_6$, which feature an ordered rock-salt like arrangement of corner-sharing $BO_6$ and $B'O_6$ units in the crystal structure are a versatile class of compounds and structurally related to Heusler compounds. A large variety of physical properties can be tuned in a similar way as in Heusler compounds. Half metallic ferromagnetism was predicted in ferromagnetic $Sr_2FeMoO_6$, an oxide with a high Curie temperature. We have studied extensively $Sr_2FeOsO_6$ [14a] and $Sr_2CoOsO_6$ [14b], which provide insight into their electronic structure, the balance of exchange interactions and the coupling to lattice degrees of freedom in these magnetic DPs. Iridates have drawn the attention of the physics community due to an interplay between structure, spin–orbit coupling and correlations. With $Na_4IrO_4$ an Iridate was found with a d5 configuration, an unusual square-planar single oxoanionic $[IrO_4]^{4-}$ species. The weak Coulomb repulsion of the Ir-5d electrons can explain the structural difference to the isoelectronic Cobaltate as a result of the strong U value of Co-3d states [14c].

The interplay between spin, orbital, charge, and lattice degrees of freedom has been explored widely in strongly correlated transition metal (TM) compounds with partially filled d shells. However, similar phenomena are also observed in open shell p electron systems. An analogy can be drawn between the properties of TM compounds such as the Jahn-Teller $t_{2g}^3e_g^1$ ($Mn^{4+}$) electron configurations and alkali metal superoxides $AO_2$ with paramagnetic $O_2^-$ ions, having a degenerate $(\pi^*)^3$ electron configuration. The orbital ordering involves a reorientation of the molecular anions, which is an important degree of freedom in molecular anionic p electron systems. The main focus of our work is in alkali sesquioxides $A_4O_6$ (A = Rb, Cs), which are anionic mixed valence compounds with two paramagnetic $O_2^-$ anions and one diamagnetic $O_2^{2-}$ anion per formula unit and thus feature also the charge degree of freedom. Until recently it was thought that the $A_4O_6$ compounds adopt a cubic crystal structure (space group I-43d), which only accommodates a single site for the $O_2^{n-}$ anions. However, Raman and inelastic neutron experiments revealed the presence of distinct $O_2^-$ and $O_2^{2-}$ units. Recently we succeeded in isolating a single crystal of a tetragonal modification of $Rb_4O_6$ and determining its crystal structure (space group I-4). The formation of a tetragonal modification of $A_4O_6$ is also the clue to understanding anomalies in the magnetic and structural properties of the sesquioxides. Combining magnetization measure-ments with EPR and 133Cs NMR measurements, performed in collaboration with Denis Arcon, Ljubljana, we have shown that the magnetic properties and structural phases present depend on the chosen temperature protocol [14d]. Our studies provide profound insights into the interplay between spin, orbital, charge, and molecular orientation degrees of freedom in these anionic p electron systems. The magnetism and the orbital ordering seems to drive the complex phase transition in these open shell p-systems [14e].


[14] www.cpfs.mpg.de/1462773/oxides,
[14a] Paul, et al., Phys. Rev Lett. **111** (2013) 167205,
[14b] Yan, et al., Phys. Rev. Lett. **112** (2014) 147202;
[14c] Kanungo, et al., Angewandte Chemie **127** (2015) 5507;
[14d] Klanjsek, et al. Phys. Rev. Lett. **115** (2015) 057205,
[14e] Knaflic, et al., Physical Review B **91** (2015) 174419

## 1.4. Chemical Metals Science 2012-2015 (Y. Grin)

Realizing the institute concept of Chemical Physics of Solids, the department *Chemical Metals Science*, together with the scientific platform groups *Chemical Bonding*, *Structure* and *Metallography*, cooperated with the departments *Solid State Chemistry* (Claudia Felser), *Physics of Quantum Materials* (Andrew Mackenzie) and *Physics of Correlated Matter* (Liu Hao Tjeng), emeritus groups *Inorganic Chemistry* (Rüdiger Kniep) and *Solid State Physics* (Frank Steglich), as well as with the *Max-Planck-Fellow Group* at the Technical University Dresden (Michael Ruck) and the *MPG Partner Group* at Moscow State University (Anastasia Alekseeva). The preparation of new classes of intermetallic compounds, the elaboration of an enhanced understanding of the relationship between the atomic interactions, the organization of crystal structures, and their influence on the chemical and physical behaviour of these substances, as well as the development of experimental and theoretical techniques necessary for such investigations, are in the focus of research.

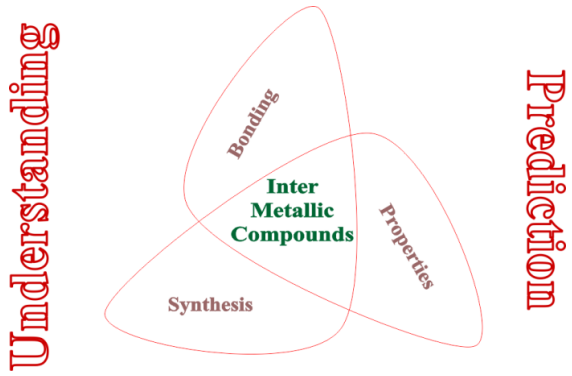


*Figure 1. Conceptual representation of the Chemical Metals Science department.*

Intermetallic compounds are the family of inorganic materials with the largest number of open questions concerning chemical and physical behaviour. To shed more light on these issues, combined experimental and theoretical studies of atomic interactions are performed (Figure 1).

Quantum chemical techniques of chemical bonding analysis in real space play an important role in the theoretical part of these studies. Beside the well-established methods of topological studies of electron density (according to the Quantum Theory of Atoms In Molecules), further new techniques were developed in the scientific platform group *Chemical Bonding*. The development of analysis tools proceeds in two steps: the theoretical derivation of the new approach and the assessment of suitability of the method for bonding analysis are followed by writing an appropriate code for routine use (***New tools for chemical bonding analysis*** by M. Kohout and co-authors [1]). The DAFH (domain averaged Fermi hole) analysis was derived and implemented as a new tool for solid state calculations (Figure 2 [2]).

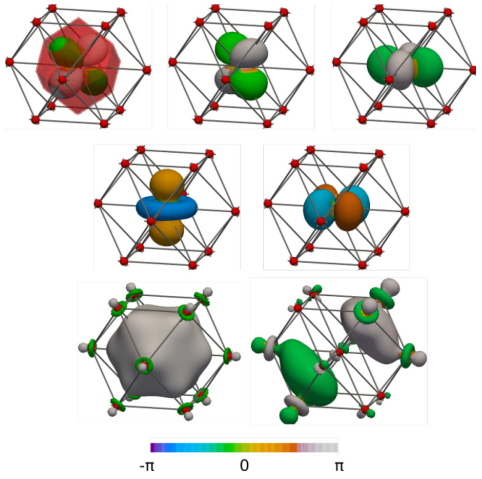


*Figure 2. DAFH orbitals for the Cu QTAIM basin (shown as transparent object) in fcc Cu: (top and middle) 3d Fermi orbitals; (bottom) s-type-like and p-type-like Fermi orbitals; the isosurfaces of the orbital amplitude 0.05 are coloured with the orbital phase.*

Moreover, improvements are made on the basic tools established earlier. Employing scalar-relativistic methods, the electron localizability indicator (ELI-D) for spatially anti-symmetrized electrons yields the ELI-D for tripled-coupled electrons, which can be applied to the results of, e.g., two-component Pauli equations with spin-orbit interaction. The systematic analysis of the atomic shell structures of the elements of the 4th to the 7th period has shown that the difference between outer shell parameters from scalar-relativistic and fully relativistic results is fairly small, but for the elements of the 7th period it becomes more pronounced, especially for the shell radii. The ω-restricted space partitioning (ωRSP) based on the so-called electron density inhomogeneity measure was applied for the sampling of the electron density to yield, after proper rescaling, a discrete distribution proportional to the charges in region of constant inhomogeneity. The corresponding functional

called $C_{0.6}$ – a new tool developed recently – closely resembles the atomic shell structure as given by the ELI-D and it was applied for the description of the bonding situation in molecules and solids. The delocalization index (DI) – a tool already well implemented for the two-centre interactions – has been recently extended for explicit analysis of three-center bonding (***Chemical Bonding in Intermetallic Phases*** by F. R. Wagner and co-authors [3]). The combined application of quantum chemical tools in real space allows to develop new approaches for the definition of covalence and ionicity as well as for the description and quantification of bond polarity (non-polar, i.e. covalent, and polar, i.e. lone-pair-like components of the bonding) and multi-centre bonding – two main challenges in the chemistry of intermetallic compounds. Systematic studies of the bonding in Heusler phases (experimentally investigated in the department *Solid State Chemistry*) lead to a better understanding of the 8-*N* rule in the real space (Figure 3). The analysis of atomic interactions in boron-rich compounds $MB_2$ and $MB_6$ (*M* is a metal), and in aluminium-rich cobalt phases revealed the role of three-centre bonds in the formation and metric of crystal structures of electron-deficient intermetallic compounds.

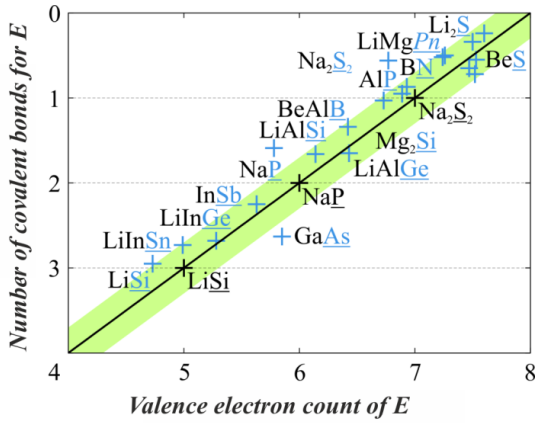


*Figure 3. Position-space representation of the 8−N rule for main-group compounds: $P_E(E)$ – charge claim of the element E; $N_{val}(E)$ – number of valence electrons; $N_{lp}(E)$ – number of lone pairs; the black line and crosses represent the formal 8−N rule; red data points represent the position-space view [4].*

Further possibilities of enhancing the output of diffraction experiments with respect to bonding analysis were found in the scientific platform group *Structure* (***Reconstruction of electron density from diffraction data*** by H. Borrmann and co-authors [5]). Using high-resolution laboratory diffraction experiments and the dedicated software developed for this purpose, the electron density of the vanadium borides VB, $V_3B_4$ and $VB_2$, as well as that of $TiB_2$ and $RuAl_2$ is reconstructed (Figure 4). These studies do not only allow for the recognition of extremely fine structural variations (crystallographic disorder) in $RuAl_2$ but also yield the basic information about the applicability of such information for bonding analysis.

Transmission electron microscopy offers another possibility to shed light on the real structure of intermetallic compounds and its influence on the chemical and physical behaviour. Here, the most important development is achieved by the installation of the new high-end microscope JEM-ARM-300F with the TEM and STEM resolution of 0.5 Å (***Atomic resolution microscopy of local atomic arrangements in solids*** by R. Ramlau and co-authors [7]). Earlier studies of the atomic order in the compounds $TmAlB_4$ and $YbAlB_4$ were made

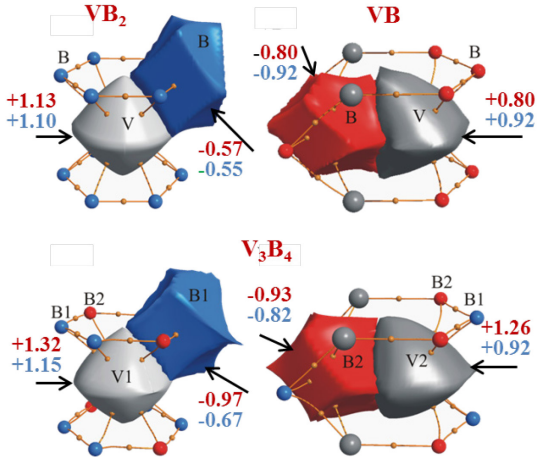


*Figure 4. Atomic basins in the electron density distribution in $VB_2$, VB and $V_3B_4$ reconstructed from experimental X-ray diffraction data: the bond critical points are denoted by orange spheres; experimentally reconstructed and theoretically obtained atomic charges are given in brown and light blue colours, respectively [6,3].*

in cooperation with the group of T. Mori (*NIMS*, Tsukuba). Recently, investigations of the boron and carbon ordering in boron carbide (in combination with high-resolution diffraction experiment and theoretical studies) reveal a much more complex atomic pattern than expected from the previous studies. This project was realized in cooperation with the groups of M. Scheffler (*Theory Department, Fritz-Haber Institute of the MPG*). New structural information was obtained on the atomic distribution in the light-element clathrate $K_7B_7Si_{39}$ as well as the promising thermoelectric clathrate $Ba_8Au_xGe_{46-x-y}\square_y$ (Figure 5).

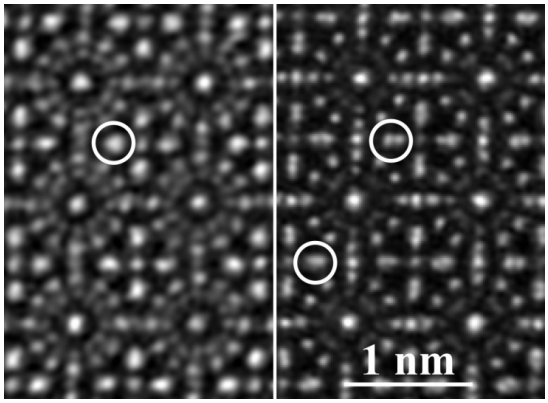


*Figure 5. Aberration-corrected STEM (HAADF) images of clathrates $K_7B_7Si_{39}$ (left) and $Ba_8Au_{0.5}Ge_{43}\square_{2.5}$ (right) in [100] direction: while the Si-K overlap with the projected interatomic distance of 0.50 Å is not fully resolved, the resolution level of the Ge-Ba overlap depends on the species at the neighbouring site (Ge, Au or vacancy □) and the projected interatomic distance varying from 0.61 Å to 0.89 Å.*

The development of new preparation routes and synthesis of new materials are one of the main topics of the research within the *Chemical Metals Science*.

Applying high-pressure high-temperature synthesis several compounds of Ba and Eu were manufactured in amounts facilitating the study of crystal structure and physical properties (***New germanium networks by high-pressure synthesis*** by U. Schwarz and co-authors [8]). So, for the known low-temperature superconductor $Ba_{8-x}Si_{46}$, the homogeneity range was investigated in detail and the thermoelectric properties were measured up to 400 K. An interesting trend was found for the germanium-rich phases *hp*-$BaGe_5$, $BaGe_{5.5}$ and $BaGe_6$. While $BaGe_6$ was found to be an electron-excess compound with respect to the Zintl count, the reduction of the Ba:Ge ratio (*hp*-$BaGe_5$) and the increase of the structural complexity (modulated $BaGe_{5.5}$) support the formation of a (pseudo)gap in the band structure (Figure 6). In the electron-balanced modifications of $BaGe_3$ and $EuGe_3$, two different Ge clusters are found to be in competition – $Ge_2$ dumbbells and $Ge_3$ triangles.

The need for thermoelectric materials resulted in the synthesis and complete characterization of a large group of intermetallic clathrates and other cage compounds (***Cage compounds and redox synthesis*** by M. Baitinger and co-authors [10]). Application of redox processes allowed to fill-up the empty cages in the metastable modification of

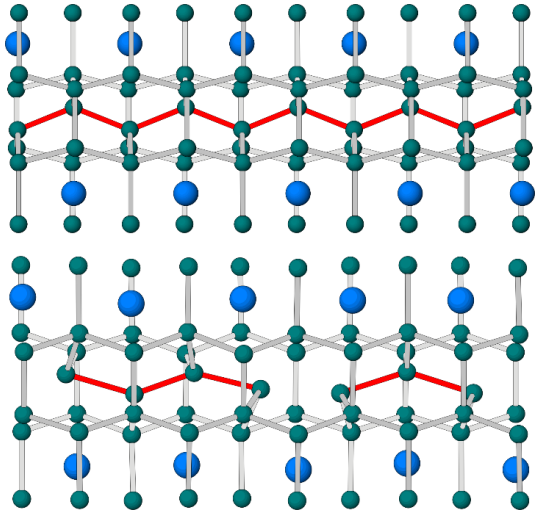

*Figure 6. Frameworks in $BaGe_6$ (top) and $BaGe_{5.5}$ (bottom): the formation of defects gives rise to an incommensurate translation symmetry and causes a metal-to-semiconductor transition [9].*

germanium $\square_{24}Ge_{136}$ and to obtain the clathrates-II $M_{24-x}Ge_{136}$ for Na, K, Rb and - most probably – also for Li. Remarkably, applying direct reactions between the elements leads to so far unknown clathrates, in which electropositive lithium replaces partially the tetrel element in the framework rather than filling-up the cages [11], and playing a role similar to the transition elements (Figure 7). Clathrate phases with in-framework substitution such as $Ba_8M_xGe_{46-x}$ and $Ba_8M_xSi_{46-x}$ were also prepared with transition metals *M*. Their homogeneity ranges were established, the ordering of the *M* components was investigated and thermoelectric properties [23], as well as chemical bonding [3] were studied in detail. In particular, NMR experiments made essential contributions to the clarification of the ordering of Al and Si within the framework of $Ba_8Al_xSi_{46-x}$, and a TEM study contributed decisively to the atomic distribution picture of $K_7B_7Si_{39}$ [4]. These studies were realized by cooperation of members from four departments and four science platform groups of our institute.

In the reported period, new developments were also made in the preparation of metal nitrides and nitridometallates. Systematic studies were performed in different systems varying from low nitrogen concentrations (reducing conditions) to large nitrogen excess (strongly oxidizing conditions). A special focus was put on the development of manufacturing techniques for mm-sized single crystals, which allow for the measurements of intrinsic properties of these mate-

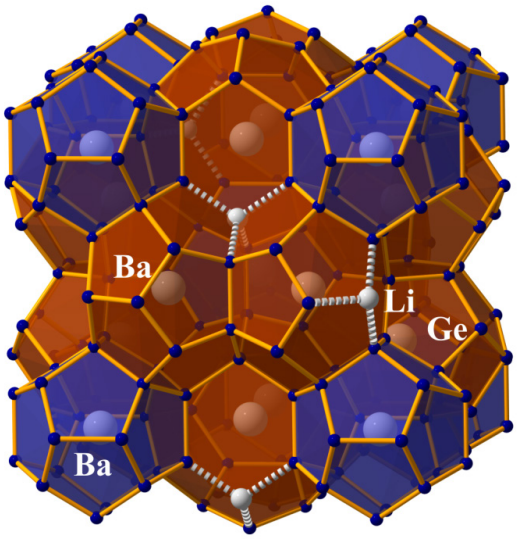


*Figure 7. Crystal structure of the clathrate $Ba_8Li_xGe_{46-x}$ [11] with the lithium atoms occupying the 6c site within the framework (Ba – large spheres, Ge – small blue spheres, Li – white spheres).*

rials (Figure 8). This issue was the main experimental drawback in the past, because the preparation of single-phase polycrystalline specimens is most challenging in this family of inorganic substances (***Nitridometallates and related compounds*** by P. Höhn and co-authors [12]).

First successes were achieved in the development of the electrochemical preparation of intermetallic compounds. This project was pursued within the *MPG Partner Group* at the Moscow State University (***Electrochemical preparation of intermetallic compounds*** by A. M. Alekseeva and co-authors [13]). By electrochemical intercalation of Li in $Fe_{1+\delta}Se$, the new ternary superconductor $Li_xFe_{1+\delta}Se$ ($x \leq 0.07$) was synthesized with a superconducting transition temperature of up to 44 K.

Another important preparation technique – chemical transport reactions – was systematically used for manufacturing materials in form of single crystals, which allows the advanced investigation of the intrinsic properties. More than 20 substances were prepared for further dedicated studies in all four departments of the institute and the scientific platform groups (***Chemical Transport*** by M. Schmidt and co-authors [14]). In particular, single crystal growth contributed essential to the studies of the catalytic properties of $Pd_2Ga$ (Figure 9).

A large group of intermetallic compounds of different families was recently prepared and structurally and chemically characterized in order

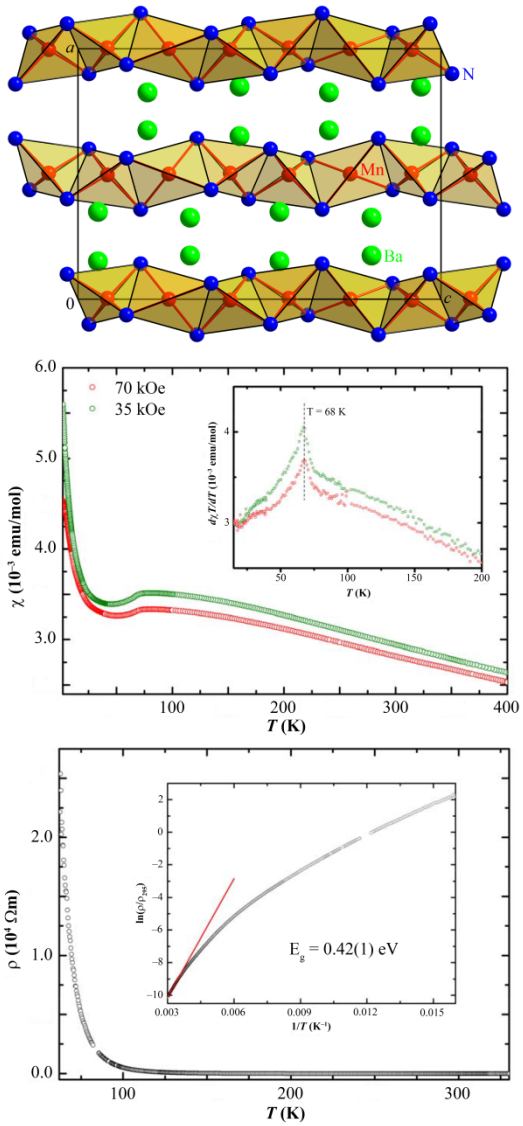


*Figure 8. $Ba_4Mn_3N_6$, a mixed-valent nitridomanganate with a one-dimensional anionic framework. Electric conductivity data show semiconducting behaviour, magnetic susceptibility data indicate an antiferromagnetic transition at 68 K being in agreement with the DFT calculations.*

to find substances with special features of their electronic structures, allowing either promising thermoelectric properties or unusual electronic states of the components (***Synthesis and properties of new intermetallic compounds*** by Yu. Prots and co-authors [15]). Two atomic arrangements were found near the equiatomic composition in the strontium – lithium – arsenic system: orthorhombic *o*-SrLiAs and the hexagonal modification *h*-$SrLi_{1-x}As$ [16] with 3D and 2D anionic LiAs frameworks, respectively, embedding Sr cations (Figure 10). The crystal structures of the new compounds $Yb_2Al_{15}Pt_6$ and $Yb_2Ga_{15}Pt_6$ adopt intergrowth variants. The distinct faults in the sequence of the structural segments lead to the

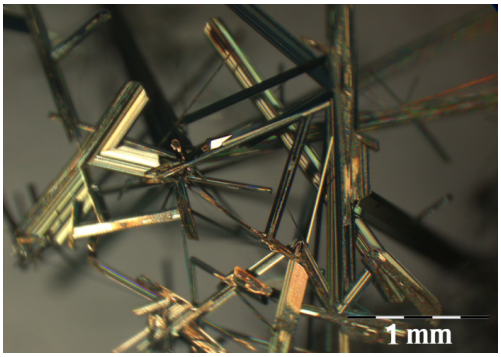


*Figure 9. Single crystals of $Pd_2Ga$ manufactured by chemical transport reaction.*

different local environments of the Yb atom which - in turn - may cause different electronic states of the rare-earth atoms. This project was performed in cooperation with the department *Physics of Correlated Matter*.

The chemistry and physics of intermetallic phases of boron were studied experimentally with transition-metal- and aluminum- or gallium-containing compounds (***New intermetallic compounds of boron*** by A. Leithe-Jasper and co-authors [17]). Together with the scientific platform group *Chemical Bonding* [3] the features of the B-B interactions in complex borides were studied in compounds *MM'*B (*M* – Nb, Ta, *M'* – Rh, Ir). Especially interesting are the compounds $MNi_9B_8$ (*M* – Al, Ga) revealing a three-dimensional interpenetration of $[B_8]$ anions comprising two- and three-bonded boron atoms with the three-dimensional $[MNi_9]$ cation formed by condensed *M*-filled Ni icosahedra (Figure 11 [18]). The reduced thermal conductivity of this metallic material is attributed to the chemical separation of the constituents in the crystal structure.

The large family of the $Yb_3Rh_4Ge_{13}$-type variants – the so-called Remeika phases – are synthesized, as well as structurally and physically characterized (***Chemistry and physics of Remeika phases*** by R. Gumeniuk and co-authors [19]). A special focus was located on the identification of the tiny structural differences between phases with different rare-earth metals or between the different modifications of the same compound (Figure 12 [20]). These studies involved scientists of the department *Physics of Quantum Materials*. The group leader – Dr. R. Gumeniuk – obtained a junior professorship in Crystal Physics at the Freiberg TU Mining Academy. The research in the laboratory of high safety standards was focused on actinide containing intermetallic compounds with the aim to shed light on the dual nature of the 5f electronic states (***Chemical physics of actinide-based intermetallic compounds*** by A. Leithe Jasper and co-authors [21]). A new structure type

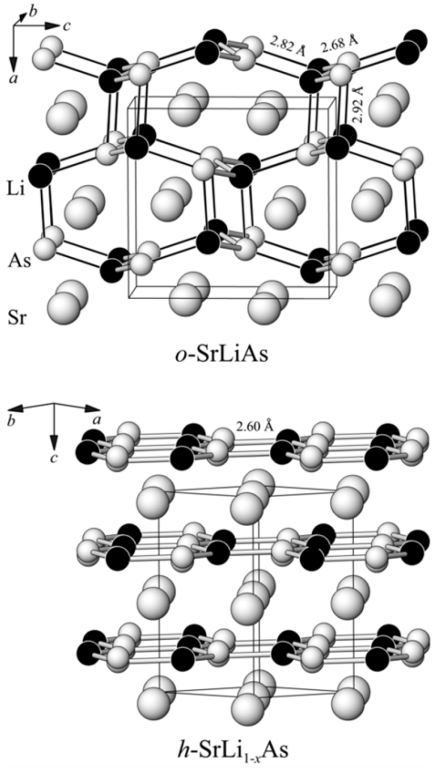


*Figure 10. Crystal structures of o-SrLiAs (TiNiSi type) and h-$SrLi_{1-x}As$ (ZrBeSi type): Li and As atoms form 3D and quasi-2D frameworks, respectively.*

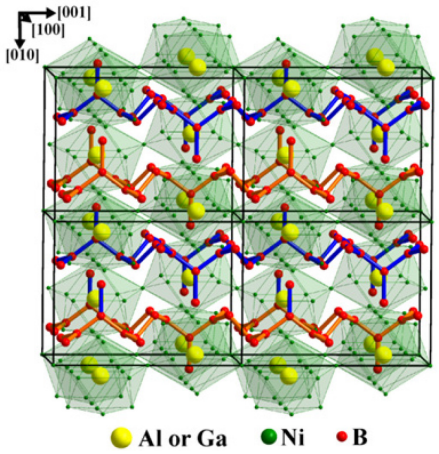


*Figure 11. Crystal structure of $AlNi_9B_8$ and $GaNi_9B_8$: Al or Ga atoms (yellow) reside in distorted $[Ni_{12}]$ icosahedra (green); boron atoms form alternating two-dimensional networks.*

was found for the binary phase $ThPt_2$ (Figure 13 [22]), and the structural and physical features of cage compounds $Th_3Rh_4Ge_{13}$ and $U_3Rh_4Ge_{13}$ were studied in detail. This project is realized in cooperation with the departments *Physics of Quantum Materials* and *Solid State Chemistry*. A new collaboration is also developed with the Max-Planck Research Group *Physics of Unconventional Metals and Superconductors*.

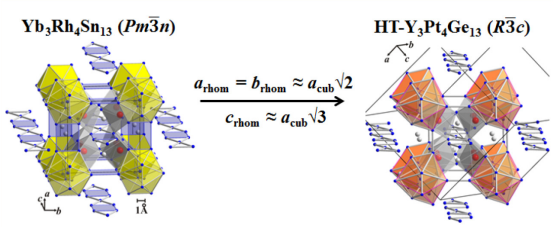


*Figure 12. Lattice transformation between the prototype structure $Yb_3Rh_4Sn_{13}$ and its derivative HT-$Y_3Pt_4Ge_{13}$.*

The third pillar of the research in the department *Chemical Metals Science* was the characterization of the chemical and physical properties of intermetallic compounds and the development of their understanding on basis of the knowledge regarding atomic interactions.

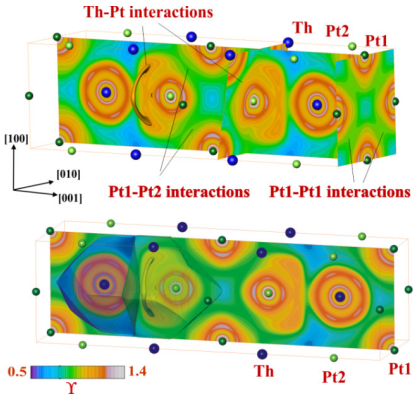


Figure 13. *Crystal structure and chemical bonding in $ThPt_2$.*

The physical phenomenon of thermoelectricity and the search for new thermoelectric materials are recently in the focus of research in connection with the problems of energy conversion. In cooperation with the departments *Physics of Quantum Materials*, *Solid State Chemistry* and scientific platform groups, thermoelectric properties of several groups of intermetallic compounds were studied (***Thermoelectric properties of inorganic compounds*** by R. Cardoso, I. Veremchuk and co-authors [23]). In particular, the representatives of the structure type $IrIn_3$ were in the focus of this project (Figure 14). An interconnection between the thermoelectric and other features was attributed to the influence of the chemical bonding on properties which are relevant for thermoelectric behaviour. The study of chemical bonding in a series of Ba clathrates resulted in the recognition of dative Ba-*M* interactions and their role in thermoelectric behaviour. The anisotropy and inhomogeneity of the interatomic interactions seem to influence the thermal conductivity of these materials decisively, in particular its lattice component. This was shown by the analysis of chemical bonding in real space [3], but also studied experimentally by means of spectroscopic techniques (***Vibrational dynamics of cage compounds*** by A. Leithe-Jasper and co-authors [25]). In contrary to previous investigations, application of inelastic neutron scattering on cm-sized single crystals of $Ba_8Ni_{3.5}\square_{0.4}Ge_{42.1}$ and $Ba_{7.81}Au_{5.33}Ge_{40.70}$ reveals that there exists no evidence for an interpretation of the thermal properties in terms of an isolated oscillator since rather coherent modes of guest and host systems were found [26]. These studies were performed within the *European Integrated Centre for the Development of Metallic Alloys and Compounds* (C-MAC).

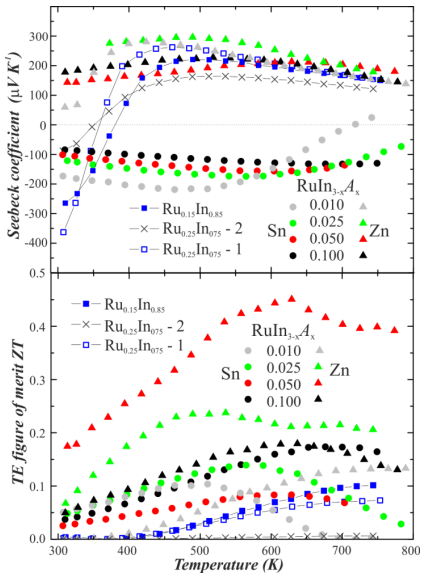


*Figure 14. Temperature dependence of the Seebeck coefficient (top) and the dimensionless figure of merit ZT (bottom) for $Ru_{1-y}In_3$, $RuIn_{3-x}Sn_x$, and $RuIn_{3-x}Zn_x$.*

The influence of the microstructure on materials properties was investigated in the scientific platform group *Metallography* (***Metallographic characterization of intermetallic materials*** by U. Burkhardt and co-authors [27]). The 'two-phase-single-crystal' material $Pd_2Ga$-$Pd_5Ga_3$ reveals an *in natura* intergrowth of different structural segments along one crystallographic direction (Figure 15). This feature results in strongly anisotropic thermal conductivity of the material being in agreement with the studies on thermoelectric materials [23].

Chemical properties of intermetallic compounds were systematically studied with respect to their catalytic activity (***Contributing to a future hydrogen-based energy infrastructure*** by M. Armbrüster and co-authors [28]). In the report pe-

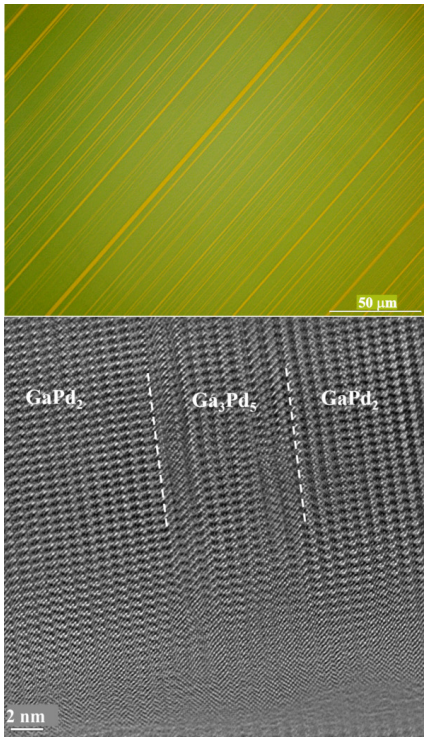


*Figure 15. Polarized-light optical (top) and TEM (bottom) images of the 'intergrowth-single-crystal' material $Pd_2Ga$-$Pd_5Ga_3$.*

riod, methanol steam reforming has been studied as an important element of future energy production. Employing the knowledge about chemical bonding a new group of catalysts based on ZnPd and related compounds was introduced (Figure 16 [29]). These studies were performed in cooperation with the group of R. Schlögl (*Inorganic Chemistry Department, Fritz- Haber Institute of the MPG*). The group leader – Dr. M. Armbrüster – obtained a professorship in Materials for Innovative Energy Concepts at the Chemnitz Technical University.

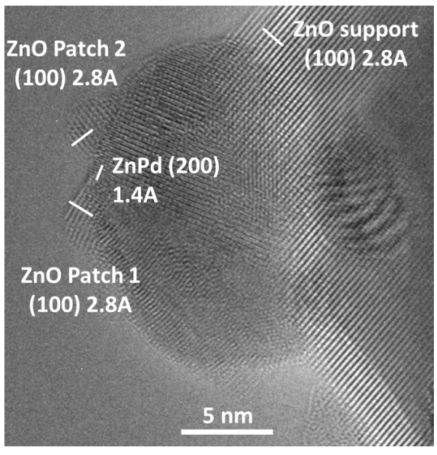


*Figure 16. HRTEM image of the team-work system ZnPd-ZnO.*

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[2] A. I. Baranov, R. Ponec, M. Kohout, *J. Chem. Phys.* 137 (2012) 214109.
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[15]www.cpfs.mpg.de/chem_metals_science/sci_rep/2015/new_compounds.
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[28]www.cpfs.mpg.de/chem_metals_science/sci_rep/2015/catalytic_properties.
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## 1.5. Max Planck Research Group for Physics of Unconventional Metals and Superconductors (E. Hassinger)

### 1.5.1. Introduction

The newly formed Max-Planck Research Group (MPRG) led by Dr. Elena Hassinger, started in December 2014. It has now two additional members: a postdoc (Frank Arnold, since February 2015) and a PhD student (Marcel Naumann, since June 2015, officially supervised by Prof. Laubschat at the TU Dresden).

Unconventional metals show a number of novel states of matter at low temperature that cannot be understood within an established quantum mechanical treatment. Examples are unusual ordered phases, non-Fermi-liquid behavior and unconventional superconductivity or topologically nontrivial phases. It is the interaction (correlation) between the electrons which makes these interesting quantum many body states emerge.

Our group strives for further understanding of these novel states of matter by experimental investigations at very low temperature and under high magnetic field and high pressure. Particularly, our aim is to understand the electronic behavior in novel states of matter through a direct detection of the Fermi surface via quantum oscillations, a fundamental "fingerprint" of a material. The powerful quantum oscillation technique gives information on the 3D Fermi surface topology and anisotropy, quasiparticle effective masses, quasiparticle scattering and magnetic interactions, the number of charge carriers, the ground state, the mobility and more.

Doing these demanding experiments requires creating a very low noise environment and requires extremely pure crystals. We can also work under high pressure (up to 3 GPa), enabling us to change the lattice constants and therefore the interaction of the electrons. By tuning the ground states with pressure, we are able to study the interplay and competition of their according order parameters and the changes of the Fermi surface.

### 1.5.2. Methods and ongoing projects

1) The main experimental apparatus needed for this project, a dilution refrigerator with a 17T magnet, is ordered and will arrive at the end of 2015. For future investigation of strongly correlated systems with high effective masses, the quantum oscillations in the magnetic susceptibility will be investigated with a modulated field method.

2) During the first year, a micro-cantilever torque method has been successfully set up and used to fully characterize the Fermi surface of $PtCoO_2$, in a collaborative project with the group of Andy Mackenzie. The 5d electrons in this material are quasi 2D and have an incredibly high conductivity. They behave almost like free electrons. A paper using information from our measurements about the parameters of the Fermi surface has been published in Science Advances. The measurements were carried out in high field and very low temperature refrigerators existing at the institute. This technique is perfect for the measurement of samples with a size < 0.5 mm, where other techniques are at their limit. Therefore it strengthens the connection between chemistry and physics, because very often it is difficult to grow large single crystals of a new material.

3) The existing characterization equipment of the institute (PPMS, Squid-VSM) has been adapted for torque measurements of larger samples with low effective masses. It has been used to measure the band structure of the proposed Weyl semi metal TaP. The combination of resistivity, magnetization and torque measurements and the very effective collaboration with the group of Binghai Yan from Claudia Felser's department who performed bandstructure calculations resulted in unprecedented precision of the knowledge about details of the Fermi surface compared to the various other groups active in this field. This information is crucial when studying properties appearing as a consequence of the Weyl points and and for further studies of the quantum limit. This highlight is described in more detail in the collaborative project about Weyl semi-metals.

4) Future projects are planned with the department of Juri Grin on uranium based strongly correlated electron systems.

### 1.5.3. Future development

We will continue working on the questions and ongoing projects outlined above, and aim to expand our group as our core equipment arrives in the Institute. In particular, we aim to recruit one more postdoc and another PhD student in the near future.

## 1.6. Collaborative (inter-departmental/group) research activities

In the years 2012 (from Sep.1), 2013, 2014, and 2015 (until Sep.29) we have 680 peer reviewed publications, of which 153 involve authors from two or more different departments/research groups, i.e. 22.5 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.

### *1.6.1. Fe-chalcogenide (11-type) based superconductors (Physics of Correlated Matter, Chemical Metals Science, Physics of Quantum Materials, Solid State Physics)*

Stimulated by the observation of superconductivity in iron-based compounds, 11-type iron chalcogenides were studied with a focus on determining the homogeneity range of the compounds, establishing structure-property correlations as well as investigations of competing interactions which facilitate superconductivity in FeSe. To this end, techniques such as high-pressure synchrotron x-ray diffraction, high-pressure magnetization/transport, neutron scattering, Mössbauer spectroscopy, and scanning tunneling microscopy-spectroscopy have been employed. Our measurements indicate that in $Fe_{1+y}Te$, the coupled magneto-structural phase transitions can be tuned by either varying the amount of excess Fe or by the application of external pressure [1-3]. Additionally, a multi-dimensional solitonic spin-liquid state was identified as a precursor to the incommensurate antiferromagnetic phase [4]. In single crystalline FeSe, a density-wave type incipient ordering mode preceding superconductivity was detected using scanning tunneling spectroscopy. Our results suggest that both charge as well as spin fluctuations play a key role in the mechanism favoring superconductivity in FeSe [5].

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


[1] *Pressure-induced successive structural transitions and high-pressure tetragonal phase of $Fe_{1.08}Te$*
C. Koz, S. Rößler, A. A. Tsirlin, D. Kasinathan, C. Börnert, M. Hanfland, H. Rosner, S. Wirth and U. Schwarz, Phys. Rev. B **86**, 094505 (2012).

[2] *Low-temperature phase diagram of $Fe_{1+y}Te$ studied using x-ray diffraction*
C. Koz, S. Rößler, A. A. Tsirlin, S. Wirth and U. Schwarz, Phys. Rev. B **88**, 094509 (2013).

[3] *Synthesis and Crystal Growth of Tetragonal β-$Fe_{1.00}Se$*
C. Koz, M. Schmidt, H. Borrmann, U. Burkhardt, S. Rößler, W. Carrillo-Cabrera, W. Schnelle, U. Schwarz, and Yu. Grin, Z. Anorg. Allg. Chem. **640**, 1600 (2014).

[4] *Solitonic spin-liquid state due to violated Lifshitz condition in $Fe_{1+y}Te$*
Ph. Materne, C. Koz, U. K. Rößler, M. Doerr, T. Goltz, H. H. Klauss, U. Schwarz, S. Wirth and S. Rößler, accepted for publication in Phys. Rev. Lett. (2015).

[5] *Emergence of an incipient ordering mode in FeSe*
S. Rößler, C. Koz, L. Jiao, U. K. Rößler, F. Steglich, U. Schwarz and S. Wirth, Phys. Rev. B **92** 060505(R) (2015).


### *1.6.2. Heavy fermion materials (Physics of Correlated Matter, Physics of Quantum Materials, Chemical Metals Science, Solid State Physics)*

We continued our study of strong correlations in heavy fermion metals, in particular by scanning tunneling microscopy and magnetotransport [6]. Thermal and electrical transport measurements on $YbRh_2Si_2$ combined with renormalized band structure calculations revealed three Lifshitz transitions associated with the heavy fermion bands [7,8]. In the Ce-based "115" heavy fermion superconductors two structural modifications could be identified by combining STM and state-of-the-art chemical characterization techniques [9].

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


[6] *Hall effect in heavy fermion metals*
S. Nair, S. Wirth, S. Friedemann, F. Steglich, Q. Si and A.J. Schofield, Adv. Phys. **61**, 583 (2012).

[7] *Lifshitz transitions and quasiparticle de-renormalization in $YbRh_2Si_2$*
H. R. Naren, S. Friedemann, G. Zwicknagl, C. Krellner, C. Geibel, F. Steglich and S. Wirth, New J. Phys. **15** (2013) 093032.

[8] *Interplay between Kondo suppression and Lifshitz transitions in $YbRh_2Si_2$ at high magnetic fields*
H. Pfau, R. Daou, S. Lausberg, H. R. Naren, M. Brando, S. Friedemann, S. Wirth, T. Westerkamp, U. Stockert, P. Gegenwart, C. Krellner, C. Geibel, G. Zwicknagl and F. Steglich, Phys. Rev. Lett. **110** (2013) 256403.

[9] *Structural investigations of $CeIrIn_5$ and $CeCoIn_5$ on macroscopic and atomic length scales*
S. Wirth, Y. Prots, M. Wedel, S. Ernst, S. Kirchner, Z. Fisk, J.D. Thompson, F. Steglich and Y. Grin, J. Phys. Soc. Jpn. **83**, 061009 (2014).

### *1.6.3. New materials with composite anionic lattices (Physics of Correlated Matter, Chemical Metals Science, Solid State Chemistry, Inorganic Chemistry)*

The aim of this project is to design and understand the appearance of super lattices of two or more anions**.** The mixture of at least two anions will, unless a solid solution results, cause new crystal structures to occur with unusual local coordination of the cations, potentially leading to novel properties. Using several alternative synthesis methods we have succeeded in synthesizing, for example, sulfide-oxide and selenium-oxide based low-dimensional spin systems with frustration [10-13].

http://www.cpfs.mpg.de/pcm/CAL-Valldor

[10] *S = 2 Spin ladders in the sulfide oxide $BaFe_2S_2O$*
M. Valldor, P. Adler, Y. Prots, U. Burkhardt, and L.H. Tjeng, Eur. J. Inorg. Chem. **36**, 6150 (2014).

[11] *$Ba_3V_2S_4O_3$: A Mott insulating frustrated quasi-one-dimensional S=1 magnet*
E.J. Hopkins, Y. Prots, U. Burkhardt, Y. Watier, Z. Hu, C.-Y. Kuo, J.-C. Chiang, T.-W. Pi, A. Tanaka, L.H. Tjeng, and M. Valldor, Chem. Eur. J. **21**, 7938 (2015).

[12] *Synthesis and characterization of frustrated spin ladders $SrFe_2S_2O$ and $SrFe_2Se_2O$*
S.J. Huh, Y. Prots, P. Adler, L.H. Tjeng, and M. Valldor, *Eur. J. Inorg. Chem.* **18**, 2982 (2015).

[13] *Synthesis and characterization of Ba[CoSO]: magnetic complexity in the presence of chalcogen ordering*
M. Valldor, U.K. Rößler, Y. Prots, C.-Y. Kuo, J.-C. Chiang, Z. Hu, T.-W. Pi, R. Kniep, and L.H. Tjeng, Chem. Eur. J. **21**, 10821 (2015).

### *1.6.4. Osmates and novel transition metal oxides (Solid State Chemistry, Physics of Correlated Matter)*

With the iridates showing very intriguing magnetic properties due to the presence of strong spin-orbit coupling in the Ir 5d shell, we also would like to explore the physical properties of the osmates. The Os valence can be 4+, 5+ and 6+, thereby giving possibilities for singlet magnetism to occur ($5d^4$, $J_{eff}$=0), spin-only magnetism ($5d^3$, $S$=3/2), and magnetism with orbital degrees of freedom ($5d^2$, $S$=1/$J_{eff}$=1), assuming an octahedral-like coordination of the Os ions in an insulating compound. We started our project with synthesizing and studying the osmates in the double perovskite structure. Putting in non-magnetic ions on the B sites, we can nicely observe magnetic frustration phenomena for Os $5d^3$ [14] and $5d^2$ [15]. Experiments with Os $5d^4$ ($La_2MgOsO_6$ and $La_2ZnOsO_6$) are underway. In the near future, we will insert different types of magnetic ions on the B sites to also generate a variety of ferromagnetic insulators. Parallel to the double perovskites, we will study osmates in other crystal structures to understand better the interplay between local (atomic) physics and band formation, and in particular, the effectiveness of the spin-orbit coupling in determining the properties. We would like to mention that within this collaboration we also explore new synthesis routes in order to obtain oxides with meta-stable structures [16].

www.cpfs.mpg.de/1462773/oxides
http://www.cpfs.mpg.de/pcm/Os-spin-orbit

[14] *Magnetically frustrated double perovskites: synthesis, structural properties, and magnetic order of $Sr_2BOsO_6$ (B = Y, In, Sc)*
A.K. Paul, A. Sarapulova, P. Adler, M. Reehuis, S. Kanungo, D. Mikhailova, W. Schnelle, Z. Hu, C.-Y. Kuo, V. Siruguri, S. Rayaprol, Y. Soo, B.H. Yan, C. Felser, L. H. Tjeng, and M. Jansen, Z. Anorg. Allg. Chem. ***641***, 197 (2015)

[15] *$Sr_2MgOsO_6$: A frustrated $Os^{6+}$ ($5d^2$) double perovskite with strong antiferromagnetic interactions*
A. Sarapulova, P. Adler, W. Schnelle, D. Mikhailova, C. Felser, L.H. Tjeng, and M. Jansen, Z. Anorg. Allg. Chem. ***641***, 769 (2015)

[16] *$Pb_2PdO_2(OH)_2$ and $Pb_2PdO(OH)_4(H_2O)$: synthesis and crystal growth at ambient conditions*
A.C. Komarek, P. Merz, H.J. Guo, E. Suard, J.-M. Chen, C. Felser, and M. Jansen, Z. Anorg. Allg. Chem. ***641***, 1473 (2015)

### *1.6.5. High-field investigation of Heusler compounds for magnetoelectronics and magnetocalorics (Solid State Chemistry, Physics of Quantum Materials)*

Experiments in high magnetic fields are essential for the understanding of the multi-functional properties found in Heusler alloys. In close cooperation with the Solid State Chemistry Department we investigated the exchange-bias effect in Mn–Pt–Ga Heusler alloys in static and pulsed magnetic fields at the High-Magnetic Field Laboratories in Nijmegen and Dresden. Our finding of an exceptionally high exchange-bias in a compensated ferrimagnet may lead to the development of magneto-electronic devices and rare earth-free exchange-biased hard magnets [17,18]. Pulsed-field experiments, furthermore, permit us to study materials on fast time scales between 10 ms and 1s, which allowed us to probe Ni-Mn-In shape-memory Heusler alloys for the prospective use in magnetocaloric cooling devices. Our results show that the structural and magnetic contributions to the magnetocaloric effect as well as the irreversible behavior observed at the

martensitic transition have to be carefully considered for future cooling applications [19].

http://www.cpfs.mpg.de/pqm/Heuslers-Nicklas
www.cpfs.mpg.de/nayak

[17] *Large Zero-Field Cooled Exchange-Bias in Bulk $Mn_2PtGa$*
A. K. Nayak, M. Nicklas, S. Chadov, C. Shekhar, Y. Skourski, J. Winterlik, and C. Felser, Phys. Rev. Lett. **110**,127204 (2013).

[18] *Design of compensated ferrimagnetic Heusler alloys for giant tunable exchange bias*
A. K. Nayak, M. Nicklas, S. Chadov, P. Khuntia, C. Shekhar, A. Kalache, M. Baenitz, Y. Skourski, V. K. Guduru, A. Puri, U. Zeitler, J. M. D. Coey and C. Felser, Nature Mater. **14**, 679 (2015).

[19] *Direct measurements of the magnetocaloric effect in pulsed magnetic fields: The example of the Heusler alloy $Ni_{50}Mn_{35}In_{15}$*
M. Ghorbani Zavareh, C. Salazar Mejía, A. K. Nayak, Y. Skourski, J. Wosnitza, C. Felser, and M. Nicklas, Appl. Phys. Lett. 106, 071904 (2015).

### *1.6.6. Topological Weyl Semimetals (Solid State Chemistry, Physics of Quantum Materials, Physics of Unconventional Metals and Superconductors, Chemical Metals Science)*

In condensed matter science, topological materials including Weyl semimetals are a hot topic. Several groups of the institute have joined forces to form a team working at the forefront of Weyl semimetal research. The Weyl fermion, which was first introduced in theoretical high-energy physics, has now been discovered as an emergent quasiparticle in a material class including NbP, TaP and TaAs. A Weyl semimetal (WSM) is a semimetal regarded as the 3D analogue of graphene, wherein the electronic bands linearly disperse around pairs of nodes, the Weyl points, of fixed (left or right) chirality. We have been carrying out pioneering experimental research on WSM materials (Nb,Ta)(P,As) with the guidance of theoretical calculations [20]. A giant, positive magneto-resistance (MR), and ultrahigh mobility, accompanied by strong Shubnikov–de Haas (SdH) and de Haas-van Alphen oscillations was found in NbP [21]. An important piece of the puzzle was the precise determination of the Fermi surface and the distance of the Weyl points to the Fermi energy in TaP [22]. Potential applications are in electronics such as valleytronics and spintronics.

www.cpfs.mpg.de/yan
www.cpfs.mpg.de/Weyl_semi_metals_Hassinger

[20] *Topological surface states and Fermi arcs of the noncentrosymmetric Weyl semimetals TaAs, TaP, NbAs, and NbP,*
Y. Sun, S.-C. Wu, and B. Yan,, Phys. Rev. B 92, 115428 (2015)

[21] *Extremely large magnetoresistance and ultrahigh mobility in the topological Weyl semimetal NbP,*
Ch. Shekhar, A. K. Nayak, Y. Sun, M. Schmidt, M. Nicklas, I. Leermakers, U. Zeitler, Yu. Skourski, J. Wosnitza, H. Borrmann, W. Schnelle, Yu. Grin, C. Felser, B. Yan, Nature Physics **11** (2015) 645, DOI:10.1038/nphys3372 preprint arXiv:1502.04361

[22] *Large and unsaturated negative magnetoresistance induced by the chiral anomaly in the Weyl semimetal TaP,*
Ch. Shekhar, F. Arnold, S.-C. Wu, Y. Sun, M. Schmidt, N. Kumar, A. G. Grushin, J. H. Bardarson, R. Donizeth dos Reis, M. Naumann, M. Baenitz, H. Borrmann, M. Nicklas, E. Hassinger, C. Felser, B. Yan, under review, preprint arXiv: 1506.06577

### *1.6.7. NMR as a local probe for ferromagnetic quantum criticality in Fe-based systems (Physics of Quantum Materials, Chemical Metals Science, Physics of Correlated Matter)*

Our ongoing NMR study on various 3d-electron systems focuses mainly on understanding ferromagnetic quantum criticality. In particular, we study the local fluctuations around a quantum critical point (QCP) and aim to expose the real nature of the magnetic fluctuations (antiferromagnetic (afm) - versus ferromagnetic (fm) - correlations) by temperature- and field-scaling. Among Fe-based systems our search for new quantum critical matter has various approaches. The first is to study weak itinerant 3d-paramagnets at the verge of magnetic order, the second one involves studying Fe containing cage systems (aluminides) [23] and the third one is on doped Fe-based semimetals [24].

http://www.cpfs.mpg.de/pqm/Fe-crit-Baenitz

[23] *Contiguous 3d and 4f Magnetism: Strongly Correlated 3d Electrons in $YbFe_2Al_{10}$*
P. Khuntia, P. Peratheepan, A. M. Strydom, Y. Utsumi, K.-T. Ko, K.-D. Tsuei, L.H. Tjeng, F. Steglich, and M. Baenitz, Phys. Rev. Lett. **113**, 216403 (2014).

[24] *Towards ferromagnetic quantum criticality in $FeGa_{3-x}Ge_x$: $^{71}Ga$ NQR as a zero-field microscopic probe*
M. Majumder, M. Wagner-Reetz, R. Cardoso-Gil, P. Gille, F. Steglich, Yu. Grin, and M. Baenitz, submitted to Phys. Rev. Lett. (2015) / arXiv:1510.01974.

## 1.7. Emeritus Research Group Solid State Physics (F. Steglich)

Since his retirement in 2012 Frank Steglich has been Director Emeritus at the MPI for Chemical Physics of Solids. At the same time, he became Distinguished Guest Professor at the Institute of Physics (IOP), Chinese Academy of Sciences (CAS), Beijing (China) as well as Quishi Distinguished Guest Professor and Founding Director of the Center for Correlated Matter (CCM) at Zhejiang University (ZJU), Hangzhou (China). His research activities at these affiliations have been devoted to phenomena of and materials containing strongly correlated electron systems. Here, the major topics are the entanglement of itinerant and localized electrons in metallic systems with open *f*- or *d*-shells (Kondo effect, Kondo lattice), the Mott-type metal-insulator transition, the magnetic and superconducting properties associated with both phenomena, non-centrosymmetric superconductors as well as thermoelectric materials.

In strongly correlated materials, unconventional superconductivity frequently develops at the border of magnetic, mainly antiferromagnetic (AF), order. As exemplified by the *f*-electron based heavy-fermion (HF) metals, the suppression of the AF order by some non-thermal control parameter like pressure or magnetic field opens up a wide parameter range where the physics is governed by an underlying quantum critical point (QCP). Two variants of AF QCPs have been predicted theoretically and, meanwhile, established experimentally, i.e., the itinerant, spin-density-wave (SDW), QCP (J.A. Hertz, Phys. Rev. B **14**, 1165 (1976, A.J. Millis, Phys. Rev. B **48**, 7183 (1993)) and its local, Kondo-destroying, counterpart (Q. Si et al., Nature **413**, 804 (2001); P. Coleman et al., J. Phys.: Condens. Matter **13**, R 723 (2001)). Unconventional superconductivity in very different material classes, e.g., HFs, cuprates, organics and Fe-based superconductors, is often discussed in terms of an attractive electron-electron interaction provided by quantum critical fluctuations associated with an SDW-type instability. This could be nicely exemplified by O. Stockert via inelastic neutron scattering for $CeCu_2Si_2$ [1]. Also, in collaboration with the teams lead by E. Schuberth (Walter Meissner Institute, Bavarian Academy of Sciences, Garching), Q. Si (Rice University) and the group of M. Brando (MPI CPfS) we could very recently demonstrate that in the canonical material for *local* quantum criticality, $YbRh_2Si_2$, HF superconductivity occurs at $T_c$=2mK, i.e., well below the Néel temperature $T_N$=70mK [2]. Here, some unique form of AF order between nuclear spins strongly competes with the primary electronic order and, thus, enables the system to approach its underlying QCP and eventually become a superconductor. Our findings highlight a novel approach of magnetic-field-induced QCPs and provide a new link between the unconventional superconductivity of the HF metals and that occurring in other material classes like those mentioned before.

The Kondo destroying quantum criticality in $YbRh_2Si_2$ was intensively studied during the last period, via combined heat and charge transport at very low temperatures and in magnetic fields in the Dissertation of H. Pfau [3]. She discovered for the first time ever a violation of the Wiedemann Franz law, a principle of fundamental importance in metal physics. This implies a shortcoming of both, Landau's celebrated Fermi liquid theory and his standard model to adequately describe critical phenomena based on the fluctuations of an order parameter [4]. This discovery has helped to unravel the *dynamical* nature of the Kondo breakdown QCP in $YbRh_2Si_2$, i.e., being due to quasiparticle-quasiparticle scatterings that persist down to zero temperature and cause an almost ≈ 10% enhancement of the residual electronic thermal resistivity compared to its electrical counterpart. Alternative theoretical concepts of the unconventional QCP in this material, invoking either a Lifshitz transition (A. Hackl and M. Vojta, Phys. Rev. Lett. **106**, 137002 (2011)) or a "critical Fermi liquid" (P. Wölfle and E. Abrahams, Phys. Rev. B **84**, 041101 (2011)), could be recently excluded [5-7]: The latter are not apt to explain the experimentally demonstrated abrupt Fermi-surface change at the QCP of $YbRh_2Si_2$ (see previous Scientific Reports and [4,8,9]). Further consequences of the Kondo-breakdown quantum criticality, e.g., for the occurrence of a ferromagnetic instability [10-12] which is prohibited in itinerant metals (D. Belitz et al., Phys. Rev. Lett. **82**, 4707 (1999)), have to be explored by future work. In addition, multiple quantum phase transitions utilizing different tuning parameters [13] non-Fermi-liquid phases arising under chemical pressure due to Kondo disorder [14] and intermediate valence [15] are timely topics and deserve further investigation.

Unconventional (i.e., non-phonon mediated) superconductivity discovered in our group [16} - with a seemingly *conventional*, i.e., isotropic, energy gap as recently observed for $CeCu_2Si_2$ [17] is the subject of ongoing theoretical studies by Q. Si and collaborators at Rice University, Houston (USA) as well as penetration-depth measurements by H.Q. Yuan's team at CCM, Hangzhou (China). This latter group has also been focusing, within the MPI CPfS Partner Group at ZJU and in collaboration with M. Nicklas, on superconductivity in materials that lack inversion

symmetry [18]. They include classical, phonon-mediated, superconductors with *unconventional*, i.e., odd-parity, pair states and are also discussed in the context of topological superconductors.

One of the most promising future topics in the physics of correlated matter is to explore heavy-fermion phenomena, as those exemplified in *f*-electron-based lanthanide and actinide materials, in *d*-electron-based transition metal compounds ("*f-d* connection"). The latter include HF superconductors, like $YFe_2Ge_2$ as discovered by M. Grosche's group at the University of Cambridge, UK (Y. Zou et al., Phys. Status Solidi RRL **8**, 928 (2014)), as well as the Cr- and Mn-based high-pressure superconductors CrAs (W. Wu et al., Nature Commun. **5**: 5508 (2014)) and MnP (J.-G. Cheng et al., Phys. Rev. Lett. **114**, 117001 (2015)), discovered by the group of J.L. Luo at the IOP in Beijing, China in collaboration with the one lead by Y. Uwatoko at ISSP, University of Tokyo (Japan). Furthermore, G.H. Cao's team at ZJU in Hangzhou (China) reported the first Cr-based HF superconductor at ambient pressure: $K_2Cr_3As_3$ (J.-B. Bao et al., Phys. Rev. X **5**, 011013 (2015)). Some Fe-based compounds, in which a low-temperature crossover from itinerant to localized 3*d*-electrons was recognized, have also become of timely interest. Thus, for instance, the exemplary material $YbFe_2Al_{10}$ was intensively studied by M. Baenitz and coworkers, in collaboration with L.H. Tjeng's group and A.M. Strydom from the University of Johannesburg (South Africa) [19]. Of great relevance for both basic science and technical applications are some Fe-based correlated semiconductors, such as FeSi [20] and $FeSb_2$ [21]. Thorough studies on these materials in collaboration with P. Sun, IOP, CAS, Beijing (China) have opened a new way towards large Seebeck coefficients and thermoelectric power factors through charge-mobility engineering, as exemplified for Ni-doped $CoSb_3$ [22]. A striking example for this scheme was provided with $CeCu_2Si_2$, where the fundamental process of on-site Kondo scattering of the unrenormalized conduction electrons from the localized 4*f*-shells of the $Ce^{3+}$ ions was found to semi-quantitatively explain the bizarre Seebeck coefficient down to temperatures which are, at least, an order of magnitude *lower* than the coherence temperature $T_{coh}$ [23]. For $CeCu_2Si_2$, the latter turned out to be identical to the Kondo temperature $T_K \approx 20$K, as expected for stoichiometric Kondo lattice systems, such as $CeNi_2Ge_2$ (A.P. Pikul et al., PRL **108**, 066405 (2012)) and $YbRh_2Si_2$ (S. Ernst et al., Nature **474**, 362 (2011)). The Fe-based small-gap semiconductors discussed above are phenomenologically related to the *f*-electron-based "Kondo insulators", which had been explored in great detail together with Yu. Grin's group in the past (see previous Scientific Reports). Among them, $SmB_6$ plays a special role as the first potential *Topological Kondo Insulator*. This compound has been intensively studied via scanning tunneling microscopy (STM) and spectroscopy (STS), powerful new techniques to explore strongly correlated electron systems as recently demonstrated by S. Wirth's group [24]. Concerning further novel experimental probes developed at MPI CPfS, we mention the one introduced by R. Küchler. He has modified a capacitance-based high-resolution dilatometry cell, developed by M. Lang during his PhD work in our group many years ago (M. Lang, Dissertation, TH Darmstadt, 1991, unpublished), to miniaturized dimensions such that it can now be used in commercial PPMS set-ups [25]. He applied this to study details of the Fermi surface of elemental Bi through thermal-expansion-based magnetic quantum oscillation measurements [26].

Joint research between physicists and chemists is at the heart of the MPI CPfS's mission. In this context, the long standing problem of a "non-magnetic Kondo effect" in certain transition metal-pnictogen-chalcogenides, studied together with the groups of R. Kniep and T. Cichorek (Institute for Low Temperature and Structure Physics, Polish Academy of Sciences, Wrocław (Poland)) was finally solved by S. Kirchner, now at CCM, Hangzhou (China). He could show that the striking two-channel Kondo anomalies in the low-temperature resistivity of ZrAsSe are caused by a dynamic Jahn-Teller effect which incorporates fluctuating bonds in a plane occupied by As only [27]. Detailed investigations on cage-structured clathrates [28] and skutterudites [14] in part discovered in Yu. Grin's group, continue to be exciting. In our joint efforts to uncover new materials with functional properties, the first binary Co-Bi compound, the superconductor $CoBi_3$ was discovered [29,30]. Further on, two structural modifications of the Ce-based "115" HF superconductors first recognized by STM in S. Wirth's group could eventually be unraveled through a careful investigation of the chemical phase diagram, utilizing state-of-the-art characterization techniques by Yu. Grin and collaborators [31]. Also, combined STM, magnetization and transport studies performed by S. Wirth's team in cooperation with U. Schwarz (Department of Chemical Metals Science) reveal for the simplest Fe-based superconducting compound FeSe the occurrence of some type of density wave whose exact nature has yet to be resolved but which, no doubt, is strongly coupled to the spin degrees of freedom [32].

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## 1.8. Emeritus Research Group Inorganic Chemistry (R. Kniep)

### *"From basic research to medical aspects"*

The emeritus position at our institute was first awarded in June 2012 and will end in May 2016. A laboratory for experimental work on principles of biomineralisation together with a qualified technican was available till July 2015. Most of the research projects from previous years have been finished, except for "nitrides" which are continuously under investigation in the group of Juri Grin. The main focus of current research activities was directed on otoconia and their biomimetic analogues. Thousands of these µm-sized, calcite-based specimens (mesocrystals with hierarchical inner architecture) are present in the inner ear of vertebrates, acting as receptor systems for acceleration movements and balance.

The former in-house project "borophosphates" which was part of the BMBF-Verbundprojekt "Resource-efficient Alkane-Selective Oxidation" (033R028C) was closed with a final common publication of the BMBF-project members [1]. Other former projects, such as "low-valency nitridometalates" and "carbometalates" were closed by authorship of a review [2], and a contribution on $Fe_6$-cluster compounds [3], respectively. A common project on "two-channel Kondo physics in ternary pnictide chalcogenides" together with Frank Steglich and the Max-Planck-Partner-Group at the Institute of Low Temperature and Structure Research in Wroclaw (Poland) is close to being completed with a final publication. PbS-organic mesocrystals ("superlattice arrays") were investigated together with TU Dresden; this topic [4, 5] is now continued at University of Konstanz (Dr. Elena Rosseeva). In the research field "biomimetic inorganic/organic composites", the work on calcium oxalate-based pathologic biominerals was finished with a publication on the morphogenesis of CaOx-dihydrate in the presence of PAA [6]. Our extended investigations in "fluorapatite-gelatine nanocomposites" were summarized as a case study in biomimetic crystal research [7]; the hierarchical structure with ordered integration of a protein-fibril pattern gave rise to a recent publication on its polar nature which is closely related to the polar state of natural hard-tissue [8]; details on the real structure of the biomimetic matrix-material representing the so-called mesocrystalline state were also published only recently [9].

The main focus of research activities since 2012 was directed on "otoconia". A close cooperation was established with the University Medicine Mannheim/Heidelberg (Prof. Dr. Leif Erik Walther). Biomimetic otoconia were grown by double-diffusion into gelatine-gel matrices, and represent the very first example of a successful imitation of a biomineral, not only in outer shape but also in composite structure and inner architecture [10]. Nucleation steps and the mode of interaction between ions in aqueous solution and the protein macromolecules were investigated by

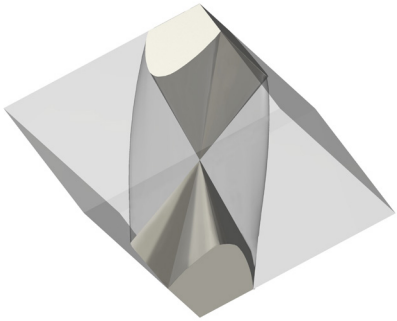

*Fig. 1: Complex inner architecture of an otoconium in crystallographic relation to a cleavage rhombohedron of calcite.*

atomistic simulations [11]. Otoconia consist of nanoparticular calcite (~ 95 wt.-%) intergrown with protein fibrils (~ 5 wt.-%) forming an ordered pattern which takes over control of the development of the inner dumbbell architecture and the surrounding porous belly area of rounded shape (see Fig. 1). As long as the liquid (endolymph) in the inner ear keeps its biogenic chemical composition, otoconia show only gradual changes in morphology (degeneration [12]) during life time. The low stability of calcite, however, clearly explains their sensitivity against any chemical attack [13, 14] which may also be related to complexing drugs [15]. Open questions which have already been started to answer [16] concern: The real density distribution within the volume of otoconia, the local response (movement) of otoconia on acceleration, the significance of intrinsic trace elements, and the development of in-vitro repair scenarios.

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## 1.9. Max Planck Fellow Research Group (M. Ruck)

### *"Resource-Efficient Syntheses and Unconventional Materials"*

Innovative approaches to synthesize inorganic materials with regard to efficient use of energy and raw materials, as well as the creation of novel materials with unforeseeable, yet in anticipation exciting chemical or physical properties are the main scientific interests of our Max Planck fellow group. In the past four years, we discovered, for instance, a benchmark catalyst, an unconventional superconductor, a room-temperature oxide ion conductor, and a new class of topological insulators. We established low-temperature material syntheses in ionic liquids — including the initiation of a DFG priority program on this topic (SPP 1708) — we refined the microwave-assisted polyol process for the directed synthesis of intermetallic nanoparticles and employed topochemistry to access unique metastable phases.

**Topological Insulators [1–5]**

Helical locking of spin and momentum as well as prohibited backscattering are the key properties of topologically protected states in topological insulators. They are expected to enable novel types of information processing such as spintronics by providing pure spin currents, or fault tolerant quantum computation by using the Majorana fermions at interfaces of topological states with superconductors.

We discovered the first so-called weak topological insulator, the bismuth rhodium iodide $Bi_{14}Rh_3I_9$, and showed, in cooperation with physicists from Dresden and Aachen, that sub-nanometer wide electron channels with natural helicity are present at surface step-edges. Scanning tunneling spectroscopy revealed the electron channels to be continuous in both energy and space within a large band gap of 200 meV, thereby, evidencing its non-trivial topology. The absence of these channels in the closely related, but topologically trivial insulator $Bi_{13}Pt_3I_7$ corroborates the channels' topological nature. The back-scatter-free electron channels provide the first observed topologically protected properties of a weak topological insulator. They are a direct consequence of the crystal structure of $Bi_{14}Rh_3I_9$, a stack of 2D topologically insulating, graphene-like bismuth-rhodium layers separated by trivial iodido-bismuthate insulators. Engraving the surface of $Bi_{14}Rh_3I_9$ with an atomic force microscope allows patterning of networks of protected channels with nm precision.

In order to understand the chemical background of the topological properties of $Bi_{14}Rh_3I_9$ related compounds with essentially the same intermetallic honeycomb nets but different spacers and electron counts have been synthesized and evaluated experimentally as well as theoretically. Among

them are $Bi_{13}Pt_3I_7$, $Bi_{38}Pt_9I_{14}$, and $Bi_{12}Pt_3I_5$. Further novel bismuth-based TIs are currently under thorough experimental investigation.

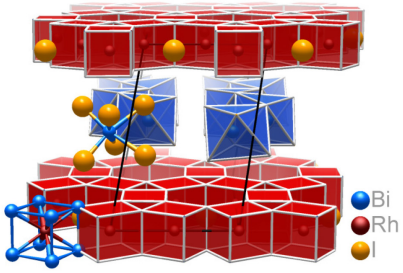



Figure 1: Honeycomb nets of rhodium-centered bismuth cubes and iodido-bismuthate spacers in the structure of the TI $Bi_{14}Rh_3I_9$.


[1] *Stacked Topological Insulator Built from Bismuth-Based Graphene-Sheet Analog.* B. Rasche, A. Isaeva, M. Ruck, S. Borisenko, V. Zabolotnyy, B. Büchner, K. Koepernik, C. Ortix, M. Richter, J. van den Brink, Nat. Mater. **12**, 422 (2013),

[2] *Bismuth-based candidates for topological insulators: Chemistry beyond $Bi_2Te_3$.* A. Isaeva, B. Rasche, M. Ruck, Phys. Status Solidi RRL **7**, 39 (2013).

[3] *Subnanometre-wide electron channels protected by topology.* C. Pauly, B. Rasche, K. Koepernik, M. Liebmann, M. Pratzer, M. Richter, J. Kellner, M. Eschbach, B. Kaufmann, L. Plucinski, C. M. Schneider, M. Ruck, J. v.d. Brink, M. Morgenstern, Nat. Phys. **11**, 338 (2015)

[4] *Crystal growth and real structure effects of the first weak 3D stacked topological insulator $Bi_{14}Rh_3I_9$.* B. Rasche, A. Gerisch, M. Kaiser, A. Isaeva, W. Van den Broek, C. Koch, U. Kaiser, M. Ruck, Chem. Mater. **25,** 2359 (2013).

[5] M. Ruck, *Between Covalent and Metallic Bonding: From Clusters to Intermetallics of Bismuth*. In J. Reedijk, (Ed.) *Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Waltham, MA: Elsevier, **2015**. http://dx.doi.org/10.1016/B978-0-12-409547-2.11445-3.


## Inorganic Materials from Ionic Liquids[6–10]

The use of ionic liquids (ILs) as reaction media for the synthesis of inorganic materials can dramatically decrease the reaction temperature and, in parallel, increase yield and purity of the products. The more efficient use of energy and resources reduces the costs of the process and the equipment. This economic advantage goes hand in hand with the ecological benefit of a more sustainable chemistry. An interesting aspect for research and development is that typical limitations of high-temperature syntheses, originating from thermodynamics or kinetics, can be overcome, providing access to low-temperature as well as metastable phases. Going beyond the (often exciting) empirical discovery of unexpected reactivity of solids in ILs and the serendipitous precipitation of known or new materials from ILs, we are interested to learn more about reaction parameters that critically influence the kind of product, its purity and the yield. The ultimate goal is a predictable synthesis of inorganic materials.

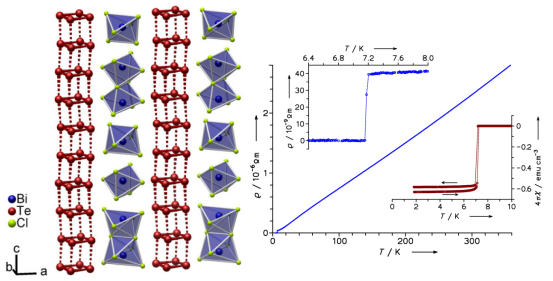



Figure 2: The superconductor $Te_4(Bi_{0.74}Cl_4)$. a) Incommensurate composite structure with $Te_4$ π-stacks. b) Electrical resistivity and low-temperature magnetic susceptibility.

We focused on the chemistry of the heavier elements of the p-block and their compounds. *These readily react in Lewis-acidic ILs, e.g.* $[BMIm]Cl{\cdot}nAlCl_3$, at room temperature or under ionothermal conditions. We learned that complex structured and/or "usually insoluble" compounds are useful starting materials in IL-based synthesis. Cluster fragments can be mobilized in ILs and then recrystallized in a new structural context. If chemical bonding in such units is not strong enough or their charge is too high, partial or full reconstruction takes place. We identified temperature, concentrations, choice of starting materials as well as the employed IL to be decisive for products' compositions and structures. Among the new materials obtained from ILs are a molecular form of the mineral $Bi_2S_3$, the first phosphorus selenium cation $[P_3Se_4]^+$, the spiro-heterocubanes $[Sb_7Se_8Br_2]^{3+}$ and $[Sb_{13}Se_{16}Br_2]^{5+}$, the cluster compounds $[Ru_2Bi_{14}Br_4](AlCl_4)_4$ and $Nb_2(Se_2)_2(AlCl_4)_4$, as well as the pseudo one-dimensional, modulated π-stack superconductor $Te_4(Bi_{0.74}Cl_4)$.


[6] *Substitution of Conventional High-Temperature Syntheses of Inorganic Compounds by Near-Room-Temperature Syntheses in Ionic Liquids.* M. Groh, E. Ahmed, A. Rothenberger, M. Ruck, Z. Naturforsch. **68b**, 1108 (2013).

[7] *Ionothermal Synthesis, Crystal Structure, and Chemical Bonding of the Niobium(IV) Complex $Nb_2(Se_2)_2(AlCl_4)_4$.* U. Müller, A. Isaeva, M. Ruck, *Z. Anorg. Allg. Chem.* **640,** 1564 (2014).

[8] *$[Sb_7Se_8Br_2]^{3+}$ and $[Sb_{13}Se_{16}Br_2]^{5+}$ — Double and Quadruple Spiro-Cubanes from Ionic Liquids.* E. Ahmed, J. Breternitz, M. F. Groh, A. Isaeva, M. Ruck, Eur. J. Inorg. Chem. 3037 (2014).

[9] *$Bi_2S_3$ Bipyramids in Layered Sulfides $M_2Bi_2S_3(AlCl_4)_2$ (M = Ag, Cu).* M. F. Groh, M. Knies, A. Isaeva, M. Ruck, Z. Anorg. Allg. Chem. **641,** 279 (2015).

[10] *Coordination Chemistry of Homoatomic Ligands of Bismuth, Selenium and Tellurium.* M. Ruck, F. Locherer, *Coord. Chem. Rev.* **285,** 1 (2015).

**Topochemical Transformations**[11–13]

Topochemical reactions allow to tailor atomic connectivity and to alter properties of a pre-synthesized compound. Topochemical synthesis starting from non-molecular solids is exceptionally challenging since it requires reorganization of the entire bulk accompanied by long-range diffusion processes. A solid precursor should have both an inert substructure and a substructure that can be altered under moderate reaction conditions. Hence weak ionic and van-der-Waals interactions in rigid frameworks and layered structures favor intercalation, de-intercalation, or substitution.

Bismuth-rich subhalides that comprise transition metals of groups 8 to 10 are prone to reductive de-intercalation of the halide ions owing to their extraordinarily robust intermetallic substructures. Because of the topochemical relation between the precursor and the product, the crystals endure the procedure. In a heterogenous reaction with n-butyllithium (nBuLi) at room temperature, the layered metal-rich compound $Bi_{13}Pt_3I_7$ transforms into the metastable phase $Bi_{12}Pt_3I_5$. While the starting material is a quasi 2D metal, the product is a metallic conductor in 3D. At about 70 °C, complete dehalogenation and formation of metastable $Bi_2Pt$(hP9) are enforced. The latter is a high-temperature phase, classically obtained by annealing at 620 °C.

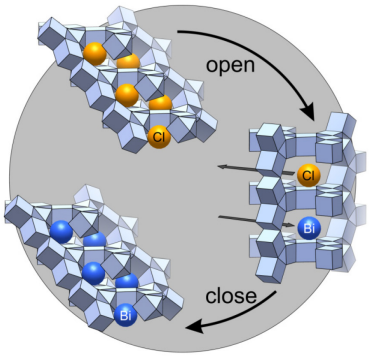



Figure 3: Topochemical transformation of $Bi_{12}Rh_3Cl_2$ into $Bi_{14}Rh_3$.

With little expectation, the topochemical approach was also applied to $Bi_{12}Rh_3Cl_2$, which has its chloride ions embedded in a dense 3D intermetallic framework. Nonetheless, nBuLi removed the chloride ions quantitatively, and, even more surprising, bismuth atoms were re-intercalated topochemically to fill the voids and yield the metastable superconductor $Bi_{14}Rh_3$. We showed that an exceptional breathing mode of the intermetallic framework, similar to those known from some metal-organic frameworks, provides the necessary diffusion paths for the enormous mass transport through the crystal.

[11] *The Topochemical Pseudomorphosis of a Chloride into a Bismuthide.* M. Kaiser, B. Rasche, M. Ruck, Angew. Chem. Int. Ed. ***53***, 3254 (2014).
[12] *Low-Temperature Topochemical Transformation of $Bi_{13}Pt_3I_7$ into the New Layered Honeycomb Metal $Bi_{12}Pt_3I_5$.* M. Kaiser, B. Rasche, A. Isaeva, M. Ruck, Chem. Eur. J. **20**, 17152 (2014).
[13] *$Bi_2Pt$(hP9) by Low-Temperature Reduction of $Bi_{13}Pt_3I_7$: Reinvestigation of the Crystal Structure and Chemical Bonding Analysis.* M. Kaiser, A. I. Baranov, M. Ruck, Z. Anorg. Allg. Chem. **640**, 2742 (2014).

**The Microwave-Assisted Polyol Process**[14-16]

By combination with microwave radiation we established the polyol process as an effective method to produce single-phase micro- or nanoscale intermetallics. Typical reaction temperatures range between 150 and 280 °C, and reaction times of few minutes are sufficient. The polyol acts as solvent, reducing agent for the metal cations, and surfactant for the nuclei and particles. The latter property, in combination with the homogeneous heating by microwaves and their interaction with the metallic seeds, results in very high yields (up to 100 %), small particle-size distributions, and well-shaped isolated crystallites.

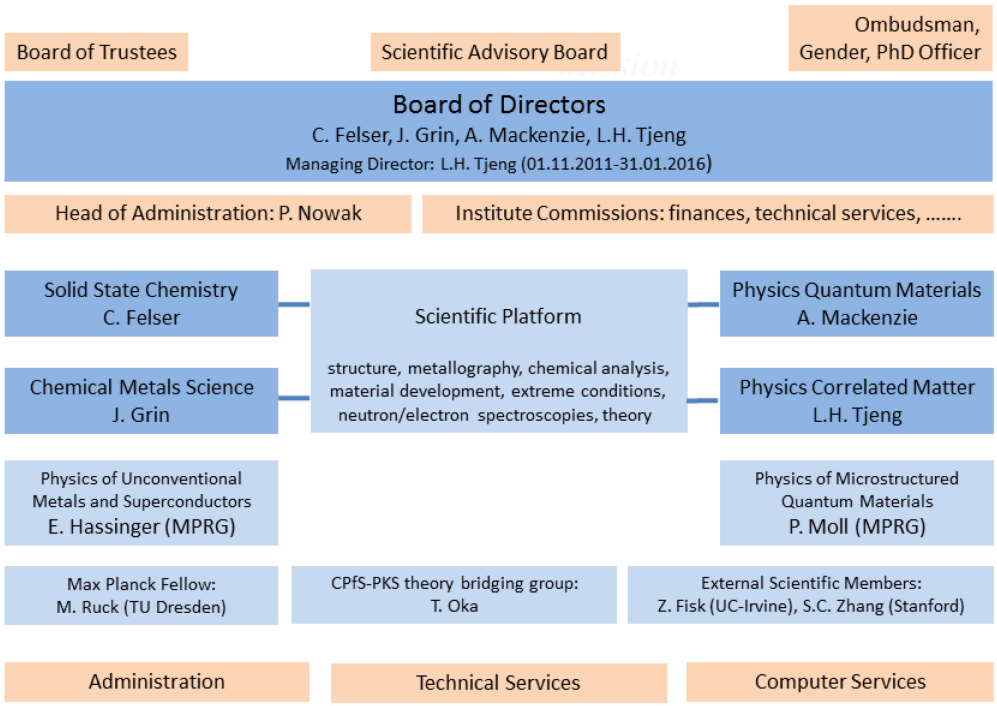
In the binary systems $Bi_nM$ with M = Ni, Rh, or Ir, extraordinary particle-size dependent properties were discovered: nanocrystalline (nc) $Bi_3Ni$ is (ferro-)magnetic, while the bulk is nonmagnetic, and moreover it shows the rare case of coexistence of the antagonists ferromagnetism and superconductivity. Nano-platelets of BiRh proved to be a superior catalyst for the semihydrogenation of acetylene to ethylene in terms of both yield and selectivity. Most intriguingly, nc-$Bi_3Ir$ reversibly activates molecular oxygen and intercalates it at room temperature, forming not only the first oxide ion conductor that operates at room temperature, but also the first that is metallic.

[14] *Semimetallic Paramagnetic Nano-$Bi_2Ir$ and Superconducting Ferromagnetic Nano-$Bi_3Ni$ by Microwave Assisted Synthesis and Room Temperature Pseudomorphosis.* R. Boldt, A. Grigas, M. Heise, T. Herrmannsdörfer, A. Isaeva, S. Kaskel, D. Köhler, M. Ruck, R. Skrotzki, J. Wosnitza, Z. Anorg. Allg. Chem. ***638***, 2035 (2012).
[15] *Full Access to Nanoscale Bismuth-Palladium Intermetallics by Low-Temperature Syntheses.* M. Heise, J.-H. Chang, R. Schönemann, T. Herrmannsdörfer, J. Wosnitza, M. Ruck, Chem. Mater. **26**, 5640 (2014).
[16] *A Metallic Room Temperature Oxide Ion Conductor.* M. Heise, B. Rasche, A. Isaeva, A. I. Baranov, M. Ruck, K. Schäfer, R. Pöttgen, J. P. Eufinger, J. Janek, Angew. Chem. Int. Ed. **53**, 7344 (2014).

# 2. Structure and Organization of the Institute

## 2.1. Structural summary

Following the structural review and staff recruitments mentioned in the Executive Summary, the structure of our Institute can now be conveniently summarized in the following diagram:




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

The Board of Directors of the Max Planck Institute for Chemical Physics of Solids (CPfS) receives advice and recommendations from the Scientific Advisory Board, the Board of Trustees, the Ombudsman (Dr. Peter Höhn), the Officer for gender equality (Dr. Gudrun Auffermann), and the Officer for doctoral matters (Dr. Burkhard Schmidt).

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 crystal structure, metallography, chemical analysis, material development, extreme conditions, neutron/electron spectroscopies, and theory.

A close scientific collaboration with the Technical University Dresden is anchored by the Max Planck Fellowship of Prof. Michael Ruck from the Chemistry Department. Common research activities with the neighboring Max Planck Institute for Physics of Complex Systems (PKS) are carried out and stimulated by the CPfS-PKS bridging group headed by Dr. Takashi Oka. 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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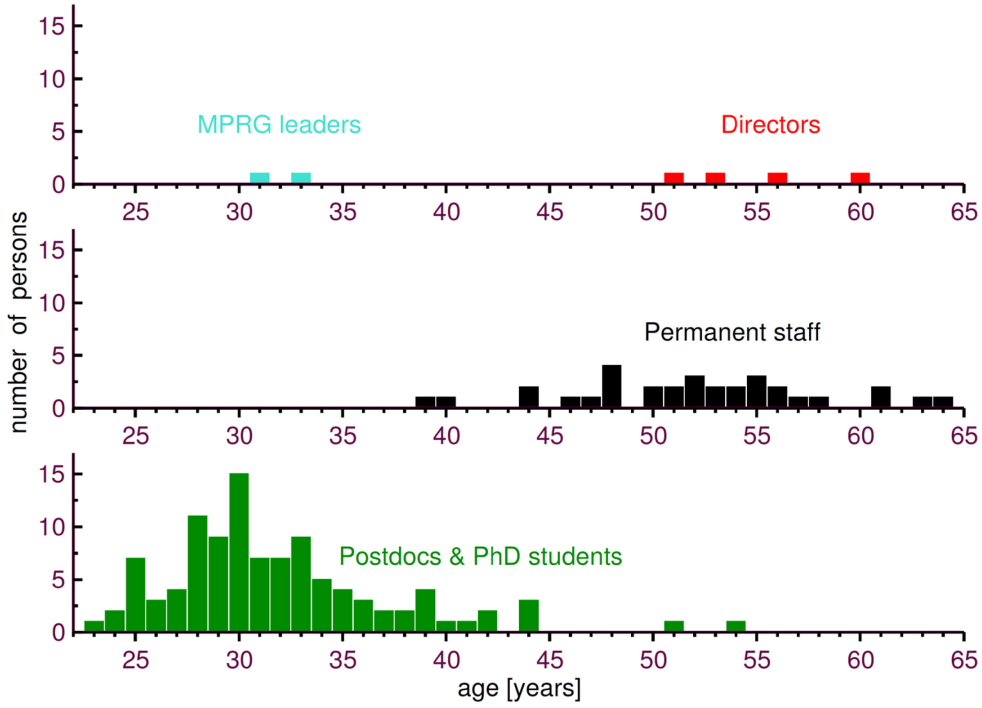
## 2.2. Personnel Structure

The overall structure of the scientific personnel of Institute is most compactly summarized in the following graph showing the age distribution of directors and MPRG leaders, 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. Physics of Quantum Materials has two permanent staff members and oversees six members of the Scientific Platform, abbreviated as (2+6). Physics of Correlated Matter has (2+3), Solid State Chemistry has (3+3) and Chemical Metals Science (5+7). Taking person-month totals and averaging over the assessment period, we had 110 graduate students and post-docs (20 in Physics of Quantum Materials, 22 in Physics of Correlated Matter, 35 in Solid State Chemistry and 33 in Chemical Metals Science).

Of the three categories shown in the above graph, 33% of the directors plus MPRG leaders, 6% of permanent staff scientists, and 36% of post-docs and students (26% of post-docs, 47% 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 Jan. 2016.

## 2.3. Junior and Guest Scientists and Career Development

Over the assessment period we have hosted on average 50 graduate students and 60 post-doctoral research scientists on contracts or stipends at any given time. Since July 2015, in line with Max Planck Society policy, we have established a guest programme in which the offering of stipends is co-ordinated centrally by the Kollegium, which must ratify the offer of any stipendiary guest position.

We take the welfare of our guests seriously, and offer them help with sourcing accommodation and language training. Unfortunately the situation for foreigners in Dresden is challenging, particularly since the rise of the Pegida movement in autumn 2014, and we have taken a number of steps to reassure our staff and attempt to ensure their safety. We would be happy to discuss these with the Advisory Board at the January meeting.

### 2.3.1. PhD students

We encourage our graduate students to co-ordinate their activities, and they run an active programme of seminars, workshops and inter-department leisure activities, co-ordinating with the national PhD net. Their elected representatives make us aware of any on-going issues. Although we believe that our relationship with them is very good, to give them an extra route to discuss potential problems of any kind, we have appointed Dr Burkhard Schmidt as the Institute PhD officer.

We believe that the employability of our graduates is excellent: of those 46 PhD students graduating from the groups of Institute staff in the 2012-2015 time period, 30 found employment in academic research science and 13 in industry, while one has just graduated and is still looking for a job. At the moment of writing we have not been able to track the remaining two PhD graduates. Full details of our PhD students are given in the Addendum.

### 2.3.1. Career development

Another area of emphasis is the career development of our non-Directorial scientific staff. They are encouraged to develop their own profiles through invited conference talks and independent applications for third party funding, as well as appropriate teaching activities. During the assessment period nine have received external job offers, and two more have completed further professional academic qualifications:

- *Marc Armbrüster:* Habilitation TU Dresden, then Professorship in Materials for Innovative Energy Concepts at TU Chemnitz
- *Alexey Baranov:* Habilitation TU Dresden
- *Raul Cardoso Gil:* Guest Professorship, Universidad Tecnica Federico Santa Maria, Valparaiso
- *Sven Friedemann:* Faculty position, Univ. Bristol
- *Roman Gumeniuk:* Professorship in Crystal Physics at TU Bergakademie Freiberg
- *Maurits Haverkort:* Junior Faculty position Vienna University of Technology (declined)
- *Stefan Kirchner:* Professorship, Zhejiang University, Hangzhou
- *Silvia Seiro*: Lectureship, Salzburg University
- *Martin Valldor:* "Venia Legendi", TU Dresden
- *Steffen Wirth:* Professorship, State University of New York, Stony Brook (declined)
- *Binghai Yan:* Associate Professorship, Shanghai Tech University. Takes up post 2016.

We have also advanced the careers of our most talented foreign postdocs by having established a Max Planck Partner Group for Dr. H. Yuan at Zhejiang University in Hangzhou (2010-2015), another for Dr. A. Alekseeva at Moscow State University (2011-2016) and a Max-Planck Indian Fellowship for Dr. Nath at the Indian Institute of Science Education and Research in Thiruvananthapuram (2011-2015).

## 2.4. Equal opportunities

One of our foremost priorities is achieving a good gender balance in our Institute. Female scientists are in notoriously short supply in our field, so our strategy is to create an environment that ensures that we attract more than our fair share of its leading female researchers. This applies at all levels of seniority – we actively recruit top females, whether PhD student, post-doc, staff scientist, group leader or director, and strive to ensure that they flourish here. As well as doing this through informal means, our Gender Equality Officers, Gudrun Auffermann and Renate Hempel-Weber, have also taken a number of formal steps:

*5th August 2013:* Inauguration of the parent-child room. Following requests from members of the Institute, we have made upgrades to adapt to the frequent usage of the room.

*21st February 2014*: Children's day in the Institute.

*4th Sept. 2014*: Talk by Dr. Ulla Weber (Central Gender Equality Officer of the MPS) on „Gender Equality at the Max Planck Institutes" for all members of the Institute.

*September 2014*: Survey on „Equality" offered to all members of the Institute.

*14th November 2014*: Information and discussion for all members of the institute on the „Evaluation of the survey on equality".

*20th March 2015:* Information session: Programmes for MPG female scientists by Anke Hübenthal (MPI for European Legal History, coordinator Minerva-FemmeNet) for all members of the Institute.

*20th March 2015:* Individual consultation with Anke Hübenthal for junior female scientists on promotion within the framework of Minerva-FemmeNet.

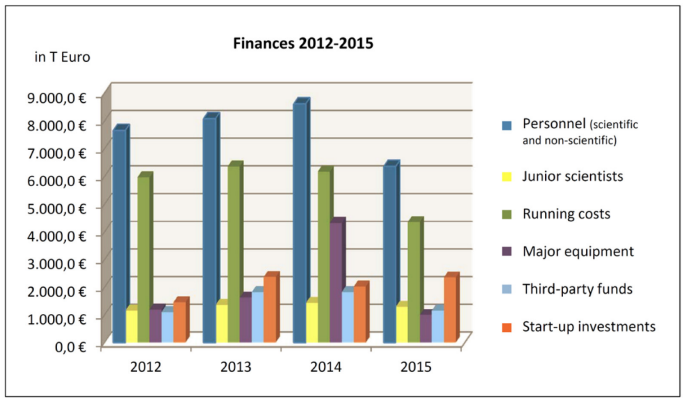
*12th-13th August 2015:* Workshop „Research Funding & Career Development" for junior female scientists, Coach Dr. Beate Scholz, ctc, Bonn/Trier, organization Anke Hübenthal (MPI for European Legal History, coordinator Minerva-FemmeNet).

In addition to these in-house activities, our MPRG leader Elena Hassinger co-ordinates actively with the Max Planck Society's overall MPRG representative Maria Bergemann on gender and child-care issues across the Society, promoting examples of good practice learned from the Canadian Institute for Advanced Research.

As already mentioned above, the current employment situation in our Institute is that 33% of the directors plus MPRG leaders are female, 6% of permanent staff scientists, 26% of post-docs, and 47% of PhD students.

## 2.5. Structure of the Budget, Material Resources, Equipment and Spatial Arrangements

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 January 2016.




The main changes in the physical infrastructure over the assessment period have been the construction and commissioning of new transmission electron microscopy facilities (led by Juri Grin), a thin film laboratory (led by Claudia Felser) and a microstructuring clean room (led by Andy Mackenzie). Spatial arrangments for laboratories are otherwise unchanged and divided pro-rata between departments. The two new Max Planck Research Groups specialize mainly in physics, so have been accommodated in laboratory space from the physics allocation. Office space is at a premium in the building, so Juri Grin led a space efficiency review whose first phase resulted in the creation of 12 new places, and whose second phase will create approximately 50 new spaces in an extension to our building planned for 2016.

## 2.6. Cooperation with National and International Research Institutes and Companies

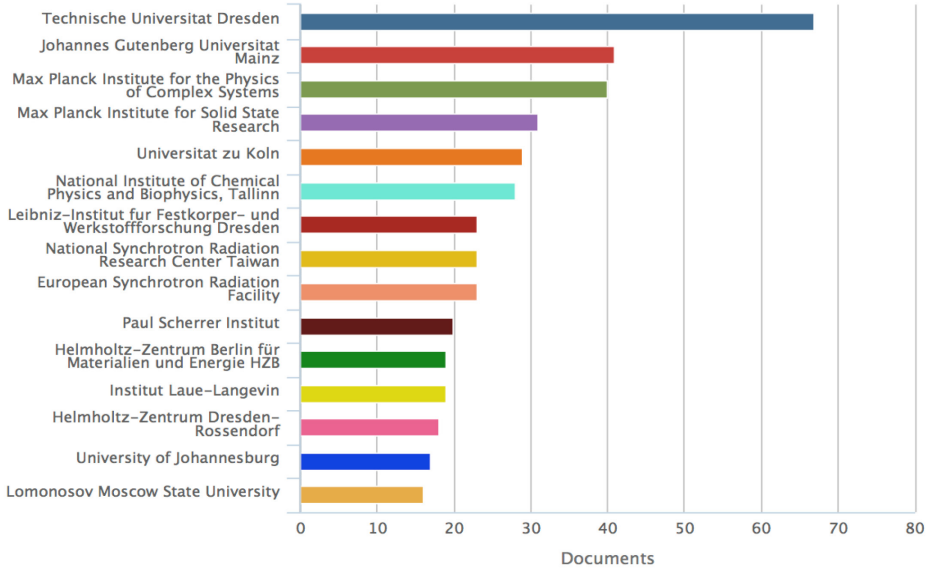
In keeping with the nature of our field, a large proportion of our work is collaborative with partners outside our Institute. We prefer to keep these collaborations informal and therefore administratively light-touch wherever possible, but also run a number of formalized collaborations when the links 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 NSRRC-Taiwan and NSTU-Taiwan, and the establishment of the Max-Planck-Center POSTECH Complex Phase Materials in Korea. Juri Grin leads the collaboration with the National Institute of Materials Science in Japan, Shanghai University in China, ITNBS of the Polish Academy of Science, and Andy Mackenzie co-ordinates the Institute's collaboration with the University of St Andrews under the umbrella agreement of the International Max Planck Partnership between the Max Planck Society and the Scottish Universities Physics Alliance. A formal agreement will also be drawn up with TU Dresden and the University of St Andrews as part of setting up the International Max Planck Research School on Chemistry and Physics of Quantum Materials.

### 2.6.2. Scientific Partners (from publications)

The most concrete evidence of our collaborative science comes from an analysis of our publications. During the assessmemt period, we jointly authored papers with more than 150 institutions elsewhere in Germany and beyond. The top 15 of these are shown below; a full list in alphabetical order can be found in the Addendum.




### 2.6.3. Industrial Partners and Patents

Our main industrial collaborations are with major international companies such as Bosch, IBM, Schott, Western Digital (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.

Clifford Hicks has applied for patents in 2013 and 2015 involving piezoelectric actuators, and Claudia Felser *et al.* in 2015 for rare-earth free permanent magnets. Juri Grin *et al.,* received between 2012 and 2015 several patents on intermetallic compounds as catalysts.

### 2.6.4. Research Grants

Our members are partners in one DFG Collaborative Research Center (with TU Dresden), one DFG Transregional Collaborative Research Center, one Research Training Group (with TU Dresden), three DFG Research Units, seven DFG Priority Programmes, six DFG Individual Grants, one Volkwagen-Stiftung and three BMBF projects. In addition, we are partners in four EU and international grants including one ERC Advanced Grant (held by Claudia Felser).

## 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 and individual institutions. 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 highlight research and associated publications. In the table below, we provide statistics on our volume of publication from September 2012 to September 2015, in a format that shows the extent of inter-departmental publication. The Institute totals are shown in bold; the total outputs of individual departments shown at the end of the table involve some double counting because of the collaborative work.

Definition of labels:
---
M - Physics of Quantum Materials, T - Physics of Correlated Matter, G - Chemical Metals Science, F - Inorganic Chemistry, R – Ruck, K - Kirchner

| Dep. | 2012 | 2013 | 2014 | 2015 | sum |
|---|---|---|---|---|---|
| M | 15 | 38 | 32 | 30 | 115 |
| T | 5 | 30 | 35 | 18 | 88 |
| G | 21 | 50 | 35 | 22 | 128 |
| F | 14 | 61 | 41 | 39 | 155 |
| MT | 3 | 8 | 3 | 3 | 17 |
| MG | 1 | 2 | 3 | 2 | 8 |
| MF | 0 | 6 | 2 | 6 | 14 |
| TG | 4 | 10 | 10 | 5 | 29 |
| TF | 0 | 1 | 1 | 3 | 5 |
| GF | 4 | 14 | 19 | 7 | 44 |
| MTG | 0 | 3 | 1 | 1 | 5 |
| MTF | 0 | 0 | 1 | 0 | 1 |
| MGF | 2 | 3 | 1 | 3 | 9 |
| TGF | 0 | 2 | 6 | 1 | 9 |
| MTGF | 0 | 1 | 1 | 0 | 2 |
| R | 3 | 7 | 10 | 5 | 25 |
| K | 1 | 11 | 4 | 0 | 16 |
| RG | 0 | 0 | 1 | 1 | 2 |
| RF | 0 | 0 | 0 | 1 | 1 |
| MR | 1 | 0 | 0 | 0 | 1 |
| GFR | 1 | 0 | 0 | 0 | 1 |
| KMT | 0 | 2 | 1 | 0 | 3 |
| KMTG | 0 | 0 | 1 | 0 | 1 |
| MTGFK | 1 | 0 | 0 | 0 | 1 |
| **sum** | **76** | **249** | **208** | **147** | **680** |
| sum M | 23 | 63 | 46 | 45 | 177 |
| sum T | 13 | 57 | 60 | 31 | 161 |
| sum G | 34 | 85 | 78 | 42 | 239 |
| sum F | 22 | 88 | 72 | 60 | 242 |

### 2.7.2. Invited talks

During the assessment period, Directors and Emeritus Directors gave approximately 140 plenary, keynote and invited talks at international conferences and workshops, and approximately 60 at individual institutions. Non-directorial staff (staff scientists, post-docs and PhD students) gave approximately 150 conference talks and 100 at individual institutions. Extensive further details of our invited talks and publications can be found in the Addendum.

### 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 topic covered by it. In physics, it has become a far more widely-used verhicle for 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.

### 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:

4. Securing and storing primary data
Primary data as a basis for publications must, as far as possible, be stored for at least ten years on durable, secure carriers in the institutes or research establishments in which they arose. Either the institute or the central organization must ensure that data remains readable for at least this length of time. Access to the data has to be granted for persons with a justifiable interest. Scientific examinations, experiments and numerical calculations can only be reproduced or reconstructed if all the important steps are comprehensible. For this reason, full and adequate reports are necessary, and these reports must be kept for a minimum period of ten years, not least as a source of reference, should the published results be called into question by others. The institute management is responsible for regulating – in a manner suited to the institute's scientific orientation – and setting out in writing all further details and responsibilities, in particular for detailing proper reporting standards and access regulations for the use of data.

## 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**
2013: Fellowship of the American Physical Society (Condensed Matter Physics)
2014: Alexander M. Cruickshank Lecturer Award, Gordon Research Conference
2015: Tsungmin Tu research prize (75 000$) by Ministry of Science and Technology of Taiwan (the highest academic honor granted to foreign researchers in Taiwan)

**Andy Mackenzie**
2012: Fellowship of the American Physical Society (Condensed Matter Physics)
2015: Fellowship of the Royal Society of London

**Juri Grin**
2012 : Guest Professorship at the École Nationale d'Ingénieurs de Caen
2015: Adjunct Professorship of the University of Shanghai for the period 2015-2018

**Hao Tjeng**
2012: Honorary Professorship, National Chiao Tung University, Hsinchu, Taiwan

**Rüdiger Kniep**
2013: Dr. rer. nat. h.c., Universität Stuttgart

**Frank Steglich**
2015: Fellowship of the American Physical Society (Condensed Matter Physics)

**Binghai Yan**
2013: ARCHES Prize from the BMBF

**Alexander Steppke**
2015: Otto Hahn Medal - Max Planck Society

**Catalina Salazar-Mejia**
2013: Best doctoral thesis award 2010-2013: Rosa Elena Simeón, Centro Latino-americano de Física

## 2.9. Service: Committee Work and Teaching

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

### 2.9.1. Committee Work

The Directors and senior scientists of the Institute are members of numerous national and international committees and panels. A list is included in the Addendum.

We would like to mention that Steffen Wirth has received in 2015 the "Outstanding Referee Award" from the American Physical Society.

### 2.9.2. Teaching

Members of our Institute are carrying 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 career 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 September 2012 – September 2015 period, Institute members have given more than 40 lecture courses with a total teaching load of more than 140 SWS (Semester Wochen Stunde = hours per week per semester). This converts approximately to 6-7 different lectures per semester with 3.5 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.

In addition to our teaching in Dresden, we seconded senior scientist Manuel Brando to teach a semester full-time in Goettingen, following a request from the university. Brando is working on his Habilitation and this teaching experience was important for his professional development.

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 neighbouring 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 Programme and Advisory Committees of the majority of the large international conferences in our field.

### 2.10.1. Conferences, Workshops

In the September 2012 – September 2015 period, our Institute has hosted more than 30 workshops and meetings, varying in length between 2 and 5 days and with 30 to 120 participants. A list is given in the Addendum. We would also like to mention that Juri Grin and his team has organized the "34$^{th}$ Annual International Coference on Thermoelectrics and 13$^{th}$ European Conference on Thermoelectrics". This event took place at the Dresden Congress Center from June 28 to July 2, 2015, with more than 800 participants.

### 2.10.2. Seminars

Our Institute has hosted more than 150 seminars and colloquia from external scientists in the assessment period. A list can be found in the Addendum.

## 2.11. Public Relations Work

During the assessment period we have been active in public relations work of various kinds, most standard for a scientific institution, but others, sadly, less so. Our standard work involved making 53 press releases http://www.cpfs.mpg.de/en/pr_events/news and hosting 10 public events. The non-standard activities have been press contact and a number of private meetings with Dresden and Saxony politicians expressing our concerns about the negative effect on our activities of the xenophobia that has been on the increase in the city since the well-publicised rise of the PEGIDA movement.

**TV and newspaper coverage** on current events (PEGIDA) with interviews of institute members

http://www.zdf.de/ZDFmediathek/beitrag/video/2518292/ZDF-heute-journal-vom-19.-Oktober-2015?bc=svp;sv0&ipad=true

http://www.3sat.de/mediathek/?mode=play&obj=54786

http://www.welt.de/politik/deutschland/article148020501/Dresden-zahlt-hohen-Preis-fuer-sein-Pegida-Problem.html

***Juniordoktor activities***

http://www.juniordoktor.de/

2012/13: 2x „Ausflug in die Welt der Symmetrie“,
2x „Reise in die Welt der Symmetrie“,
1x „Diamanten-Vorlesung“
2013/14: „Ausflug in die Welt der Symmetrie“,
„Reise in die Welt der Symmetrie“
2014/15: „Ausflug in die Welt der Symmetrie“,
„Reise in die Welt der Symmetrie“

**Events:**

***Dresden Long Night of Science***
http://www.wissenschaftsnacht-dresden.de/
06.07.2012, 18.00 - 1.00 Uhr, ca. 2600 visitors
05.07.2013, 18.00 - 1.00 Uhr, ca. 3000 visitors
04.07.2014, 18.00 - 1.00 Uhr, 3 shows to 200 visitors; Harry Potter Lectures and experiments

Junior Doctor Seminar at MPI CPfS 2015 (photo: MPI CPfS)

Harry Potter Show, LNW 2014 (photos: MPI CPfS)

Junior Doctor Award 2015 (photo: Matthias Popp)