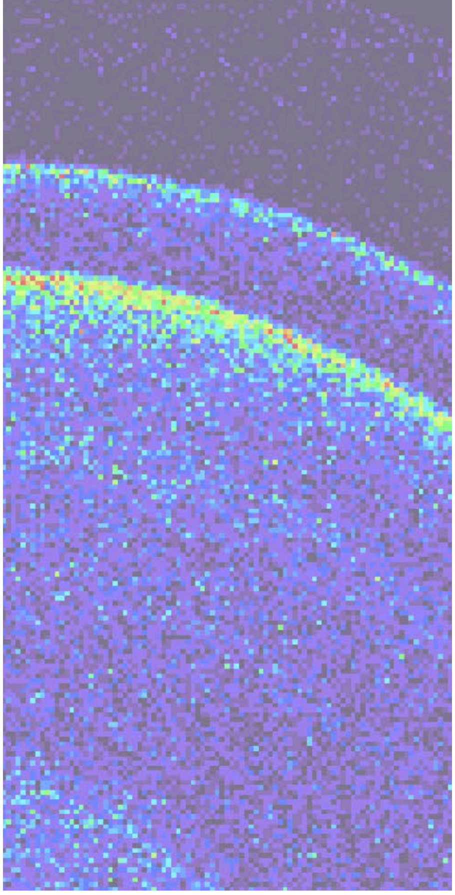
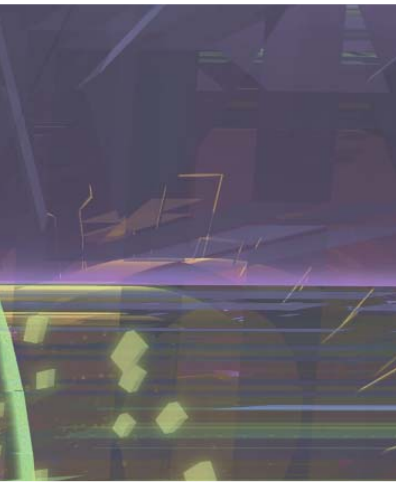
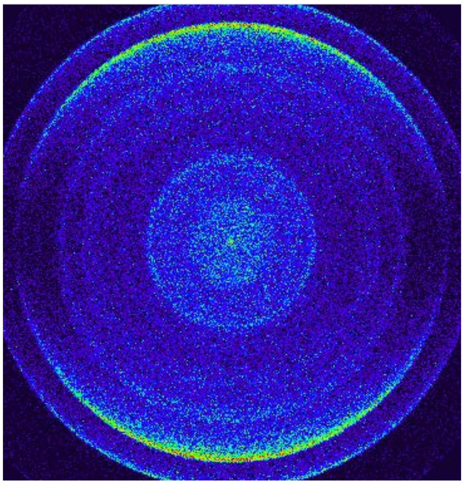
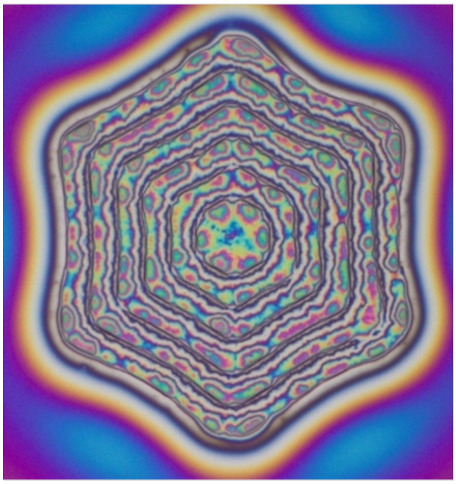
Freiburg Institute of Physics

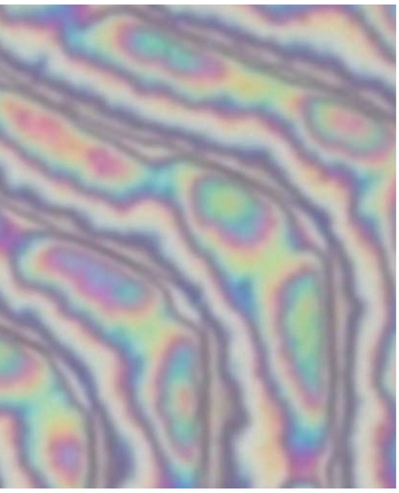
Activity Report 2014-2017

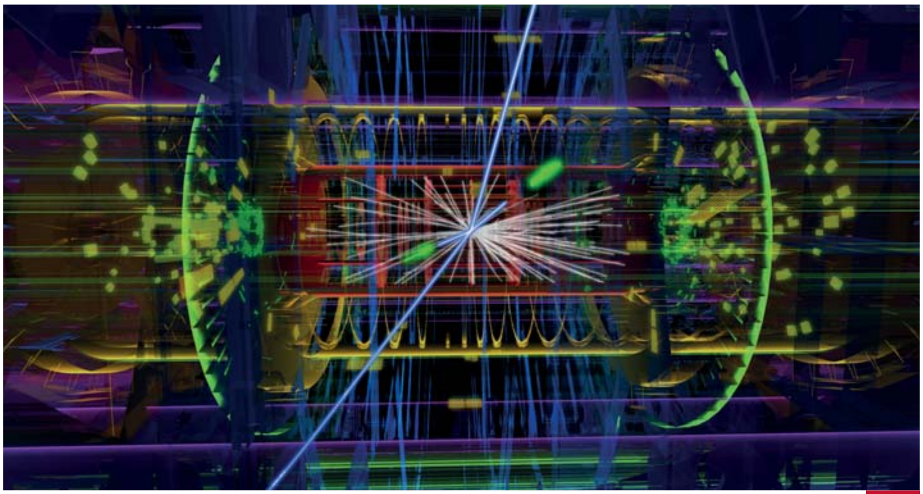












Albert-Ludwigs-Universität Freiburg

UNI
FREIBURG

INSTITUTE OF PHYSICS
UNIVERSITY OF FREIBURG

ACTIVITY REPORT
2014 - 2017

Institute of Physics
Albert-Ludwigs-Universität Freiburg
Hermann-Herder-Str. 3
79104 Freiburg

Front cover
Velocity map imaging detection of photoelectrons emitted from a size-selected Na_3^- cluster, fascinating morphologies of polymer crystals, and a candidate event for a Higgs boson produced in the ATLAS experiment, symbolising the three research areas of the Institute of Physics.

IMPRESSUM

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The Institute of Physics of the University of Freiburg, with the explicit support of the Rectorate of the University, has decided to install an international Scientific Advisory Board (SAB), to consult and advise the institute in all aspects of its academic research and education, on a regular basis.

The present activity report provides a concise description of the scientific activities of the research groups during the years 2014 to 2017, of the teaching and outreach programme, and of the available infrastructure. The part of the scientific activities is divided into three main chapters dedicated to the three main research areas of the institute. The variable structure of these chapters reflects the diverse and lively scientific cultures of the different areas which meet under the roof of this institute.

Following the inaugural meeting of the Scientific Advisory Board on February 17./18., 2014, its 2nd meeting is scheduled for April 12./13., 2018.

Contents

Part I

The Institute of Physics

Chapter caption: Collection of photos providing an impression of the Freiburg Institute of Physics

1.1 Overview of the Institute

The Institute of Physics is part of the Faculty of Mathematics and Physics of the University of Freiburg. Its members conduct research in a wide range of areas, from particle physics and field theory to organic electronics and nano-physics. With currently 22 full professors and 4 co-opted members, the department is of moderate size compared to others in Germany, however, it offers its students a broad range of topics in lectures, seminars and laboratories. The research diversity of the institute which is embedded in the interdisciplinary research landscape defined through the University of Freiburg and other institutions in the larger Freiburg area, e.g., the five Fraunhofer Institutes, as well as the quality of its teaching programme make the institute attractive for national and international researchers and students.

At the end of the year 2017, 575 students are enrolled in Bachelor of Science, Master of Science or Teacher-training studies ("Lehramt"). A total of 125 young researchers work towards their PhD degree, and 62 institute members are at the PostDoc stage of their career. Together with faculty and the administrative and technical staff, our team comprises about 240 individuals who are committed to foster and deliver high-quality academic training and research.

1.1.1 Location and Organization

The Institute of Physics is structured as department, composed of 14 experimental and 9 theoretical research groups which ideally should be located at the central site of the Institute at Hermann-Herder-Straße 3 and 6 (see site map, Fig. 1.1). However, due to substantial lack of laboratory space at the central site, all experimental groups suffer from severe space constraints. This required, for example, to place two groups (Sansone, von Issendorff) outside of the physics campus. The related handicaps have been identified and the accepted, the long standing plan to ease this challenge is a new building right next to the main physics campus (see Fig. 1.1, blue circle). Fortunately, all teaching activities can be carried out at the central site, where also the library of the institute is located. This allows for regular direct contacts between lecturers, the local research staff and students.

Support for the experimental research of the institute is provided by a mechanics and an electronics workshop which both represent crucial elements of the research infrastructure. The central IT-support group, recently formed from personnel previously based at some of the former chairs, is envisioned to ensure the support of the entire institute. It also focuses to support an increasing number of theory groups and their increasing computational demands. The central administration takes care of general management duties, ranging from infrastructure maintenance, management of manpower and staff, to organizing the financial budgets provided by the university as well as third-party funding. It is also responsible for the organization of the teaching programme of the institute, which includes dealing with compatibility issues between the curricula of various study programmes also at other faculties, as the institute offers physics courses for many other faculties (e.g., medicine, biology, chemistry). The central administration is led by the Director of the institute, assisted by the senior manager and the deputy senior manager/head of technical services, while the teaching administration is overseen by the Dean of Studies (see organisation chart, Fig. 1.2). The offices of the Director and the Dean of Studies are executed by professors of the institute for a period of two years (presently by Prof. T. Schätz and Prof. J. Timmer, respectively).

On the institutional level within the University, the Institute of Physics is integrated into the Faculty for Mathematics and Physics. The executive body of the faculty is the Faculty Board, with the Director and

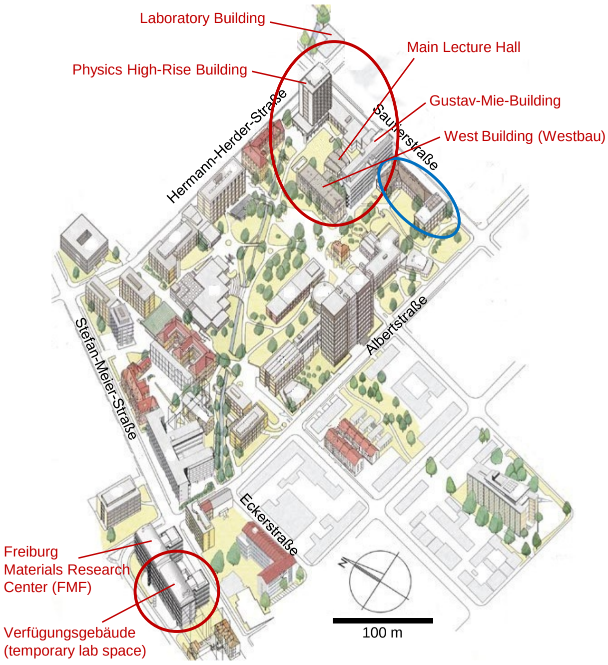


Figure 1.1: Map of the Natural Sciences Campus showing buildings currently employed by the Institute of Physics (red) and site of the prospected new physics building (blue).

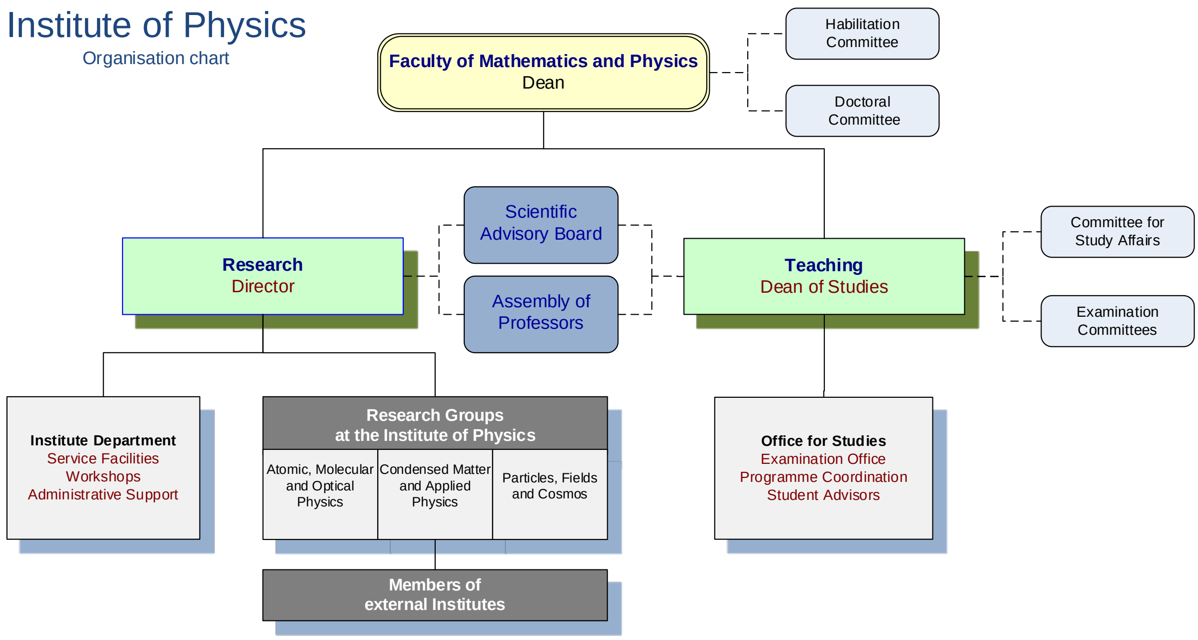


Figure 1.2: Organisation chart of the Institute of Physics. Together with the Institute of Mathematics, the Institute of Physics constitutes the Faculty of Mathematics and Physics.

the Dean of Studies as official members. The Offices of Dean (at present, Prof. G. Herten, Institute of Physics) and Vice-Dean (at present, Prof. W. Soergel, Institute of Mathematics) of the faculty alternate between the Institutes of Mathematics and Physics, in intervals of two years.

1.1.2 Research

The research at the Institute of Physics is organized within three main areas (see Fig. 1.3):

Atomic, Molecular and Optical Sciences: The atomic and molecular physics group, with expertise ranging from mathematical physics over ion trap, Bose-Einstein condensation and Rydberg physics to femtosecond spectroscopy of macromolecular structures, strongly relies on light-matter-interaction. The groups share expertise and interest in controlling systems on the level of individual quanta to permit the detailed analysis from few atoms up to complex structures and transport processes on very diverse scales. The groups combine forces with the Kiepenheuer Institute for Solar Physics, KIS (see Part I, Sec. 1.2).

Condensed Matter and Applied Physics: The broad context of the condensed matter and applied physics research area is the study of classical and quantum theories of complex systems, with a strong computational component, in combination with experimental polymer science, nano-magnetism and photovoltaic research.

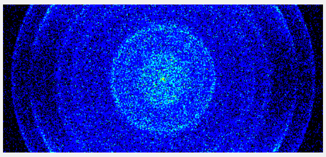
Particles, Fields, Cosmos: The institute accommodates several internationally very visible experimental and theoretical particle physics groups. The experimental programme is mainly focused on experiments at the European Centre for particle physics, CERN, in Geneva/Switzerland. Physicists from the institute have contributed significantly to the discovery of the Higgs boson via their strong involvement in the ATLAS experiment. The newly established astroparticle physics group concentrates on the direct search for dark matter. The theoretical particle physics activities range from precision studies of the strong and electroweak interactions and quantum-field-theoretical aspects to the exploration of model extensions with new theoretical structures.

During this reporting period, the researchers of the Institute of Physics published more than 700 articles in international, peer-reviewed journals. (This does not include publications by researchers from the external institutes, see Section 1.2). Competitive funding from national and international sources (BMBF, DFG, EU, State of Baden-Württemberg, etc.) was attracted, significantly exceeding the direct funding provided by the University. A total of three ERC-grants were received by members of the institute: one Advanced Grant (COCONIS: Stienkemeier, 2016) and two Consolidator Grants (TIAMO: Schätz, 2015; ULTIMATE: Schumann, 2016).

In addition, two important prizes were awarded to

Research Groups at the Institute of Physics

Atomic, Molecular and Optical Physics



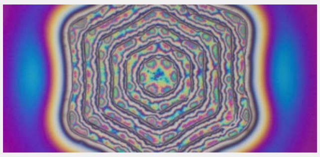
Experimental Physics

- **Cluster and Synchrotron Spectroscopy**
  Prof. T. Lau (PI and HZB)
- **Experimental Attosecond and Laser Physics**
  Prof. G. Sansone
  (successor Helm)
- **Experimental Atomic, Molecular and Optical Physics**
  Prof. T. Schätz
- **Molecular and Nanophysics**
  Prof. F. Stienkemeier
- **Clusterphysics**
  apl. Prof. B. von Issendorff
- **Solar Physics**
  Prof. O. von der Lühe (PI and KIS)
  Prof. S. Berdyugina (PI and KIS)

Theoretical Physics

- **Quantum Optics and Statistics**
  Prof. A. Buchleitner
  apl. Prof. H.-P. Breuer
  Dr. S.Y. Buhmann
  PD A. Rodriguez
  PD T. Wellens

Condensed Matter and Applied Physics



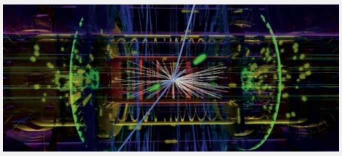
Experimental Physics

- **Experimental Polymer Physics**
  Prof. G. Reiter
- **Nanophysics and Molecular Nanomagnets**
  Prof. O. Waldmann

Theoretical Physics

- **Functional Nanosystems**
  Prof. M. Moseler (PI and IWM)
  PD M. Walter
- **Statistical Physics of Soft Matter and Complex Systems**
  Prof. T. Schilling
  (successor Blumen)
- **Biomolecular Dynamics**
  Prof. G. Stock
- **Theoretical Condensed Matter Physics**
  Prof. M. Thoss
  (successor Grabert)
- **Dynamics in the Life Sciences**
  Prof. J. Timmer
  apl. Prof. T. Filk
- **Theoretical Applied Physics – Computational Physics**
  N.N.

Particles, Fields and Cosmos



Experimental Physics

- **Experimental Particle Physics**
  Prof. B. Heinemann (PI and DESY)
- **Experimental Particle Physics**
  Prof. G. Herten,
  apl. Prof. U. Landgraf
- **Experimental Particle Physics**
  Prof. K. Jakobs,
  Dr. C. Weiser (Interim Professor),
  Hon.-Prof. P. Jenni
- **Experimental Particle Physics**
  Prof. M. Schumacher
- **Experimental Astroparticle Physics**
  Prof. M. Schumann (successor Königsmann)
  apl. Prof. H. Fischer

Theoretical Physics

- **Theory of Particle Physics and Quantum Field Theory**
  Prof. S. Dittmaier
- **Quantum Fields and Particle Phenomenology**
  Prof. H. Ita,
  visiting Prof. F. Febres Cordero
- **Elementary Particle Phenomenology**
  Prof. J. van der Bij

Members of external Institutes

Kiepenheuer Institute, KIS

- **Solar Physics (KIS)**
  Prof. S. Berdyugina,
  apl. Prof. M. Roth,
  apl. Prof. W. Schmidt,
  Prof. O. von der Lühe

University of Freiburg

- **Medical Physics (University Hospital)**
  Prof. M. Bock*
  Prof. J. Hennig*,
- **Bio and Nanophotonics (IMTEK)**
  Prof. A. Rohrbach*
- **Computational Neuroscience (Faculty of Biology)**
  Prof. S. Rotter*

Fraunhofer Institutes

- **Applied Solid State Physics (Fraunhofer IAF)**
  apl. Prof. J. Wagner
- **Theoretical Materials Physics (Fraunhofer IWM)**
  apl. Prof. C. Elsässer,
  Prof. M. Moseler
- **Spectroscopy of Optical Materials (Fraunhofer IPM)**
  PD F. Kühnemann
- **Solar Energy Systems (Fraunhofer ISE)**
  N.N. (successor Weber)

* co-opted members of the Institute of Physics

Figure 1.3: Research groups at the Institute of Physics and at external institutes - status as of January 2018. (PI = Institute of Physics, KIS = Kiepenheuer Institute for Solar Physics, IMTEK = Department of Microsystems Engineering, IWM = Fraunhofer Institute for Mechanics of Materials, IAF = Fraunhofer Institute for Applied Solid State Physics, IPM = Fraunhofer Institute for Physical Measurement Techniques, ISE = Fraunhofer Institute for Solar Energy Systems. Institutes outside of Freiburg: HZB = Helmhotz-Zentrum Berlin, DESY = Deutsches Elektronen Synchrotron Hamburg)

members of the institute: Prof. Jakobs, currently the spokesperson of the ATLAS experiment at CERN, received the Stern-Gerlach-Medal in 2015, the most prestigious award for experimental physics awarded by the German Physics Society (DPG). In 2017, Hon. Prof. Jenni received the W.H.K. Panofsky Prize of the American Physical Society, in recognition of outstanding achievements in experimental particle physics.

During the past years, the institute has seen several important developments:

(i) Four colleagues were retired within the reporting period (Blumen 2016, Grabert 2016, Helm 2015, Königsmann 2015). Identifying and recruiting four full professor was an enormous opportunity to optimize the strategic long-term development of the institute. The newly appointed colleagues are Prof. Tanja Schilling (successor Blumen, from University of Luxembourg), Prof. Michael Thoss (successor Grabert, from University of Erlangen/Nürnberg), Prof. Giuseppe Sansone (successor Helm, from Politecnico di Milano) and Prof. Marc Schumann (successor Königsmann, from University of Bern). Their research topics nicely complement the existing groups, as summarized in Figure 1.3.

(ii) For each of the three research fields, an additional, new position for a professor at the Institute of Physics could be established. These were filled by the new colleagues Prof. Tobias Lau (from Helmholtz Center Berlin) and Prof. Beate Heinemann (from University of California/Berkeley), to further strengthen the collaboration within the fields. The third professorship on Computational Physics is currently being filled.

(iii) With a total of five institutes, Freiburg is the largest site of the Fraunhofer Gesellschaft for applied research in Germany. To further strengthen the cooperation with the local Fraunhofer Institutes, a permanent Fraunhofer professorship was installed at the institute and staffed with Prof. Moseler.

(iv) With the new Master for Applied Physics, an additional master course has been created. It builds on and further deepens the collaboration with the external institutes in Freiburg (KIS, Fraunhofer, etc., see Section 1.2) and was able to attract a sizeable number of students already.

(v) In the context of the new Master for Applied Physics, two new co-optations[1] have been realized to link additional institutes to the Institute of Physics (Medical Physics – Prof. Bock, Bernstein Centre – Prof. Rotter). A third co-optation is in preparation (Fraunhofer ISE – succession of Prof. Weber).

(vi) After approximately three decades of service, the institute's senior manager Klaus Scharpf retired in 2017. Fortunately, we were able to recruit Dr. Vanessa Holzer as highly qualified successor.

1.1.3 Education and Qualification of Young Researchers

The Institute of Physics succeeded to establish two new PhD-schools during this reporting period; a third one could be prolonged:

- The Research Training Group (RTG) *Mass and Symmetries after the Discovery of the Higgs Particle at the LHC* (RTG 2044, funding period 2015–2019),
- the International Research Training Group (IRTG) *Cold Controlled Ensembles in Physics and Chemistry* (IRTG 2079, together with partners at the University of British Columbia at Vancouver, funding period 2015–2019) and
- the International Research Training Group (IRTG) *Soft Matter Science: Concepts for the Design of Functional Materials* (IRTG 1642, together with the Faculty of Chemistry and Pharmacy of the University of Freiburg, and partner groups at Strasbourg and Mulhouse, funding period 2010–2019).

In addition, the institute contributed to the International Training Network (ITN) *HiggsTools* (together with nine partners from eight European countries; funding period 2014–2017). A postdoc cluster on *Quantum Science and Quantum Computation* in collaboration with the University of Basel is in an advanced stage of preparation (envisioned 2018-2027).

During the reporting period, three new junior research groups (Buhmann, Febres Cordero, Kreutz) were established at the Institute of Physics, funded via different sources (DFG, Humboldt Foundation, BMBF). Five junior researchers from the institute (Schelter, Gross, Lai, Mintert and Peifer) received permanent academic positions at Wageningen, Cologne, Göttingen, London and Cologne.

Jun. Prof. Ita was tenured and will continue to work at the Institute of Physics as full Professor. Apl. Prof. Mudrich accepted a full professorship at the University of Aarhus. The institute succeeded in winning and permanently integrating the apl. Profs. Breuer and von Issendorf.

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[1] Co-opted professors have the right to supervise PhD students graduating at the Insitute of Physics and contribute to the teaching programme.

1.2 Associated Institutes and Co-opted Members

In various research fields, the institute has long-term institutional partnerships with other faculties within the University of Freiburg, as well as with external research institutions (see Fig. 1.3). Four colleagues from different Faculties, the Faculty of Biology (1), the Faculties of Medicine (2), and the Department of Microsystems Engineering, IMTEK (1) are co-opted members of the institute.

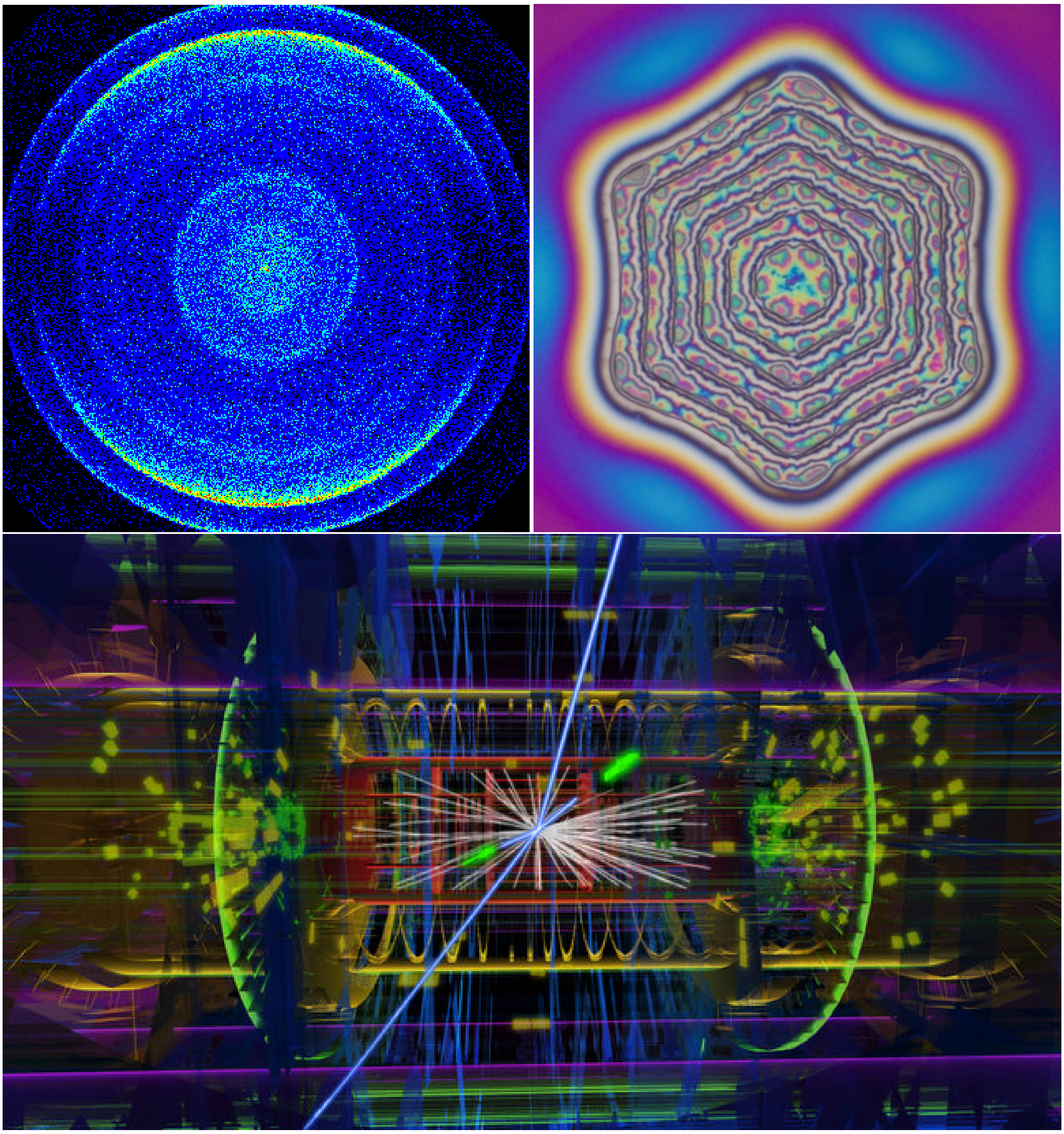
In early 2018, four professors of the Institute of Physics hold joint appointments with external institutes. These are Prof. von der Lühe (*Kiepenheuer-Institut für Sonnenphysik (KIS)* of the Leibniz-Gemeinschaft), Prof. Moseler (*Fraunhofer Institute for Material Mechanics (IWM))*, Prof. Lau (*Helmholtz Zentrum Berlin (HZB)* of the Helmholtz-Gemeinschaft), and Prof. Heinemann (*DESY Hamburg* of the Helmholtz-Gemeinschaft). A successor of Prof. Weber (*Fraunhofer Institute for Solar Energy Systems (ISE)*) has been identified; negotiations with the candidate are currently ongoing.

Several members of the institute conduct research programmes at the Research Centres of the University, such as the *Freiburg Material Research Centre (FMF)*, the *Freiburg Centre for Data Analysis and Modelling (FDM)*, and the *Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien (FIT)*.

The collaboration with the external institutes in Freiburg is further strengthened by the new Master of Applied Physics, which was established together with these institutions. The scope course programme is broadened by lectures and seminars given by the external members, and specific practical courses are installed at the related research institutes. The cooperation with several external institutes is further supported by a new professorship dedicated to computational physics. The negotiations with the applicants are currently in the final phase.

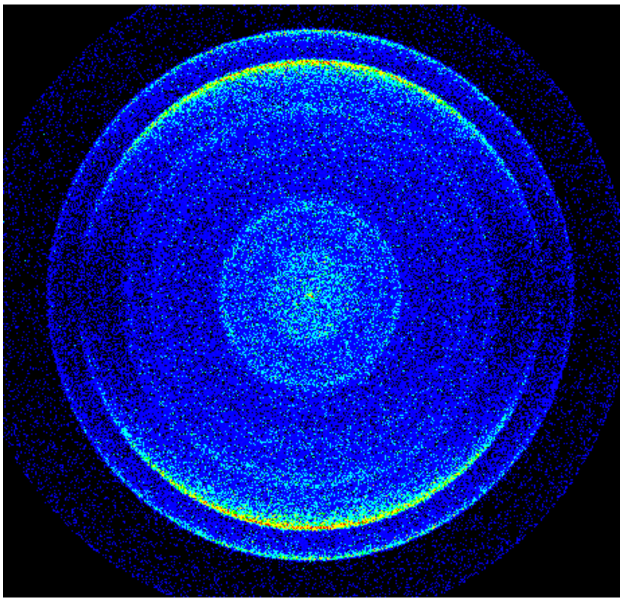
Part II

Scientific Activities 2014 - 2017



Chapter 1

Atomic, Molecular and Optical Sciences



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  Prof. T. Schätz
- **Molecular and Nanophysics**
  Prof. F. Stienkemeier
- **Clusterphysics**
  apl. Prof. B. von Issendorff
- **Solar Physics**
  Prof. S. Berdyugina (PI and KIS)
  apl. Prof. M. Roth,
  apl. Prof. W. Schmidt,
  Prof. O. von der Lühe (PI and KIS)
- **Quantum Optics and Statistics**
  Prof. A. Buchleitner,
  apl. Prof. H.-P. Breuer,
  Dr. S.Y. Buhmann,
  PD A. Rodriguez,
  PD T. Wellens

Chapter caption: Velocity map imaging detection of photoelectrons emitted from a size-selected Na_3^- cluster.

1.1 Overview

Gaining insight into the structural, dynamical and statistical properties of composite quantum systems as well as of astronomical objects lies at the heart of Atomic, Molecular and Optical Sciences (AMO). While effective single particle problems like the hydrogen atom or the two-body Kepler problem can be treated with arbitrary precision, just slightly larger systems like small molecules, clusters, few interacting ions in a trap, photonic multi-mode Fock states, let alone the hydrodynamic convection mediating solar radiation and heat transport challenge the largest supercomputers. This means that approximate descriptions have to be used, which, on the one hand, calls for an as deep as possible understanding of the behavior of small systems and of their constituents, and, on the other, for the development of effective descriptions which, by suitable coarse graining, distill the properties of relevant observables from an overwhelming background density of states. Recent years have seen enormous progresses of the experimental techniques and theoretical concepts to prepare or characterize such systems. This encompasses the preparation of atoms, ions, molecules, clusters or photons at very low temperatures or in well defined states, as well as their confinement or embedding in controlled potential landscapes or host materials, and the development of high level optical techniques and novel telescopes for the observation of stellar objects in diverse spectral ranges. The characterization of photonic, atomic and molecular AMO systems has profited strongly from the continuous development of diverse light sources – which range from single or few photon sources, over high resolution (frequency comb stabilized – with applications also in sun research) continuous, to femto- and attosecond pulsed, or free electron lasers and synchrotrons – and trap design. This is complemented by dedicated theoretical approaches towards an accurate modelling of the relevant force fields and the formulation of versatile spectroscopic protocols, which find applications in the microscopic as well as in the macroscopic realm. The Freiburg Institute of Physics is very active in employing these fantastic new experimental tools, as well as in pushing forward truly innovative theoretical approaches.

A concise description of the individual research groups and their projects will be given in the subsequent sections. Here, we concentrate on the complementary expertise of the groups in theory and experiment that permit to focus symbiotically on common topics of interest.

The theory groups of **S.Y. Buhmann**, **H.P. Breuer**, **D. Gross** (chair at the university of Cologne since 2015), and **A. Buchleitner**, together with the experimental groups of **T. Schaetz** and **H. Helm** (retired in 2015), study the dynamical and statistical features of increasingly complex, composite quantum systems, where quantum light-matter interaction and advanced, higher dimensional trap design play a prominent practical role. Building upon the accurate control of single constituents, these groups monitor complexity *in statu nascendi*, and develop tailored experimental and theoretical tools which directly address the challenge of scalable quantum control.

The extension of the study of atomic quantum objects to complex molecular systems is a central research topic in the group of **F. Stienkemeier**. Low temperature conditions allowing for well defined initial states are established in cold beams as well as helium droplets. Intense electromagnetic fields including XUV free-electron lasers broaden the range of experimental tools to form and study extreme states of matter. PD M. Mudrich, who qualified for his academic career in the Stienkemeier group during the last years, accepted a professorship at the University of Aarhus in Denmark. The group of **B. von Issendorff** has pioneered the structural and thermodynamic study of clusters of atoms, exploring the transition region between the nanoscopic and the microscopic regime, where fundamental properties of matter strongly change as function of size and temperature. The group of **G. Sansone** (succession Helm in 2016) will focus on the generation of trains and isolated attosecond pulses for the time-resolved investigation of nuclear and electronic dynamics in molecules and clusters. In particular, coincidence techniques will be implemented for the characterization of molecular dynamics in the molecular frame. From January 2018 **T. Lau** occupies the new professorship established together with the Helmholtz-Zentrum Berlin. He works in the field of synchrotron spectroscopy of size-selected free clusters, molecules, and complexes with a focus on understanding and controlling their electronic states and magnetic moments. The group of **G. Stock**, which had been presented as part of the AMO section before, is now listed within the ”Condensed Matter and Applied Physics” section. Close collaborations with the AMO section still exist and will be further strengthened.

The Kiepenheuer Institute for Solar Physics (KIS) is associated with the Institute of Physics and pursues topics in theoretical and experimental solar and stellar physics. KIS studies magnetism of the Sun and stars and magnetic phenomena in their atmospheres, in particular atomic and molecular radiation in the presence of magnetic fields, formation and evolution of magnetic structures, magneto-acoustic wave propagation in complex magnetic fields, as well as polarimetric signatures of exoplanets, photosynthetic biopigments and exoplanet surface imaging. KIS designed, built and operates the largest solar telescope in Europe (second largest in the world) and works on image stabilization of ground- and satellite-based observatories using wave-front sensors and adaptive optics.

All of these topics of AMO Sciences at the Institute of Physics are covering a considerable spectrum while remaining closely interlinked. In addition, they are getting strengthened by local, national and international collaborations (elucidated further below). One vision is to address fundamental models and processes in physics and to reveal processes in physical chemistry, sharing the same underlying principles, which could advance our understanding and interdisciplinary interest in chemistry and biological physics. Another motivation is to develop and engineer quantum devices of increasing scale. Two of the recent common research initiatives are briefly presented in the following subsections.

Centre of Excellence for “Quantum Science and Quantum Computing” of the Universities Freiburg and Basel, under the roof of EUCOR - The European Campus (funding period 2018 – 2027).

Largely funded by the Georg H. Endress foundation, quantum research at the Universities of Basel and Freiburg launches the *Georg H. Endress PostDoc Cluster for Quantum Science and Quantum Computing* as the nucleus of a Centre of Excellence dedicated to cross-border, long-term research into modern Quantum Science, integrated into the partner Universities’ long-term strategy to foster focused academic cooperation in the European Campus area. Given the immediate geographic vicinity of both partner institutions, we anticipate that an internationally visible, lively research unit can be established, which merges both sites’ specific and internationally renowned know-how on quantum computation (Basel) and complex quantum systems (Freiburg). The PostDoc cluster will recruit approx. eight to ten PostDocs who will be the pillars of this cooperative endeavour and who will enjoy exposure to the diverse subdisciplines of Quantum Science as represented by the PIs on both sides. On a mid-term perspective, we aim at complementing the PostDoc cluster by other cooperative funding schemes, such as to develop an integrated research and teaching programme which attracts the best talents from the EUCOR area and beyond.

DFG-funded IRTG 2079 ”Cold Controlled Ensembles in Physics and Chemistry“ (funding period 2015 – 2019)

Research Profile

The International Research Training Group (IRTG) aims at significantly advancing the technology and the fundamental understanding of Cold Controlled Atomic and Molecular Ensembles. A wide range of quantum phenomena in physics and chemistry are addressed in a joint binational endeavor. The programme combines experimental groups of the fields of ultracold atoms, ion traps, cold molecules and clusters, and quantum control with femtosecond lasers, and microscopy. The complementary expertise of the theory groups involved (DFT calculations, quantum chemistry, molecular dynamics, reactive scattering, quantum many-body simulations, quantum statistics, molecules in strong fields, macroscopic QED) adds a solid theoretical background to the research program. While the scientific background of all investigators involved is rather broad, they all share the common passion of finding new strategies and conceptions for controlling complex quantum systems.

Training Profile

The IRTG provides a structured doctoral programme including seminars, summer schools, meetings and guest programs. The research is of interdisciplinary character and connects to diverse fields of atomic and molecular physics, quantum optics, condensed-matter physics, and physical chemistry. The involved groups efficiently foster synergy effects in technological developments, scientific achievements as well as for creating a unique training environment for young scientists. All doctoral projects are embedded into binational collaborations and include long-term stays at both locations. Doctoral projects are co-supervised, having one German and one Canadian supervisor. The extended working periods in Freiburg and Vancouver offer a tremendous advantage for the qualification of the doctoral students both for a future career in academia as well as in industry due to the added interdisciplinary and intercultural experiences. In addition, the collaborative research is enhancing the educational programme of the Institute of Physics, from the Bachelor to the PhD level, by dedicated seminars, summer schools, meetings and guest lectures.

Participants
The spokespersons of the international Research Training Network are: F. Stienkemeier (Institute of Physics, Freiburg) and T. Momose (UBC, Vancouver); the group of project leader consists of: A. Buchleitner, S.Y. Buhmann, K. Dulitz, B. v. Issendorff, M. Mudrich, T. Schaetz (Institute of Physics); M. Walter (Fraunhofer Institute for Mechanics of Materials, Freiburg), E. Grant, J. Hepburn, D. Jones, R. Krems, K. Madison, V. Milner (UBC, Department of Chemistry and Department of Physics & Astronomy); Associated Researchers: M. Berciu, M. Litinskaya (UBC, Department of Physics & Astronomy), M. Moseler (Institute of Physics and Fraunhofer Institute for Mechanics of Materials, Freiburg). The recently hired new colleagues G. Sansone and M. Thoss have already joint the program. The graduate school includes more than 20 PhD students and several Postdoctoral fellows in Freiburg and at UBC.

The progress report as well as the proposal for the second 4.5 years funding period has to be filed in this year expecting a continuation of funding until 2024.

1.2 Research Groups

1.2.1 Quantum Optics and Statistics (QOS)

The **Department for Quantum Optics and Statistics (coached by Andreas Buchleitner, together with Heinz-Peter Breuer, Alberto Rodríguez González, Thomas Wellens**, and proudly hosting **Stefan Buhmann's Emmy Noether group**) performs Quantum Optics research over a wide spectrum, reaching from mathematical over experimental to applied aspects. A common motivation for our work is to contribute to the conceptual and quantitative understanding of quantum phenomena in complex systems, where different length, energy and time scales compete, and quantum states tend to explore a large portion of Hilbert space. Our research branches up into quantum phenomena on macroscopic scales, with links to molecular, bio- and solar energy physics, the theory of open and of disordered quantum systems as a natural ingredient from a certain level of complexity onwards, and the quantum statistics (encompassing quantum information-related aspects) of few to many-particle quantum systems. Our methodological toolbox samples from results in mathematical physics to high performance computing, and is enriched by the exchange with colleagues notably from biochemistry and photovoltaic light-energy conversion.

Macroscopic quantum electrodynamics - Stefan Yoshi Buhmann

The **Emmy Noether group of Stefan Yoshi Buhmann** uses macroscopic quantum electrodynamics (QED) as an effective field theory at the intersection of atomic, molecular and solid-state physics and quantum optics to study the quantum vacuum [syb2] and its interaction with microscopic (atoms, molecules, quantum dots . . .) and macroscopic objects (bodies, media, surfaces, gratings . . .).

Non-reciprocal media and topological insulators

Media with a non-reciprocal electromagnetic response lead to a violation of Lorentz reciprocity, so that optical paths are no longer reversible. We have generalized QED to such media and considered the examples of photonic and plasmonic topological insulators as well as the idealized perfect electromagnetic conductor. In particular, we find that the Casimir force in the latter case may be repulsive and that the force between two photonic topological insulators can be tuned via applied magnetic fields.

Chiral media, on the other hand, exhibit an electromagnetic cross-susceptibility which is reciprocal. We have proposed that such materials can be used to mediate a discriminatory force between a chiral molecule and an achiral atom which can facilitate enantiomer separation [syb10].

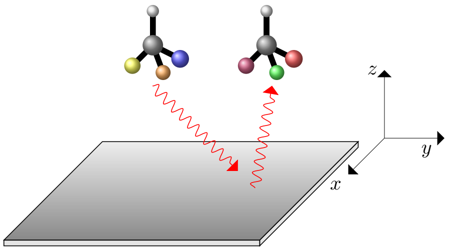

Figure 1.1: Surface-mediated van der Waals interactions for chiral molecules [syb10].

Casimir–Polder forces and photon recoil

An excited atom with a circularly polarised dipole moment that is close to the surface of a plane substrate or a cylindrical nanofiber emits into a preferential direction with respect to the fibre or surface. We have quantified this effect and shown that it will lead to a lateral Casimir–Polder force on the atom which is entirely due to photon recoil [syb4]. A similar photon recoil force also resolves the long-standing debate whether the van der Waals force involving an excited atom shows spatial oscillations due to interference: we find that the force on the excited atom oscillates while that on the ground-state atom is monotonous, with the imbalance being due to photon recoil [syb5].

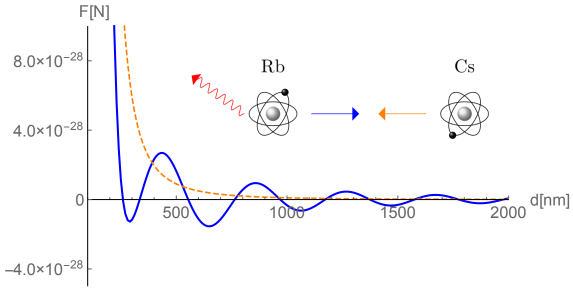

Figure 1.2: Van der Waals forces between an excited and a ground-state atom [syb5].

Dispersion forces in media

In collaboration with a consortium around Mathias Boström at NTNU Trondheim and Michael Walter from the University of Freiburg, we have studied the dispersion interaction of particles in a solvent medium, combining quantum optics descriptions with a molecular dynamics perspective based on density functional theory. We have developed and compared different models for the polarisability of the particles in the medium which account for local-field effects, finite size and simulated continuous expulsion profiles of the solvent density to obtain realistic predictions for van der Waals interactions.

By a related hybrid approach, we have shown that chemically inert polymer films can be used to realise powerful Casimir-based glues for nanotechnology [syb9].

Quantum friction

Quantum friction is an elusive and highly debated phenomenon whereby an atom moving parallel to a perfectly the smooth surface is conjectured to be subject to a dissipative force. We have resolved the discrepancy between different predictions for the velocity-dependence of the effect by showing that three very distinct asymptotic regimes exist in the dynamics. We have further proposed an indirect method for verifying this effect for the first time by observing the motion-induced Purcell-type modifications of atomic linewidths and shifts [syb7]. In collaboration with the group of Martial Ducloy at Université Paris 13 Nord, we are working towards an experimental implementation.

Matter-wave scattering

In order to push the quantum–classical divide, modern matter-wave scattering experiments aim towards observing quantum interference of objects with ever-increasing mass. In order to unambiguously attribute the observed signal to quantum effects, the Casimir–Polder interaction between matter wave and scatterer has to be taken into account. In collaboration with the experimental groups of Claus Zimmermann in Tübingen and Thomas Reisinger at the Karslruhe Institute for Technology, we have demonstrated that reflective gratings for matter waves can be implemented by combining Casimir–Polder and optical forces (see Fig. 1.3) [syb1] and that the Poisson spot behind a spherical scatterer is a sensitive probe of atom–surface interactions [syb6].

Driven atoms and collective effects

In current schemes, atoms are trapped and manipulating in optical fields at ever decreasing distances from surfaces. In this context, the optical trapping potential and the surface-induced potential are typically regarded as independent. We have found a new non-additive laser-induced atom surface interaction that is similar to optical trapping potentials.

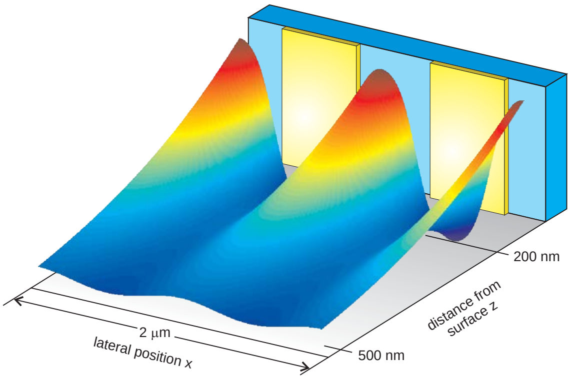

Figure 1.3: Casimir–Polder and optical potentials combine to form a potential for reflective grating for matter-wave scattering [syb1].

We are now investigating effects due to the coherent manipulation of a whole ensemble of atoms. We predict a super-radiant force burst under suitable conditions and enhanced Rabi oscillations for atoms in a cavity.

Interatomic Coulomb decay

Interatomic Coulomb decay is a recently predicted and experimentally confirmed phenomenon whereby a highly excited ion transmits its energy to a neighboring atom, ionizing the latter. The process had previously only been considered in free space on the basis of molecular dynamics. We have applied macroscopic QED to the problem in order to describe the effect in the presence of solvent media and surfaces. Our description also applies to the very similar process of resonant energy transfer.

Quantum Theory of Open Systems - Heinz-Peter Breuer

The group **Quantum Theory of Open Systems** is studying the foundations and applications of the quantum dynamics of open systems. An open quantum system is a quantum system which is coupled to some other quantum system, its environment, leading to large a variety of important physical phenomena such as dissipation, relaxation, decoherence, and the emergence of equilibrium and non-equilibrium stationary states.

Current research topics of our group are the quantum dynamics of Markovian and non-Markovian quantum processes, dynamical detection of quantum correlations and entanglement, quantum transport and control in complex quantum systems [breuer8, breuer7]. The most important achievements in recent years are the characterisation, classification and quantification of quantum memory effects through the information flow between an open quantum system and its environment, and the development of various schemes for the detection of quantum correlations by local operations. These theoretical results have led to a large number of applications and experimental realisations, e.g. in quantum optics and quantum information [breuer4, breuer1], photonics [breuer5], Bose-Einstein condensates [breuer6, breuer9], trapped-ion systems [breuer10, breuer3], condensed matter theory and quantum metrology [breuer2].

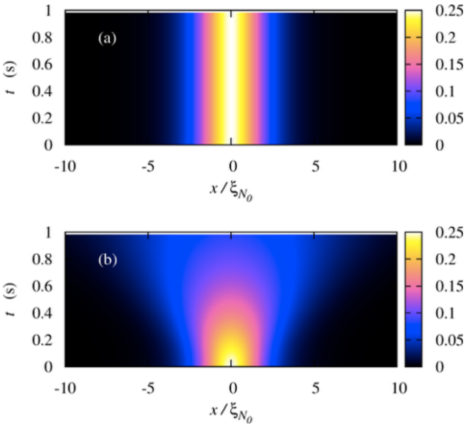

Figure 1.4: Center-of-mass motion of a bright soliton without decoherence. The picture shows the projection of the single-particle density as a function of time and distance from the origin. (a) On the mean field level (GPE), the soliton remains stationary. (b) On the many-particle quantum level, the ballistically expanding center-of-mass wave function smears out the single-particle density [breuer6].

Foundations of the theory of open quantum systems

We are interested in fundamental questions and conceptual problems of the theory of open quantum systems, as well as in the development of mathematical tools and numerical techniques allowing an efficient simulation of the dynamics of open systems. Fundamental aspects of the theory of dissipation, relaxation and decoherence in quantum mechanics are, for example, the classification of quantum dynamical maps, the description of multitime correlation functions, the dynamical impact of system-environment correlations, and the influence of decoherence on quantum transport. An example for the transition from diffusive to ballistic transport of the center-of-mass motion of a quantum matter-wave bright soliton induced by particle losses is discussed in [breuer6] (see also Fig. 1.4).

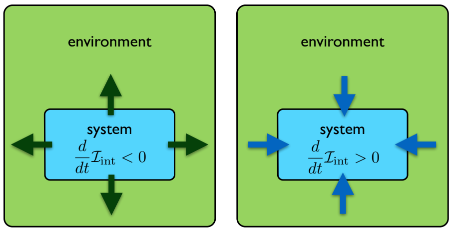

Figure 1.5: The information flow between an open system and its environment. Left: The open system loses information to the environment, corresponding to a decrease of information $I_{\text{int}}(t)$ inside the open system and Markovian dynamics. Right: Non-Markovian dynamics is characterized by a backflow of information from the environment to the system and a corresponding increase of $I_{\text{int}}(t)$ [breuer8].

Non-Markovian quantum processes

The standard approach to the quantum dynamics of dissipative systems is based on the assumption of a memoryless time evolution. However, many realistic systems are influenced by strong system–environment correlations and involved quantum memory effects. In our group we have developed a general theoretical approach in which quantum memory effects are connected to the flow of information between an open system and its environment, as is illustrated in Fig. 1.5. Thus, quantum non-Markovianity is characterised and quantified by the amount of information which flows back from the environment into the open system. This concept has led to many theoretical and experimental works summarised in a recent review [breuer8]. Examples of interesting features of non-Markovianity are nonlocal quantum memory effects (see Fig. 1.6) and their applications to teleportation with mixed quantum states [breuer4].

Quantum Optics and Statistics (QOS) - Andreas Buchleitner

During the reporting period, the Quantum Optics and Statistics group has in particular contributed novel diagnostic tools for the characterisation of complex quantum systems, and to the understanding and/or optimisation of transport phenomena which are strongly affected by quantum interference effects, on the single as well as on the many particle level, in idealised, biological, and applied physics contexts.

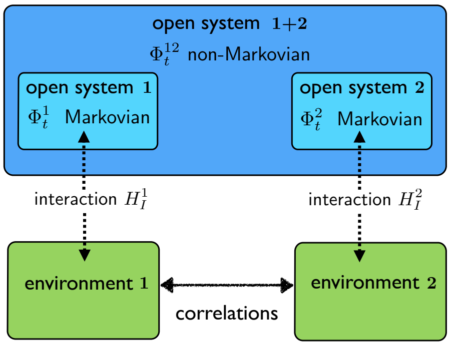

Figure 1.6: Scheme of a composite system showing nonlocal memory effects. The open systems 1 and 2 locally interact with their respective environments through local Hamiltonians H_I^1 and H_I^2. Initial correlations between the local environments then lead to the emergence of nonlocal memory effects: While both dynamical maps Φ_t^1 and Φ_t^2 of the two subsystems are Markovian (memoryless), the dynamical map of the composite system exhibits strong memory effects [breuer8].

Entanglement dynamics and transmission

Our research on the dynamical evolution of entanglement (or weaker types of quantum correlations) under incoherent perturbations addressed two main questions: First, which are the conditions for entangled quantum states to exhibit robustness under experimentally generic open system dynamics, and, second, how to accurately model and control the transmission of entangled states of photons across a turbulent atmosphere? While the first question is of relevance for the experimental control of scalable quantum information processing architectures, the latter addresses an important aspect of free-space quantum communication.

In the framework of one M.Sc. (Carnio) and two PhD (Gessner, Kropf) theses, we derived an analytical description of the dynamics of an N-qubit quantum register under collective dephasing, and infered the structure of those entangled register states which do preserve their entanglement properties even asymptotically.

With the help of one B.Sc. (Bachmann) and two (Campaioli, Leonhard) M.Sc./diploma students, we succeeded to analytically derive a general scaling law for entanglement decay under weak atmospheric turbulence [abu3], which relies on a comparison of structural features of the OAM (orbital angular momentum)-entangled photons' wave fronts with the phase noise imparted upon the photons by the atmospheric density fluctuations. This work is currently continued with one M.Sc. (Eichhorn) and one PhD (Sorelli) student, in cooperation with the National Metrology Institute of South Africa (Pretoria) and the Fraunhofer Institute for Applied Optics and Precision Engineering (Jena), to go beyond the weak turbulence scenario, and to identify OAM entanglement classes which allow screening against the detrimental effects of atmospheric turbulence.

Control of open quantum systems

Under a more fundamental perspective upon open quantum systems, we conceived a general framework to describe the effective time evolution of disordered systems (PhD Kropf), and to feedback-control the coherence and entanglement properties of simple quantum systems under decoherence (M.Sc. Brünner). Very recently, we initiated a cooperation with Y. Gefen's group at the Weizmann Institute of Sciences (Rehovot) on measurement-induced geometric phases (M.Sc. Gebhart), in physical settings inspired by toy models from quantum optics and mesoscopic physics.

Photovoltaic upconversion

Fostered by the group's initiative for a FRIAS research focus on *Designed quantum transport in complex materials* (Oct. 2014 until Sept. 2015), we did launch a cooperative project, under the umbrella of the Sustainability Centre Freiburg, on photovoltaic upconversion, with J.-C. Goldschmidt's group at Fraunhofer ISE, on the improvement of photovoltaic upconversion devices. This interest was seeded by a cooperation with G. Scholes (Toronto/Princeton) on optimal topologies for upconverter materials [abu2], which we studied and conceived, in a statistical approach, in the framework of a first PhD thesis (J. Zimmermann). A second, ongoing PhD (Spallek) and a recent B.Sc. (Fries) thesis focus on the interference-aided tailoring of desired photonic densities in realistic upconverter structures. First results [abu9] demonstrate that importing expertise from modern disorder physics can considerably improve over state of the art engineering approaches.

Controlling quantum transport by structure and disorder

Closely related are the group's activities on the characterisation and control of (single particle or excitation) quantum transport on structured and/or disordered, continuous or discrete, infinite of finite potential landscapes. Diagrammatic, statistical and advanced computational methods are combined to assess (possibly multi-fractal) spectral as well as dynamical features. Physical scenarios reach from multiple scattering of photons (M.Sc. Knothe) over exciton transport on driven molecular networks (M.Sc. Kristjánsson) or in cold Rydberg gases and/or arrays, to Anderson localization of ultracold atoms or electrons on 1D (PhD Valdes) and 3D lattices/networks. Original results include, inter alia, a statistical theory of robust and efficient transport across networks with constrained randomness (PhD Walschaers), an analytical theory of tailored resonances on designed Rydberg lattices (B.Sc.'s Schäfer, Bäuerle, M.Sc. Hess), and a fractal dimension analysis of the 3D Anderson transition, as well as of the ground state of the many particle Bose Hubbard Hamiltonian (B.Sc. and M.Sc. Lindinger, habilitation Rodriguez)

Multidimensional spectroscopy and coherent control with quantum light

With ever more complex quantum systems under study in biomolecular spectroscopy as well as in highly controlled quantum optics, diagnostic tools which are optimally tailored to targeted features are in need. In the framework of two PhD theses (Gessner, Schlawin - both awarded with a Springer Thesis Award 2016), and in cooperation with H. Häffner (Berkeley) and S. Mukamel (Irvine), we imported and adapted multidimensional spectroscopy from chemical physics to the study of interacting many-body systems in a quantum optics context [abu1]. Beyond Ramsey-like techniques, this approach paves the way for the monitoring and discrimination of coherent vs. incoherent quantum path ways, e.g. on multiple excitation manifolds of ion chains, and allows for the unambiguous identification of distinct, correlated many-particle phases. Under a related perspective, we presented the first theoretical analysis of coherent control by optimally shaped, quantum correlated two-photon states which can outperform optimal classical pulses [abu6]. Furthermore, we were actively involved in a broad, interdisciplinary discussion on the potential of nontrivial coherence effects to enhance function in complex chemical systems [abu7].

Many particle quantum dynamics and statistics

Much of the recent interest in "complexity" on the quantum level is spurred by the improved experimental control over few to many-particle quantum systems. Given the rapid growth of the Hilbert space dimension with the number of constituents, it is clear that deterministic descriptions rapidly hit the ceiling, if one wishes to model truly complex - rather than just complicated - system states and evolution. Furthermore, while interacting many-particle quantum systems are often invoked as testbeds for "new physics", it is surprising that the distinct roles of the particles' indistinguishability, on the one hand, and of interactions, on the other, so far remain unresolved in the literature, in particular when it comes to understanding the structural features of the many-particle time evolution. Consequently, we set out for a systematic theoretical approach which combines tools from semiclassical [abu8], statistical, many particle, scattering and open quantum systems' theory, with the aim to identify robust and distinctive features of few- or many-particle quantum states and dynamics, amenable to scalable experimental validation when knowledge of the full quantum state is prohibitive. Different physical settings are here considered, from doubly excited Rydberg states of helium under electromagnetic driving over – possibly dressed – Bose-Hubbard physics and multi-band many particle dynamics in 1D potentials, to many particle dynamics on highly symmetric or random graphs. Some of our theoretical analyses [abu5, abu10] led to fruitful cooperations with the experimental groups of Yoon-Ho Kim (Pohang), Gregor Weihs (Innsbruck), and Fabio Sciarrino (Rome), and have been or are being implemented in the lab. Altogether, five PhD theses (Mayer, Jörder, Fischer, Walschaers, Knothe), two M.Sc. theses (Heitz, Streif), and two B.Sc. theses (Dirkmann, Dohse, Karle), generated new insights into various aspects of this in many respects uncharted territory, and one PhD thesis (Brünner) and two M.Sc. theses (Mielke, Schäfer) are currently dedicated to this field.

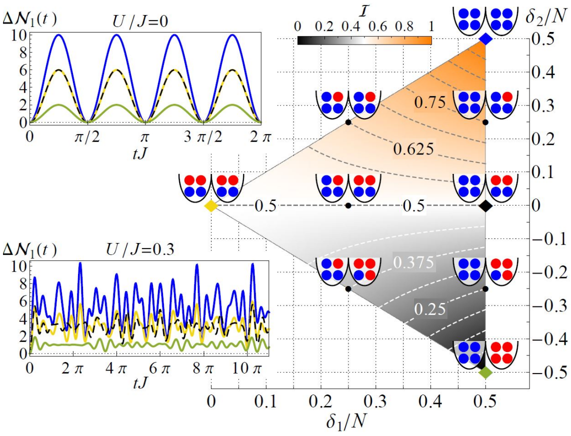

Figure 1.7: Representation of our indistinguishability measure for Fock states in a two-species bosonic Josephson junction. The insets show the time evolution of the local density fluctuations in the absence (top) and in the presence (bottom) of interactions for the indicated (by colour) initial configurations [Brünner, Dufour, Rodriguez, Buchleitner (2017)].

1.2.2 Experimental Attosecond and Laser Physics

The **Attosecond and Ultrafast Science Group by Giuseppe Sansone** aims at investigating electronic and nuclear dynamics on the ultrafast timescale (from the femtosecond down to the attosecond timescale), by using few-cycle pulses in the near-infrared and visible spectral range, in combination with trains and isolated attosecond pulses generated by high-order harmonic generation (HHG) in gases. To this purpose two attosecond lasers source operating at 1 kHz and 100 kHz will be designed and implemented in the next years. Using these novel sources the research group will investigate ultrafast dynamics in dilute samples (size-selected clusters and conformer-selected beams) and will perform detailed characterisation of molecular dynamics in the molecular frame by exploiting coincidence photoelectron-photoion spectroscopy. The research group has recently moved (2016-2017) from the Physics Department Politecnico Milano and it is currently involved in the design of the new attosecond laser sources and attosecond beamlines. The new systems will be installed in the new laboratory space currently under renovation. The main research activities of the group will be complemented by experimental activities carried out at large scale facilities delivering ultrashort visible and extreme ultraviolet pulses.

Photoelectron-Photoion Coincidence Spectroscopy using Attosecond Pulses

Generation of high-order harmonics at high-repetition rates ($\gg 1$ kHz) has attracted increasing interest in the last years for different scientific applications, including photoelectron spectroscopy from surfaces, coherent diffractive imaging, and photoelectron/photoion coincidence spectroscopy. Photoelectron-photoion coincidence spectroscopy requires to operate in single-event conditions (i.e. a single photoionisation events per laser shot), thus limiting the photon flux and/or the density of the target. High-repetition-rate attosecond sources are required for these experiments in order to increase the number of measured single events, thus reducing the acquisition time. Depending on the characteristics of the specific experiment, the mass of the systems under investigation, and the required momentum resolution, the optimal repetition rate of the attosecond source is in the 50-200 kHz range. For these repetition rates, two approaches have been developed for the generation of attosecond pulses (trains and isolated pulses): a) the first one is based on the optical parametric amplification (OPA) or optical parametric chirped pulse amplification (OPCPA) of a seed pulse generated by a broadband few-cycle femtosecond oscillator (typically a titanium-sapphire (Ti:Sa) oscillator). The pump of the OPA/OPCPA is, typically, the output of an ytterbium (Yb) amplifier (or amplifier chain), which is seeded by a small fraction (at 1030 nm) of the seed oscillator. Using this approach, optical synchronisation between the seed and pump pulses is achieved. Moreover, carrier-envelope phase (CEP)-stable output pulses are obtained using a CEP-stabilised oscillator, as OPA/OPCPA preserves the CEP drift of the seed pulse. b) the second one is based on the temporal compression of pulses emitted by a single or a coherent-combination of large-pitch fibers, using a single or a cascaded hollow fiber configuration. Using this approach, few-cycle pulses at high-average power have been demonstrated.

In our research group, we plan to investigate both approaches for the generation of trains and isolated attosecond pulses, starting from a common Yb-based driving source. For the generation of trains of attosecond pulses, a single hollow-fiber compression stage will be used for the temporal compression of pulses from ≈ 300 fs down to $\approx 30-40$ fs. Pulses with energies up to 100 μJ at 100 kHz are expected. For the generation of isolated attosecond pulses, we plan to develop a passively CEP-stabilised seed by difference frequency generation of a white-light continuum created in a non-linear medium. The seed will be then amplified in two (three) nonlinear crystals. Energies up to 100 μJ at 100 kHz and pulse duration below 10 fs are expected by broadband parametric amplification. This pulse duration, in combination with polarisation gating techniques, should give access to the isolated attosecond pulses.

The source will be given by the combination of two synchronised Yb systems delivering short pulses (300 fs) low-power (20 W) and long pulses (1 ps) and high-average power (200 W). This combination will ensure a great flexibility for the implementation of different temporal compression strategies and also for the development of OPAs with different central wavelengths, on a long-term perspective.

The attosecond pulses created by the high-repetition rate laser source will be used in combination with a Reaction Microscope for the investigation of attosecond and femtosecond dynamics in small molecules.

Time-resolved dynamics on the femtosecond and attosecond timescale in dilute targets

The research group will be involved also in the generation of trains and isolated attosecond pulses with energies ranging from a few to a few tens of nJ for the investigation of attosecond dynamics in dilute targets, such as beams of conformer-selected molecules and size-selected clusters. The attosecond source for these experiments will operate at 1 kHz and it will be driven by a multi-mJ, CEP-stable driving laser system.

Theoretical and experimental studies have shown that electronic hole migration dynamics in molecular systems can be triggered on the attosecond timescale by the absorption of XUV light. In this process an electron-hole, which is initially localised in one part of the molecule, can spread over the entire molecule within a timescale that can range from a few hundreds of attoseconds to a few femtoseconds. The ultrafast electron dynamics couples to the vibrational modes of the molecule, which may lead to a charge localisation on a different site of the molecule. The charge concentration can ultimately lead to a bond breaking away from the original excitation (or ionisation) site. Although first experiments, discussing the electron dynamics in large molecules of biological interest after an initial photoionisation event, have been reported, the various stages of the charge migration and the coupling of electron and vibrational dynamics have not yet been fully characterised.

Moreover the charge-migration characteristics strongly depends on the specific structure of the molecule. The generation of cold molecular beam of conformer-selected molecules has been demonstrated using field deflectors. This approach also offers the possibility for an improved alignment and orientation of the molecular system. We plan to take advantage of these techniques for the time-resolved investigation of conformer-selected electronic dynamics in molecule. This work will be also supported by the Marie Sklodowska Curie Innovative Training Network MEDEA project, in which the research group is currently active.

In collaboration with the research groups of Prof. Stienkemeier and Prof. von Issendorf, we plan to investigate femtosecond and attosecond dynamics initiated by photoionisation by trains and isolated attosecond pulses in large clusters of noble gas atoms and size-selected metallic clusters.

Nonlinear interactions in the extreme ultraviolet and X-ray spectral range

The process of high-order harmonic generation gives access to extreme ultraviolet radiation with durations as short as a few tens of attosecond, but it suffers from the limited conversion efficiency (typically $10^{-5} - 10^{-6}$), which makes challenging the generation of isolated and trains of attosecond pulses in the μJ energy range. The low energies per pulse makes challenging the development of nonlinear attosecond metrology and the investigation of nonlinear effects in the XUV spectral range using HHG-based sources. FELs, and in particular seeded FEL, offers an important alternative to high-order harmonic generation for the synthesis and application of XUV pulses with ultrashort pulse duration and energies up to the few hundreds of μJ and even mJ. In the framework of a large collaboration, the research group has realised the first demonstration of coherent control in the extreme ultraviolet range, exploiting the unique characteristics of the seeded-FEL FERMI at Elettra, Italy (K. Prince *et al.* Nat. Photon. **10**, 176–179 (2016)). In the experiments, two coherent harmonics (19.6 eV and 39.2 eV) were generated by the same electron bunch tuning at the first and second harmonic the first five and last undulator of FERMI, respectively. The relative phase was adjusted by slightly delaying the electron bunch trajectories between the fifth and sixth undulator, thus delaying the electron bunch with respect to the first harmonic. Using this approach the delay between the first harmonic (generated in the first five undulators) and the second harmonic (generated in the last undulator) can be controlled with a precision of few attoseconds. Using this radiation, two possible photoionisation pathways are possible in Neon: single photon ionisation, corresponding to the absorption of a photon of the second harmonic, or two-photon single ionisation due to the absorption of two photons of the first harmonic. The two pathways lead to the same photoelectron energy and interfere, determining an asymmetric photoelectron emission (K. Prince *et al.* Nat. Photon. **10**, 176–179 (2016)). The research group has recently investigated the role of atomic resonances in the evolution of the asymmetric photoelectron emission. Preliminary data analysis indicates that the resonance (corresponding to the excitation of a $2p$ electron to the the $4s$ level) leads to a significant modification of the amplitude and of the phase of the asymmetry. The data analysis is still ongoing.

On a long-term perspective, the research group plans to implement techniques well-established in the attosecond community, to experiments realised at FERMI. In a future experiment we plan the generation of three coherent harmonics for the synthesis of trains of attosecond pulses. The group plans to extend the investigation of nonlinear XUV and X-ray processes also at other large scale facilities, which will be become full operational in the next few years (for example XFEL in Hamburg, Germany and ELI-ALPS in Szeged, Hungary).

1.2.3 Experimental Atomic, Molecular and Optical Physics

The endeavor to control increasingly large systems of particles at the quantum level might be one of the driving forces for physical sciences in the coming decades. The **experimental Atomic, Molecular and Quantum Physics group of Tobias Schätz** aims (i) to gain deeper insight into complex dynamics that are influenced or even driven by quantum effects, and (ii) to control atoms and molecules at the highest level possible to set up many-body (model) systems - in a way, the ultimate form of engineering. Our work builds on different trapping technologies. On the one hand, on conventional and novel radio-frequency (rf) traps, which we exploit to trap 1D chains and 2D zigzag structures of ions, so called Coulomb crystals (see Figs.1.8 and 1.9). We further miniaturize the rf-traps to extend the ion ensembles in size and dimension, towards two-dimensional arrays of individual traps spanned by micro-fabricated surface electrodes (see Figs.1.10). On the other hand, we start to explore trapping of ions and atoms by optical means.

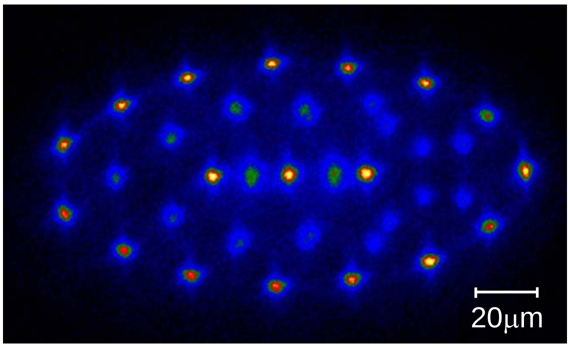

Figure 1.8: Scaling Coulomb crystals in size and dimension while maintaining the unique controllability of the individual ion might allow addressing intriguing quantum effects in many different fields of physics. Here: Fluorescence image of ≈ 40 ions within one single trapping potential of our conventional radio-frequency (rf) trap, frozen by laser cooling into a 2D- to 3D Coulomb crystal.

Experimental Quantum Simulations

Direct experimental access to the most intriguing and puzzling quantum phenomena is extremely difficult and their numerical simulation on conventional computers can easily become computationally intractable. However, one might gain deeper insight into complex quantum dynamics via experimentally simulating and modeling the quantum behavior of interest in a second quantum system. There, the significant parameters and interactions might be precisely controlled, underlaying quantum effects detected sufficiently well and, therefore, their relevance could be revealed and studied. This might remain valid even for open systems, since the environment coupled to the simulator can be tailored and exploited. Our group is dedicated to build such a model system, to derive and to perform two different classes of experimental quantum simulations addressing systems **(1)** that might still be numerically tractable, however, hard or impossible to realize in the laboratory directly and **(2)** that can be extended ion by ion to complex ensembles. Here we aim at bridging the gap between benchmarking our experimental platform by validating our results still with numerics and accessing regimes that remain numerically intractable - to study where experiments might assist in gaining deeper insights beyond numerics.

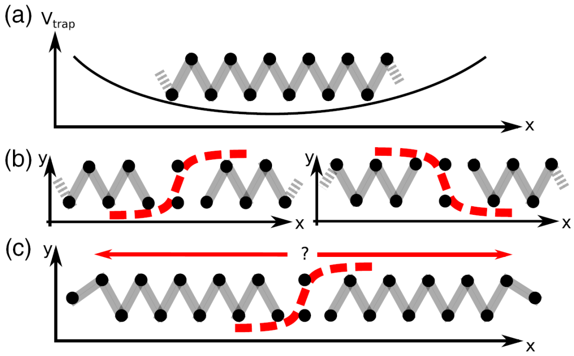

Figure 1.9: Schematic depiction of discrete solitons and their propagation in a trapped Coulomb crystal. **(a)** The self-assembled crystal features reflection symmetry and its energy minimum comes in two degenerate configurations, the ‘zigzag’ and its mirror image ‘$\overline{zigzag}$’ (only one shown). **(b)** Realizing both configurations in one crystal requires an interface, a domain wall called ‘kink’ (left) or ‘$\overline{kink}$’ (right), which is a discrete soliton, carrying a topological charge of ± 1, illustrated with a dashed red line. **(c)** We study how a resonant global excitation of radial vibrational kink modes can be rectified by the soliton and exploited to conditionally propagate it to the right or left in a noisy environment.

(as to 1) simulating discrete solitons:
We create and study topologically protected defects within Coulomb crystals by non-adiabatically crossing the structural phase-transition from a linear chain to a two-dimensional zigzag, i.e., evolving too fast for communication between different domains of the crystal (see Fig.1.9). Furthermore, the global trapping potential permits controlling the soliton dynamics and realizing directed transport depending on its topological charge [schae9]. Our work is proposed to permit accessing the quantum regime [schae1].

(as to 2) simulating quantum spin systems: effective spins interacting via phonons:

The aim is not to copy the system and its dynamics in nature with its plethora of complex interactions. The aim is to reduce the system to its essential ingredients including the relevant impact by the environment and to test, in a controllable manner, the validity of theoretical assumptions and predictions. After our proof of principle experiment on quantum spin systems in the year 2008, we further extend our simulator in size and dimensionality. Our efforts are twofold.

(i) We use a hybrid Coulomb crystal and exploit its phonons to study an isolated quantum system composed of a single spin coupled to an engineered bosonic environment [schae4]. We increase the complexity of the system by adding ion by ion and controlling coherent couplings. Thereby, we observe the emergence of thermalization: Time averages of spin observables approach microcanonical averages while related fluctuations decay. Further extending the control of system size, coupling strength, and isolation from the external world is envisioned to permit exploring the dynamics and timescales of equilibration and thermalization. The identical system is proposed to permit simulating phenomena of quantum transport [schae5].

(+) As a side-project, we investigated how to exploit the tunable sensitivity of our system to permit "Decoherence-Assisted Spectroscopy of a Single Ion [schae2]". We enhance the efficiency of the detection to the single excitation event, the latter leading to a complete loss of the coherence of a superposition of two electronic ground states.

ii) Supported by our collaborators at NIST and Sandia-National-Laboratories (SNL) we designed and realized a basic, two dimensional array of rf-surface traps (see Fig.1.10). Recently, we reported how to operate two basic 2D arrays, each hosting three trapped ions in individually controlled harmonic wells [schae6, schae7]. In our approach, we demonstrate individual control of the electronic and motional degrees of freedom, preparation of a fiducial initial state with ion motion close to the ground state, as well as a tuning of couplings between ions within experimental sequences. Our work might be extended towards a quantum simulator of two-dimensional systems designed at will.

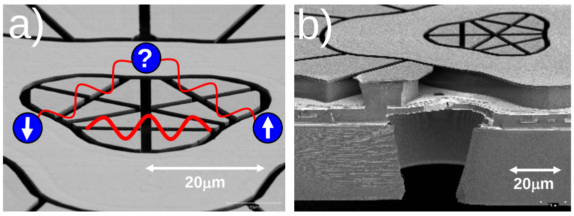

Figure 1.10: Electron-microscopic images of our novel rf-surface traps, a basic 2D array micro-fabricated by SNL. a) Bird's eye view, the gaps isolating between rf and DC patches (ions and individually controllable interactions are animated). Three ions residing in three individual traps are suited to simulate anti-ferromagnetic interactions between three quantum spins. Classically, only two neighboring spins can be orientated in an anti-ferromagnetic manner while the third spin becomes frustrated. Quantum mechanically, a superposition of all frustrated permutations, an entangled state, arises (in the envisioned, extended array, the whole ensemble of spins evolves adiabatically, via a quantum-phase-transition, into a complex state). b) (similar as (a)), providing additional insight into the underlaying structure, e.g., the electrodes' extensions shielding the insulators and the cross section through a loading hole.

Trapping Ions Atoms and Molecules Optically (TIAMO)

Our group had achieved optical trapping of an ion in a dipole trap, and within an 1D-optical lattice [schae8], as well as in a far-detuned trap [schae3] in the absence of any rf-field. There is a long-term prospect for experimental quantum simulations in 2D, based on ions and atoms in versatile optical trapping geometries. However, our current project of optically trapping an ion within a BEC of atoms is dedicated to overcome fundamental limitations set by the rf-driven micro-motion when combining optical and rf-trapping technology in state-of-the-art hybrid traps. Recently, we reported that optical trapping and isolation of ions can be performed on a level comparable to neutral atoms under similar trapping conditions, boosting the lifetime of ions in a single beam dipole trap to 3 seconds [schae10]. The trap features state-dependent optical potentials, which we experimentally prepared and characterized. In addition, we have investigated an upper bound of the heating experienced by an ion and found it to remain low compared to expected cooling rates in ion–atom interaction experiments. This opens a path to a novel regime of many-body physics and ultra-cold interactions of ions and atoms. We now aim to address the question, how interaction and reactions proceed at lowest temperatures? In collaboration with R.Cote (Univ. of Connecticut) we elaborate on options how to study the interaction of a single ion with a BEC. The subsequent quantum chemistry might permit to control reactions and their pathways by external fields, since forces and related interactions become relevant compared to the kinetic energy. In collaboration with R.Mozynski (Univ. of Warschow) we aim to study ultra-cold formation of BaRb$^+$ and the interaction between Ba$^+$ and ^{6,7}Li within our optical traps.

1.2.4 Molecular and Nanophysics

The research of the **Molecular and Nanophysics group of Frank Stienkemeier** focusses on fundamental quantum mechanical properties of atomic and molecular complexes and their interaction with light. Experimentally, to a large extend atomic, molecular and cluster beams provide targets interacting with electromagnetic radiation. Utilized light sources include spectrally highly resolving laser systems, ultrashort pulse lasers accessing real-time dynamics, as well as facility-based light sources in the XUV range (synchrotrons, free-electron lasers (FELs)). Specifically, helium nanodroplet isolation at millikelvin temperatures is pursued [sti2]. On the one hand, we are intrigued by the fundamental quantum properties of the superfluid, on the other hand, we utilize helium droplets as “nano-cryostats” for synthesizing molecular complexes in a cold and weakly interacting matrix. Experiments include the aggregation and cluster formation, microsolvation, cold chemical reactions, photo-dissociation and ionization by multiphoton absorption up to the strong-field and collective regimes. Funded by the ERC Advanced Grant COCONIS, recently a new direction towards multidimensional spectroscopy of dilute samples has been successfully started. Connected to that a new high repetition-rate laser system was installed and corresponding rearrangements of molecular beam machines as well as laser labs had to be performed. Within the IRTG CoCo collaborations with groups at UBC, specifically with Takamasa Momose and Valery Milner have been significantly intensified.

Excitation and energy transfer in organic molecular complexes

Organic molecules, complexes, and nanostructures attached to rare-gas clusters are characterized using laser-induced and dispersed fluorescence spectroscopy to determine electronic properties and geometric structures. Helium nanodroplets are used in order to obtain highly resolved vibronic spectra whereas the deposition of molecules on the surface of solid neon or argon clusters is employed in order to study intermolecular interactions. In particular, the excitation dynamics and the role of cooperative effects of acenes in a disordered array randomly distributed on a surface were studied [sti3]. Radiative lifetime measurements revealed excited-state lifetime reduction mechanisms when increasing the surface coverage. The role of superradiance, singlet fission (Fig. 1.11), as well as triplet-triplet-anihilation has been identified [sti8]. In collaboration with Michael Walter (Fraunhofer IWM), theoretical simulations aided in determining underlying processes. A continuance of previous studies has been to observe changes of electronic properties in perylene derivatives, e.g., perylenediimide (PDI) in collaboration with Prof. Y. Xu (IRTG CoCo Mercator Fellow) and Prof. W. Jaeger (University of Alberta).

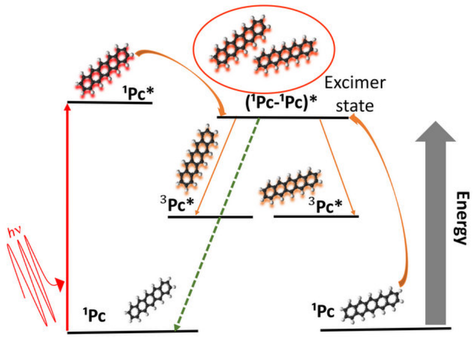

Figure 1.11: Singlet fission process and the formation of triplet states in pentacene (Pc).

Imaging spectroscopy of doped helium nanodroplets

The dynamics and energetics of different excited states of atoms and molecules attached to quantumfluid helium nanodroplets have been studied, establishing a better understanding of many-body quantum phenomena on the microscopic level. Alkali atoms and dimers attached to He nanodroplets have been investigated using pump-probe resonance enhanced multiphoton ionization (REMPI) schemes with either nanosecond or femtosecond time resolution. The velocity map imaging technique is used to extract angularly resolved energy distributions of ejected photoions and photoelectrons. Experimental studies are compared to simulations based on time dependent density functional theory (TDDFT) carried out in collaboration with Manuel Barranco (University of Barcelona) and Nadine Halberstadt (University of Toulouse). Besides a quantitative characterization of excitation and desorption dynamics, an efficient ion solvation mechanism in the vicinity of the cluster surface, the so-called fallback-effect was identified [sti10].

In a collaboration with A. Baklanov (ICKC, Novosibirsk, Russia, IRTG CoCo Mercator Fellow), the photodynamics of highly excited molecular iodine as well as iodine attached to helium nanodroplets have been studied by means of fs-pump-probe spectroscopy and ion imaging detection [sti7]. A collaboration with Robert Moshammer and Thomas Pfeifer (MPI-K Heidelberg) on strong-field effects and nanoplasma formation of helium droplets have been continued within the DFG priority program QUTIF.

Interaction with XUV radiation

After having setup the Low Density Matter (LDM) endstation at the FEL FERMI in Trieste, we have continued projects, using intense, femtosecond XUV radiation in combination with atomic, molecuar and cluster beams. Apart from our participation of beamtimes, lead by principal investigators from othere national or international groups [sti6], we continued our work on collective autotionization processes in rare gas clusters [sti1]. Using pump-probe techniques, we have characterized the rate at which collective autoionization processes occur as well as the relaxation dynamics of excitations within a helium nanodroplet.

On a different topic we have performed a series of experiments on hydrogen-bonded clusters (e.g. water, ammonia, and methanol) to study electron solvation and fragmentation dynamics in realtime, both relevant to biological systems and atmospheric chemistry. Results using XUV – UV pump probe schemes identified individual processes an corresponding formation times. At ELETTRA synchrotron, we have studied correlated decay processes in pure and doped He droplets. For pure droplets, we have shown the existence of doubly excited atoms which have similar, but broadened features to their atomic counterparts [sti5] as well as a highly efficient interatomic Coulombic decay process.

Energy dissipation and coherent processes in cluster-isolated molecular systems

In the ERC-funded project, real-time investigation of coherent dynamics in cluster-isolated systems has been started. The coherent evolution of wave packets were studied with high spectro-temporal resolution. With the implementation of a novel phase modulation technique, the sensitivity of the apparatus was improved by orders of magnitudes and selective detection of the linear and nonlinear system response was facilitated. With this unique combination of spectroscopic tools, new insights into the energetic structure and the formation dynamics of exotic alkali-helium exciplexes were gained [sti4].

A new technique to efficiently detect weak multiphoton processes or multiple quantum coherences was developed allowing to study many-body effects in low-density gas-phase systems. For the first time, collective 4-body excitations in a room-temperature atomic gas at atom densities down to $\sim 10^7$ cm^{-3} were characterized. High-resolution studies revealed, furthermore, distinct phase signatures connected to hyperfine states of the system. Assisted by simulations in collaboration with A. Eisfeld at MPI-KS in Dresden, the findings were explained by the long-range dipole interaction among the particles.

The developed phase modulation technique allows to establish coherent nonlinear spectroscopy at XUV wavelengths. Control of the properties of the XUV pulses is achieved by manipulating the driving field of the harmonic generation. The concept was demonstrated [sti9] and a specific setup has been developed to be implemented at seeded FELs (sFLASH, FERMI).

Eventually, phase-modulated 2-dimensional electronic spectroscopy (2DES) in dilute gas-phase systems has been successfully performed. 2DES provides enhanced information about coherences and couplings in quantum systems and is particularly beneficial in studies of energy and charge transfer processes. First results on alkali-doped helium droplets (Fig. 1.12) demonstrated, for the first time, sufficient sensitivity to perform 2DES on cold cluster beams, which opens a new direction in multidimensional spectroscopy.

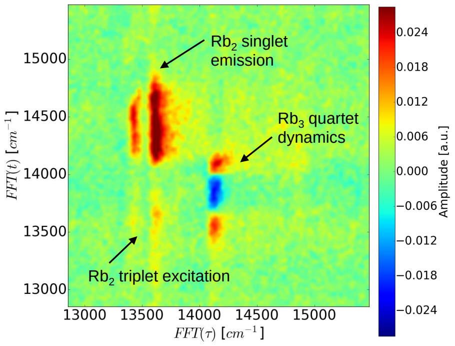

Figure 1.12: 2D Spectrum of cold high-spin Rb_2 and Rb_3 molecules isolated on He nanodroplets. An ultrafast ($\sim$200 fs) intersystem crossing in the Rb_2 system is clearly observable.

Cold collisions and cold Chemistry

The dynamics of fundamental chemical reactions has been investigated with the aim of controlling reaction rates using external fields. For these studies, a unique and versatile experimental setup composed of a supersonic beam of metastable helium atoms (He*) and a magneto-optical trap for ultracold lithium atoms (Li) has been setup allowing collision-energy-dependent and quantum-state controlled reaction experiments. Owing to electron-spin conservation rules, only certain quantum-state combinations of He* and Li are expected to form ionic reaction products. However, the influence of hyperfine interactions on the reaction rate is yet to be determined. Experimental techniques for the quantum-state selection of He* are developed in collaboration with B. Heazlewood (University of Oxford) and S. Willitsch (University of Basel).

1.2.5 Cluster Physics

The **experimental physics group of Bernd von Issendorff** performs research in Cluster Physics. Clusters with a few to a few thousand identical atoms or molecules often exhibit properties rather different to that of the corresponding bulk material, which is due to the strong influence of the surface, to an often different crystalline structure and, most spectacularly, to quantum size effects. Addition of a single atom to a cluster can often change its optical, magnetic, thermodynamic or chemical properties significantly. In order to characterize and understand such cluster properties in detail the group studies size-selected and temperature controlled clusters in the gas phase, employing a range of spectroscopic methods. In the following examples of current projects are given.

Electronic and geometric cluster structures

Photoelectron spectroscopy is a powerful tool for the study of gas phase clusters as in principle it yields a direct image of their occupied electronic density of states. This allows to directly study quantum size effects, but also, in combination with high level theory (mainly DFT calculations, performed,e.g., in the groups of Michael Moseler or Michael Walter), the determination of the geometric structure of the clusters. Systems examined range from alkaline and noble metal clusters to molecular clusters like water cluster anions. An interesting example of a recently studied system are Zn-clusters, which in a combined photoelectron spectroscopy/DFT study have been shown to exhibit very exotic properties, like the formation of only loosely interacting core-shell structures (Fig. 1.13).

The application of angle resolved photoelectron spectroscopy allows to obtain direct information about the form of the electron wavefunctions[bvi1], as demonstrated for the example of Na_5^- in Fig. 1.14.

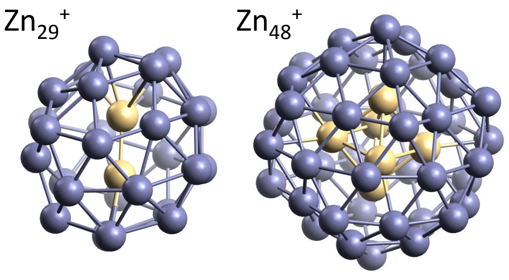

Figure 1.13: Geometric structures of zinc cluster cations with 29 and 48 atoms. Both exhibit very unusual core-shell structures, where the core is only weakly interacting with the surrounding cage. In the case of Zn_{48}^+ this even leads to different symmetries for core (octahedral) and shell (icosahedral) [bvi4].

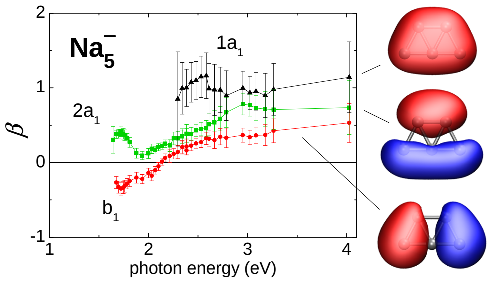

Figure 1.14: Measured photoelectron distributions (parametrized by the so-called beta-parameter) for the three valence orbitals of Na_5^- [bvi1].

But more importantly the angular distributions yield direct information about the photoemission dynamics. Very recently a breakthrough in the understanding of these distributions has been achieved; it turns out that the large variety of angular distributions can be all described by a universal function, which can be derived from a semiclassical treatment of the many-particle response of the cluster electron system to the photoemission (in preparation).

Additionally the group constantly strives towards an improvement of the experimental setups. Recently an improved version of a magnetic bottle photoelectron spectrometer has been developed, which uses a time-dependent field for the temporal focusing of electron packages. The spectrometer works very well; it delivers a resolution better than any other spectrometer of this type (Fig. 1.15). In combination with an improved low temperature ion trap for the thermalization of the clusters, which now reaches temperatures as low as 4 K, the new spectrometer will allow studying in detail vibrational patterns in photoelectron spectra as well as to do sensitive searches for the occurrence of low temperature quantum phenomena like Cooper pair formation.

Ultrafast dynamics

Electron dynamics in clusters is studied using time-resolved pump-probe photoelectron spectroscopy. Systems examined are metal, semiconductor and carbon clusters (fullerenes). In C_{60}^- for example a strong temperature dependence of the electronic relaxation time constants was observed, which makes it an ideal model system to study electron-phonon coupling in finite systems. Currently measurements on size-selected acene clusters are in preparation with the goal to study exciton dynamics.

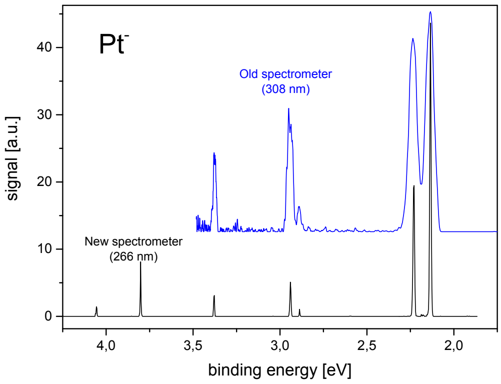

Figure 1.15: Comparison of the photoelectron spectrum of a Pt anion measured with a standard magnetic bottle spectrometer and with the newly developed one.

Caloric measurements

Traditional thermodynamics only treats infinite systems, which raises the question how this description has to be altered for finite systems. In the group a technique was developed to measure caloric curves of free clusters. This technique has been employed to study the melting phase transition in sodium clusters in detail (Fig. 1.16). Recently the focus was put on water clusters, which do not undergo melting, but have been shown to rather exhibit a glass transition. This opens a whole new direction, the study of glass transition in finite systems. Experiments are in preparation with the goal to study such effects in similar systems like ethanol clusters.

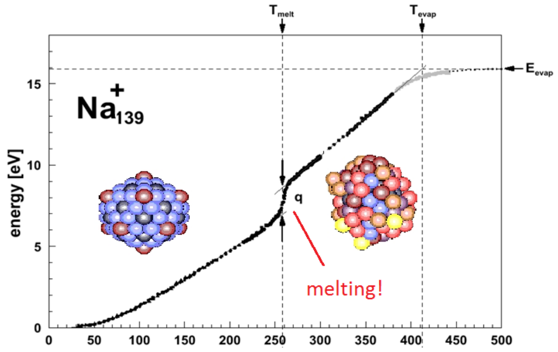

Figure 1.16: Caloric curve of a free sodium cluster.

X-ray spectroscopy

Inner shell excitation energies are element specific, which makes x-ray absorption spectroscopy an ideal tool to examine clusters incorporating different elements. An extension of the method, XMCD (x-ray magnetic circular dichroism) spectroscopy, can be used to determine the magnetic moments of the clusters. Together with the group of Tobias Lau (IP, HZB), a setup has been constructed which allows measuring XMCD spectra on size selected clusters stored in a liquid helium cooled ion trap within a 5T magnetic field. This setup is now permanently installed at a beamline of BESSYII (under the name of ”Nanoclustertrap”) and is used for a plethora of studies on semiconductor and metal clusters, transition metal complexes and simple molecular ions[bvi3, bvi5, bvi6, bvi9, bvi10]. One example of a recent result is the XMCD-spectrum of Cr_2^+ (Fig. 1.17), which exhibits a strong XMCD-effect. This directly shows that Cr_2^+ is in a high spin state, thereby solving a long-standing controversy [bvi8].

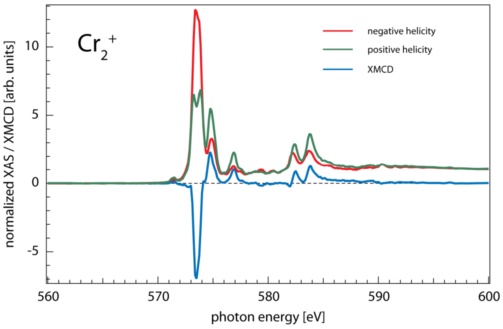

Figure 1.17: XMCD-spectrum of a Chromium dimer cation in the gas phase. The strong XMCD-effect directly demonstrates a high spin state (S=11) of the dimer [bvi8].

FEL experiments

The advent of XUV and X-ray free electron lasers offers exciting possibilities for cluster research. Full use of the time structure and intensity of FEL pulses will be made by measuring time-resolved diffraction patterns of nanoparticles, which will yield movies of the internal motion of these particles and thereby unprecedented insight into their dynamics. Experiments of this type are currently prepared in a cooperation with the group of Thomas Möller (TU Berlin), and have been funded by a Reinhart-Koselleck DFG-grant.

The high photon energies and short pulse lengths of FEL-pulses also offer enormous potential for the study of electron dynamics. The group is part of a consortium which performs photoelectron spectroscopy experiments on free size-selected clusters at the FEL FLASH in Hamburg; a central contribution will be the construction of a new type of magnetic bottle photoelectron spectrometer specially adapted to the requirements of FELs.

1.2.6 Solar Physics (KIS)

The **Kiepenheuer-Institut für Sonnenphysik (KIS) led by Svetlana Berdyugina and Oskar von der Lühe** is a member of the Leibniz Association. It conducts research on fundamental astrophysics, with particular emphasis on the major unresolved issues in solar and stellar physics: the origin, structure and evolution of the magnetic field, the hydrodynamic structure of the convection zone and operation of the dynamo, the heating of the outer atmosphere, and effects of stellar radiation and activity on planets. Accordingly, research projects of the KIS are organized into four main activities: Solar and Stellar Astrophysics, Solar Data Center, Observatory Operations and Instrument Development.
Recent research highlights include:

- The development of new helioseismic methods for investigating the dynamics in the solar interior, the solar dynamo, and the temporal and depth dependence of the meriodional flow,
- improved modeling of the effects of magnetic fields on seismic waves, enabling a first estimate on the variation of the magnetic field inside the Sun between the minimum and maximum of the solar activity cycle,
- new properties of convection in sunspot penumbrae, which is found not to be constrained by the strength of the magnetic field, but by the vertical component of the magnetic field: too large vertical field components suppress the penumbral magneto-convection,
- the first detection of (strong) magnetic fields on brown dwarfs,
- the first-ever multi-conjugate adaptive optics (MCAO) corrected observations of the Sun with the MCAO pathfinder Clear developed at KIS that show a clearly and visibly widened corrected field of view compared to quasi-simultaneous observations with classical adaptive optics correction,
- the Laser Absolute Reference Spectrograph (LARS), a combination of a prototype laser frequency comb with the echelle spectrograph of the VTT offers absolute wavelength accuracy and repeatability of 1 m/s, enabling the required long-term studies of solar material motions,
- the development of an innovative polarimetry system (INNOPOL) using advanced modulation techniques to be used at dedicated stellar telescopes as well as at GREGOR in combination with the GREGOR@NIGHT spectrograph.

The institute operates German solar telescopes at the Observatorio del Teide, Tenerife, Spain, including the 1.5-m telescope GREGOR, one of the world's most powerful solar telescopes with cutting-edge imaging quality. Among the recent technical developments are the multi-conjugate adaptive optics system for GREGOR, the laser frequency comb and the helioseismology instrument HELLRIDE at the Vacuum Tower Telescope (VTT), a stellar spectrograph at GREGOR, and high-precision polarimeters for exoplanet studies (in cooperation with the Universities of Hawaii and of Turku).

KIS researchers have been successful in acquiring third-party funding, including ERC Starting and Advanced Grants and other EC grants, and in building instruments for ground-based telescopes (DKIST/VTF) and space telescopes (Sunrise, Solar Orbiter). KIS plays a major role in international collaborative efforts to define and build the next generation of instrumentation for solar observations (EST, SPRING).

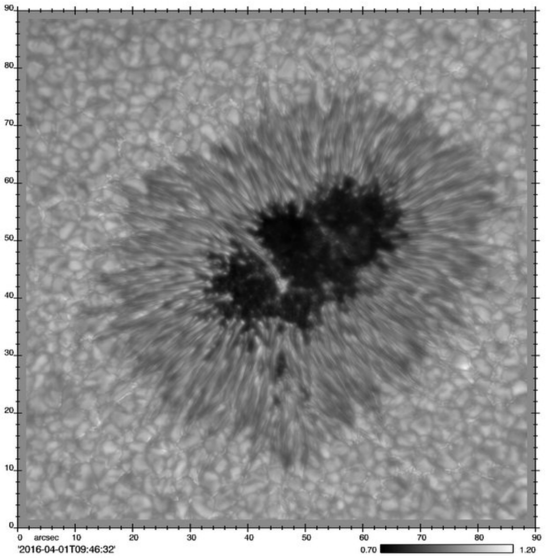

Figure 1.18: Active region NOAA 12526 on April 1, 2016, containing a single sunspot close to the solar equator. The solar disk center is located approx. 430 arcsec towards the lower right (for reference: the solar radius corresponds to 960 arcsec). The image is a speckle-reconstruction from 100 short exposures obtained with the Broadband Imager of the GREGOR telescope at a wavelength of 656 nm. Note the fine detail in the light bridge, the numerous umbral dots, and the bright magnetic features in the intergranular regions in the vicinity of the spot.

1.3 Important Publications and Conference Talks

Group Buchleitner

Publications

[abu1] M. Gessner, F. Schlawin, H. Häffner, S. Mukamel, and A. Buchleitner, “Nonlinear spectroscopy of controllable many-body quantum systems”, New J. Phys. **16** (2014) 092001.

[abu2] J. Zimmermann, R. Mulet, G. D. Scholes, T. Wellens, and A. Buchleitner, “Improving triplet-triplet-annihilation based upconversion systems by tuning their topological structure”, J. Chem. Phys. **141** (2014) 184104.

[abu3] N. Leonhard, V. N. Shatokhin, and A. Buchleitner, “Universal entanglement decay in atmospheric turbulence”, Phys. Rev. A. **91** (2015) 012345.

[abu4] U. Marzolino, and A. Buchleitner, “Quantum teleportation with identical particles”, Phys. Rev. A. **91** (2015) 032316.

[abu5] M. Walschaers, J. Kuipers, J. D. Urbina, K. Mayer, M. C. Tichy, K. Richter, and A. Buchleitner, “Statistical Benchmark for BosonSampling”, New J. Phys. **18** (2016) 032001.

[abu6] F. Schlawin, and A. Buchleitner, “Theory of coherent control with quantum light”, New J. Phys. **19** (2017) 013009.

[abu7] G. D. Scholes, G. R. Fleming, L. X. Chen, A. Aspuru-Guzik, A. Buchleitner, D. F. Coker, G. S. Engel, R. van Grondelle, A. Ishizaki, D. M. Jonas, J. S. Lundeen, J. K. McCusker,, S. Mukamel, J. P. Ogilvie, A. Olaya-Castro, M. A. Ratner, F. C. Spano, K. B. Whaley, X. Zhu, “Using coherence to enhance function in chemical and biophysical systems”, Nature. **543** (2017) 647-656.

[abu8] S. G. Fischer, C. Gneiting, and A. Buchleitner, “Semiclassical asymptotics of the Aharonov-Bohm interference process”, Ann. Phys. (Berlin) **529** (2017) 1700120.

[abu9] F. Spallek, A. Buchleitner, and A. Buchleitner, “Optimal trapping of monochromatic light in designed photonic multilayer structures”, J. Phys. B.: At. Mol. Opt. Phys. **50** (2017) 214005.

[abu10] G. Dufour, T. Brünner, C. Dittel, G. Weihs, R. Keil, and A. Buchleitner, “Many-particle interference in a two-component bosonic Josephson junction: an all-optical simulation”, New. J. Phys. **19** (2017) 125015.

Conference Talks

1. A. Buchleitner, Transport on network-like structures: from light harvesting to boson sampling, Large scale quantum phenomena in biological systems, Galiano Island, Canada, June 2014.
2. A. Buchleitner, Photosynthetic light harvesting - control through disorder, Quantum chaos: fundamentals and applications, Ecole des sciences avancées de Luchon, March 2015.
3. A. Buchleitner, Quantum effects in complex materials: Determinism, statistics, structure, Fundamental Problems in Quantum Physics, Erice, Italy, March 2015.
4. A. Buchleitner, A possible role of non-trivial quantum effects for biology?, Académie Nationale de Médecine, Paris, May 2015.
5. T. Wellens, Multiple scattering of interacting bosons in random potentials, Quantum Africa 3, Rabat, Morocco, September 2015.
6. A. Buchleitner, From many-particle interference to correlation spectroscopy, Quantum Metamaterials & Quantum Technologies, Spetses, Greece, June 2016.
7. T. Wellens, Weak localization of interacting bosons in random potentials, International Workshop on Disordered Systems 10, Brescia, Italy, June 2016.

8. A. Buchleitner, Colloquium on ”Transport on network-like structures – from light-harvesting to boson sampling, Joint Institute for Nuclear Research, Dubna, Russia, September 2016.
9. A. Buchleitner, Witnessing many-particle interference, dynamical observables, and the impact of interactions, CCPQ Workshop, Cumberland Lodge, U.K., August 2017.
10. A. Buchleitner, Quantum dynamics on networks - the interplay of structure, disorder, and statistics, ICQOQI17, Minsk, Belarus, November 2017.

Group Buhmann

Publications

[syb1] H. Bender, C. Stehle, C. Zimmermann, S. Slama, J. Fiedler, S. Scheel, S. Y. Buhmann, and V. N. Marachevsky, “Probing atom-surface interactions by diffraction of Bose-Einstein condensates”, Phys. Rev. X **4** (2014) 011029.

[syb2] S. Y. Buhmann, “Normal-mode quantum electrodynamics: the quantum vacuum and its consequences”, in: “Forces of the Quantum Vacuum: An introduction to Casimir Physics”, edited by W. Simpson and U. Leonhardt, pp. 7–59 (World Scientific Press, London, 2015).

[syb3] S. Ribeiro, S. Y. Buhmann, T. Stielow, and Stefan Scheel, “Casimir–Polder interaction from exact diagonalization and surface-induced state mixing”, Europhys. Lett. **110** (2015) 51003.

[syb4] S. Scheel, S. Y. Buhmann, C. Clausen, and P. Schneeweiss, “Directional spontaneous emission and lateral Casimir–Polder force on an atom close to a nanofiber”, Phys. Rev. A **92** (2015) 043819.

[syb5] P. Barcellona, R. Passante, L. Rizzuto, and S. Y. Buhmann, “Van der Waals interactions between excited atoms in generic environments”, Phys. Rev. A **94** (2016) 012705.

[syb6] J. L. Hemmerich, R. Bennett, T. Reisinger, S. Nimmrichter, J. Fiedler, H. Hahn, H. Gleiter, and S. Y. Buhmann, “Impact of Casimir–Polder interaction on Poisson-spot diffraction at a dielectric sphere”, Phys. Rev. A **94** (2016) 023621.

[syb7] J. Klatt, R. Bennett, and S. Y. Buhmann, “Spectroscopic signatures of quantum friction”, Phys. Rev. A **94** (2016) 063803.

[syb8] I. M. Kinchin, M. Kingsbury, and S. Y. Buhmann, “Research as pedagogy in academic development—a case study”, in: “Academic Peculiarities: Conversations at the Edge of University Teaching and Learning”, edited by E. Medland, R. Watermeyer, A. Hosein, I. M. Kinchin and S. Lygo-Baker (Sense Publishers, Rotterdam, 2017).

[syb9] J. Klatt, P. Barcellona, R. Bennett, O. S. Bokareva, H. Feth, A. Rasch, P. Reith, and S. Y. Buhmann, “Strong van der Waals adhesion of a polymer film on rough substrates”, Langmuir **33** (2017) 5298.

[syb10] P. Barcellona, H. Safari, A. Salam, and S. Y. Buhmann, “Enhanced chiral discriminatory van der Waals interactions mediated by chiral surfaces”, Phys. Rev. Lett. **118** (2017) 193401.

Conference Talks

1. S. Y. Buhmann, Atoms probing the Casimir–Polder potential above a periodically structured surface, invited talk, International Conference on Precision Physics of Simple Atomic Systems, Rio, Brazil, May 2014.
2. S. Y. Buhmann, QED effects involving non-reciprocal media, invited talk, Progress in Electromagnetics Research Symposium, Guangzhou, China, August 2014.
3. S. Y. Buhmann, Casimir–Polder potential of a sphere and its impact on the Poisson spot, invited talk, Progress in Electromagnetics Research Symposium, Prague, Czech Republic, September 2015.

4. S. Y. Buhmann, Casimir effects for unusual systems: From neutrons to Chern–Simons interactions, invited talk, Condensed Matter 26, Groningen, Netherlands, September 2016.
5. J. Fiedler, Medium-assisted van der Waals forces, invited seminar, Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo, Norway, April 2017.
6. R. Bennett, Sphere-plate heat transfer: An analytic approach, invited talk, Progress in Electromagnetics Research Symposium, St. Petersburg, Russia, May 2017.
7. S. Y. Buhmann, How philosophy could enrich physics teaching: linking Kuhn's scientific revolutions to threshold concepts and transformative learning, keynote talk, Progress in Electromagnetics Research Symposium, St. Petersburg, Russia, May 2017.
8. S. Y. Buhmann, Casimir effect and heat transfer for non-reciprocal media, invited talk, Progress in Electromagnetics Research Symposium, St. Petersburg, Russia, May 2017.
9. S. Y. Buhmann, Macroscopic quantum electrodynamics in media: basic formalism and application to the Coulomb interaction, invited talk, Workshop on Casimir/van der Waals theory, Trondheim, Norway, May 2017.
10. S. Y. Buhmann, Harnessing the quantum vacuum: from dispersion forces to interatomic Coulomb decay, Bothe Colloquium, Max-Planck Institute for Nuclear Physics, Heidelberg, November 2017.

Group Breuer

Publications

[breuer1] B.-H. Liu, S. Wißmann, X.-M. Hu, C. Zhang, Y.-F. Huang, C.-F. Li, G.-C. Guo, A. Karlsson, J. Piilo and H.-P. Breuer, "Locality and universality of quantum memory effects," Sci. Rep. **4**, 6327 (2014).

[breuer2] M. Gessner, M. Ramm, H. Häffner, A. Buchleitner and H.-P. Breuer, "Observing a quantum phase transition by measuring a single spin," EPL **107**, 40005 (2014).

[breuer3] M. Gessner, M. Ramm, T. Pruttivarasin, A. Buchleitner, H.-P. Breuer and H. Häffner, "Local detection of quantum correlations with a single trapped ion," Nat. Phys. **10**, 105 (2014).

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[breuer5] J.-S. Tang, Y.-T. Wang, G. Chen, Y. Zou, C.-F. Li, G.-C. Guo, Y. Yu, M.-F. Li, G.-W. Zha, H.-Q. Ni, Z.-C. Niu, M. Gessner and H.-P. Breuer, "Experimental detection of polarization-frequency quantum correlations in a photonic quantum channel by local operations," Optica **2**, 1014 (2015).

[breuer6] C. Weiss, S. A. Gardiner and H.-P. Breuer, "From short-time diffusive to long-time ballistic dynamics: The unusual center-of-mass motion of quantum bright solitons," Phys. Rev. A **91**, 063616 (2015).

[breuer7] S. Wißmann, B. Vacchini and H.-P. Breuer, "Generalized trace-distance measure connecting quantum and classical non-Markovianity," Phys. Rev. A **92**, 042108 (2015).

[breuer8] H.-P. Breuer, E.-M. Laine, J. Piilo and B. Vacchini, "Non-Markovian dynamics in open quantum systems", Rev. Mod. Phys. **88**, 021002 (2016).

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[breuer10] A. Abdelrahman, O. Khosravani, M. Gessner, H.-P. Breuer, A. Buchleitner, D. J. Gorman, R. Masuda, T. Pruttivarasin, M. Ramm, P. Schindler, H. Häffner, "Local probe of single phonon dynamics in warm ion crystals", Nat. Commun. **8**, 15712 (2017).

Conference Talks

1. H.-P. Breuer, Nonequilibrium Quantum dynamics of Open Systems, Workshop on Quantum and Classical Complexity: From Atoms to Biosystems, Bad Homburg, May 2014.
2. H.-P. Breuer, Markovian and Non-Markovian Dynamics in Complex Quantum Systems, Colloquium at the Instituto de Fisica, Universidad Nacional Autonoma de Mexico, January 2015.
3. H.-P. Breuer, Markovian and Non-Markovian Quantum Dynamics of Open Systems, Lectures at the 51 Winter School of Theoretical Physics on Irreversible Dynamics: Nonlinear, Nonlocal and Non-Markovian Manifestations, Ladek Zdroj, February 2015.
4. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, Mini-conference on Non-equilibrium quantum dynamics in low dimensions, Joint Quantum Centre Durham-Newcastle, Durham, July 2015.
5. H.-P. Breuer, Non-Markovian Quantum Dynamics, Lectures held at the Arctic School on Open Quantum Systems, Kilpisjärvi Biological Station, Finland, December 2015.
6. H.-P. Breuer, Theory of Open Quantum Systems, Lectures at First Isfahan-Freiburg Joint School on Quantum Science, Isfahan, May 2016.
7. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, 48th Symposium on Mathematical Physics, Torun, June 2016.
8. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, Workshop on Quantum Dynamics: From Algorithms to Applications, Alfred Krupp Wissenschaftskolleg, Greifswald, September 2016.
9. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, CECAM Workshop on Numerical Methods for Optimal Control of Open Quantum Systems, FU Berlin, September 2016.
10. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, 640. WE-Heraeus-Seminar on Non-Markovianity and Strong Coupling Effects in Thermodynamics, Bad Honnef, April 2017.

Group Sansone

Publications

[sans1] S. L. Cousin, N. Di Palo, B. Buades, S. M. Teichmann, M. Reduzzi, M. Devetta, A. Kheifets, G. Sansone, J. Biegert, “Attosecond Streaking in the Water Window: A New Regime of Attosecond Pulse Characterization”, Phys. Rev. X **7** (2017) 041030.

[sans2] P. Carpeggiani, M. Reduzzi, A. Comby, H. Ahmadi, S. Kühn, F. Calegari, M. Nisoli, F. Frassetto, L. Poletto, D. Hoff, J. Ullrich, C. D. Schröter, R. Moshammer, G. G. Paulus, G. Sansone, “Vectorial optical field reconstruction by attosecond spatial interferometry”, Nat. Photon. **11** (2017) 383-389.

[sans3] S. Kühn, M. Dumergue, S. Kahaly, S. Mondal, M.Füle, T. Csizmadia, B. Farkas, B. Major, Z. Várallyay, E. Cormier, M. Kalashnikov, F. Calegari, M. Devetta, F. Frassetto, Erik Månsson, L. Poletto, S. Stagira, C. Vozzi, M. Nisoli, P. Rudawski, S. Maclot, F. Campi, H. Wikmark, C. L Arnold, C. M Heyl, P. Johnsson, A. L’Huillier, R. Lopez-Martens, S. Haessler, M. Bocoum, F. Boehle, A. Vernier, G. Iaquaniello, E. Skantzakis, N. Papadakis, C. Kalpouzos, P. Tzallas, F. Lépine, D. Charalambidis, K, Varjú, K. Osvay, and G. Sansone, “The ELI-ALPS facility: the next generation of attosecond sources”, J. Phys. B **50** (2017) 13202.

[sans4] S. Chatziathanasiou, S. Kahaly, E. Skantzakis, G. Sansone, R. Lopez-Martens, S. Haessler, K. Varju, G. D. Tsakiris, D. Charalambidis, P. Tzallas, “Generation of Attosecond Light Pulses from Gas and Solid State Media” Photonics **4** (2017) 26.

[sans5] T. Takanashi, N.V. Golubev, C. Callegari, H. Fukuzawa, K. Motomura, D. Iablonskyi, Y. Kumagai, S. Mondal, T. Tachibana, K. Nagaya, T. Nishiyama, K. Matsunami, P. Johnsson, P. Piseri, G. Sansone, A. Dubrouil, M. Reduzzi, P. Carpeggiani, C. Vozzi, M. Devetta, M. Negro, D. Faccialà, F. Calegari, A. Trabattoni, M.C. Castrovilli, Y. Ovcharenko 0, M. Mudrich , F. Stienkemeier , M. Coreno , M. Alagia , B. Schütte , N. Berrah , O. Plekan, P. Finetti, C. Spezzani, E. Ferrari, E. Allaria, G. Penco, C. Serpico, G. De Ninno, B. Diviacco, S. Di Mitri, L. Giannessi, G. Jabbari, K.C. Prince , L.S. Cederbaum, Ph.V. Demekhin , A.I. Kuleff, and K. Ueda, “Time-Resolved Measurement of Interatomic Coulombic Decay Induced by Two-Photon Double Excitation of Ne-2”, Phys. Rev. Lett. **118** (2017) 2033202.

[sans6] C. Callegari, T. Takanashi, H. Fukuzawa, K. Motomura, D. Iablonskyi, Y. Kumagai, S. Mondal, T. Tachibana, K. Nagaya, T. Nishiyama, K. Matsunami, P. Johnsson, P. Piseri, G. Sansone, A. Dubrouil, M. Reduzzi, P. Carpeggiani, C. Vozzi, M. Devetta, D. Faccialà, F. Calegari, M. C. Castrovilli, M. Coreno, M. Alagia, B. Schütte, N. Berrah, O. Plekan, P. Finetti, E. Ferrari, K. C. Prince, K. Ueda, ”Application of Matched-Filter Concepts to Unbiased Selection of Data in Pump-Probe Experiments with Free Electron Lasers”, Applied Sciences **7** (2017) 621

Conference Talks

1. G. Sansone, ”Synthesis of intense, multicolor extre me ultraviolet fields at FERMI: a route towards attosecond coherent control of nonlinear processes” Workshop WAVEFRONT: New Frontiers and Advanced Applications of 4th generation light sources to Atomic, Molecular, Optical and Cluster Science, ICTP, Trieste, Italy, November 2016.

2. G. Sansone, ”Spatial interferometry and coincidence spectroscopy in the extreme ultraviolet range using attosecond pulses”, FRIAS Junior Researcher Conference - Beyond molecular movies: Bringing time-domain spectroscopy to diffraction imaging, Freiburg Germany, September 2017.

3. G. Sansone, ”Coherent control and attosecond spectral interferometry in the extreme ultraviolet range”, Intense field, Short Wavelength Atomic and Molecular Processes (ISWAMP) Ship Inn, South Bank, Brisbane, Australia, July 2017.

Group Schätz

Publications

[schae1] H. Landa, A. Retzker, T. Schaetz, B. Reznik, “Entanglement Generation Using Discrete Solitons in Coulomb Crystals”, Phys. Rev. Lett. **113** (2014) 053001.

[schae2] G. Clos, M. Enderlein, U. Warring, T. Schaetz, D. Leibfried, “Decoherence-assisted spectroscopy of a single Mg+ ion“ Phys. Rev. Lett. **112** (2014) 113003.

[schae3] T. Huber, A. Lambrecht, J. Schmidt, L. Karpa, T. Schaetz, “A far-off-resonance optical trap for a Ba+ ion” Nat. Commun. **5** (2014) 6587.

[schae4] G. Clos, D. Porras, U. Warring, T. Schaetz, “Time-resolved observation of thermalization in an isolated quantum system” Phys. Rev. Lett. **117** (2016) 170401.

[schae5] A. Bermudez, T. Schaetz, “Quantum Transport of Energy in Controlled Synthetic Quantum Magnets” New J. Phys. **18** (2016) 083006.

[schae6] M. Mielenz, H. Kalis, M. Wittemer, F. Hakelberg, R. Schmied, M. Blain, P. Maunz, D.L. Moehring, D. Leibfried, U. Warring, T. Schaetz, “Arrays of individually controlled ions suitable for two-dimensional quantum simulations” Nat. Commun. **7** (2016) 11839.

[schae7] H. Kalis, F. Hakelberg, M. Wittemer, M. Mielenz, U. Warring, T. Schaetz, “Motional-mode analysis of trapped ions” Phys.Rev.A **94** (2016) 023401.

[schae8] T. Schaetz, “Trapping ions and atoms optically” topical review: J. Phys. B **50** (2017) 102001.

[schae9] J. Brox, P. Kiefer, M. Bujak, H. Landa, T. Schaetz, “ Spectroscopy and Directed Transport of Topological Solitons in Crystals of Trapped Ions”, Phys. Rev. Lett. **119** (2017) 153602.

[schae10] A. Lambrecht, J. Schmidt, P. Weckesser, M. Debatin, L. Karpa, T. Schaetz, “Long lifetimes and effective isolation of ions in optical and electrostatic traps” Nature Photonics **11** (2017) 704.

Conference Talks

1. T. Schaetz, Exploiting Ions (and Atoms) in Optical and RF-Traps, 23rd International Congress of the International Commission for Optics (ICO23), Santiago de Compostela, August 2014.
2. T. Schaetz, Trapping Ions and Atoms Optically (TIAMO), 22nd International Conference on Laser Spectroscopy (ICOLS), Singapore, Juni 2015.
3. T. Schaetz, Decoherence-Assisted Spectroscopy: Demonstrated with a Single Mg+ Ion, 47th Conference of the European Group on Atomic Systems (EGAS), Riga, Juli 2015.
4. T. Schaetz, Trapping Ions in Atoms and Molecules Optically, International Workshop on “Hybrid Atomic Quantum Systems”, Hamburg, September 2015.
5. T. Schaetz, Trapping Ions Optically, 4th European Conference on Trapped Ions (ECTI), Arosa, August 2016.
6. T. Schaetz, Arrays of individually controlled ions suitable for two-dimensional quantum simulations, 635th WE-Heraeus-Seminar on “Scalable Architectures for Quantum Simulation”, Bonn, February 2017.
7. T. Schaetz, Time-resolved observation of thermalization in an isolated quantum system, American Physical Society March Meeting, New Orleans, March 2017.
8. T. Schaetz, Optically Trapping and Isolating Atoms and Ions, International Workshop on “Spectroscopy, Dynamics and Applications of Cold Molecular Ions”, Les Houches, Mai 2017.
9. T. Schaetz, Time-resolved observation of thermalization in an isolated quantum system, International Conference on “new trends in complex quantum systems dynamics”, Cartagena, Mai 2017.
10. T. Schaetz, Trapping Ions and Atoms Optically (TIAMO), International ITAMP Workshop on“Controllable Quantum Impurities in Physics and Chemistry” (CoQIPC - 2017), Wien, August 2017.

Group Stienkemeier

Publications

[sti1] A. C. LaForge, M. Drabbels, N. Brauer, M. Coreno, M. Devetta, M. Di Fraia, P. Finetti, C. Grazoli, R. Katzy, V. Lyamayev, T. Mazza, M. Mudrich, P. O'Keeffe, Y. Ovcharenko, P. Piseri, O. Plekan, K. C. Prince, R. Richter, S. Stranges, C. Callegari, T. Moeller, F. Stienkemeier, “Collective autoionization in multiply-excited system: A novel ionization process observed in helium nanodroplets”, Scientific Reports **4** (2014) 3621.

[sti2] M. Mudrich, F. Stienkemeier, “Photoionization of Pure and Doped Helium Nanodroplets”, International Reviews in Physical Chemistry **33** (3) (2014) 301-339.

[sti3] M. Müller, S. Izadnia, S. M. Vlaming, A. Eisfeld, A. C. LaForge, F. Stienkemeier, “Cooperative lifetime reduction of single acene molecules attached to the surface of neon clusters”, Phys. Rev. B **92** (2015) 121408(R).

[sti4] L. Bruder, M. Mudrich, F. Stienkemeier, “Phase-modulated electronic wave-packet interferometry reveals high resolution vibronic spectra of free Rb atoms and Rb*He molecules”, Phys. Chem. Chem. Phys. **17** (2015) 23877–23885.

[sti5] A. C. LaForge, V. Stumpf, K. Gokhberg, J. v. Vangerow, F. Stienkemeier, N. V Kryzhevoi, P. O'Keeffe, A. Ciavardini, S. R. Krishnan, M. Coreno, K. C. Prince, R. Richter, R. Moshammer, T. Pfeifer, L. S. Cederbaum, M. Mudrich, "Enhanced Ionization of Embedded Clusters by Electron-Transfer-Mediated Decay in Helium Nanodroplets", Phys. Rev. Lett. **116** (20) (2016) 203001.

[sti6] K. C. Prince, E. Allaria, C. Callegari, R. Cucini, G. De Ninno, S. Di Mitri, B. Diviacco, E. Ferrari, P. Finetti, D. Gauthier, L. Giannessi, N. Mahne, G. Penco, O. Plekan, L. Raimondi, P. Rebernik, E. Roussel, C. Svetina, M. Trovò, M. Zangrando, M. Negro, P. Carpeggiani, M. Reduzzi, G. Sansone, A. N. Grum-Grzhimailo, E. V. Gryzlova, S. I. Strakhova, K. Bartschat, N. Douguet, J. Venzke, D. Iablonskyi, Y. Kumagai, T. Takanashi, K. Ueda, A. Fischer, M. Coreno, F. Stienkemeier, Y. Ovcharenko, T. Mazza, M. Meyer, "Coherent control with a short-wavelength free-electron laser", Nat. Photonics **10** (2016) 176-179.

[sti7] J. v. Vangerow, A. S. Bogomolov, N. Dozmorov, D. Schomas, F. Stienkemeier, A. V. Baklanov, M. Mudrich, "Role of ion-pair states in the predissociation dynamics of Rydberg states of molecular iodine, Phys. Chem. Chem. Phys. **18** (2016) 18896-18904.

[sti8] S. Izadnia, D. W. Schönleber, A. Eisfeld, A. Ruf, A. C. LaForge, F. Stienkemeier, "Singlet Fission in Weakly Interacting Acene Molecules", J. Phys. Chem. Lett. **8** (9) (2017) 2068–2073.

[sti9] L. Bruder, U. Bangert, F. Stienkemeier, "Phase-modulated harmonic light spectroscopy", Opt. Express **25** (5) (2017) 5302-5315.

[sti10] J. v. Vangerow, F. Coppens, A. Leal, M. Pi, M. Barranco, N. Halberstadt, F. Stienkemeier, M. Mudrich, "Imaging Excited-State Dynamics of Doped He Nanodroplets in Real-Time", J. Phys. Chem. Lett. **8** (1) (2017) 307-312.

Conference Talks

1. F. Stienkemeier,"Doped Rare Gas Clusters in Intense Laser Fields from IR to XUV", Gordon Research Conference *Photoionization & Photodetachment*, Galveston, Texas, USA, February 2014.

2. F. Stienkemeier, "Cluster Experiments at the Free-Electron Laser FERMI", Gordon Research Conference *Molecular & Ionic Clusters*, Lucca, Barga, Italy, April 2014.

3. F. Stienkemeier, "Cluster Experiments at the Free-Electron Laser FERMI", Science@FELS 2014 conference at Paul Scherrer Institute, Villigen, Switzerland, September 2014.

4. M. Mudrich, "Time-resolved and EUV spectroscopy of helium nanodroplets", International Conference on Quantum Fluid Clusters, QFC2015, Toulouse, France, June 2015.

5. F. Stienkemeier, "Excitation and Ionization Dynamics in Helium Nanodroplets", PACIFICHEM, Honolulu, Hawai, December 2015.

6. F. Stienkemeier, "Superradiance, singlet fission and triplet annihilation processes of organic molecules attached to rare gas clusters", S3C, Davos, Switzerland, February 2016.

7. F. Stienkemeier, "Superradiance, singlet fission and triplet annihilation processes of organic molecules attached to rare gas clusters", International School of Solid State Physics: 71st. Workshop: Delocalized Electrons in Atomic and Molecular Nanoclusters, Erice, Italy, July 2016.

8. F. Stienkemeier, "XUV-induced Electron Solvation Dynamics in Water Clusters and New Perspectives in Higher Harmonic Pulse Manipulation", WAVEFRONT: New Frontiers and Advanced Applications of 4th generation light sources to Atomic, Molecular, Optical and Cluster Science, ICTP, Trieste, Italy, November 2016.

9. K. Dulitz, "Reactive Scattering between Metastable Helium and State-Selected, Magneto-Optically Trapped Lithium", International Meeting on Atomic and Molecular Physics and Chemistry, IMAMPC, Torun, Polen, June 2017.

10. F. Stienkemeier, “Electronic Wave Packet Interferometry of Gas Phase Samples: High-Resolution Spectra and Collective Effects”, 72nd International Symposium on Molecular Spectroscopy, Illinois, USA, Plenary Talk, June 2017.

Group von Issendorff

Publications

[bvi1] C. Bartels, C. Hock, R. Kuhnen, and B. von Issendorff, “Photoelectron Imaging Spectroscopy of the Small Sodium Cluster Anions Na_3^-, Na_5^-, and Na_7^-”, J. Phys. Chem. A **118** (2014) 8270–8276.

[bvi2] N. Dörre, J. Rodewald, P. Geyer, B. von Issendorff, P. Haslinger, and M. Arndt, “Photofragmentation Beam Splitters for Matter-Wave Interferometry”, Phys. Rev. Lett. **113** (2014) 233001.

[bvi3] A. Langenberg, K. Hirsch, A. Lawicki, V. Zamudio-Bayer, M. Niemeyer, P. Chmiela, B. Langbehn, A. Terasaki, B. von Issendorff, and J. T. Lau, “Spin and orbital magnetic moments of size-selected iron, cobalt, and nickel clusters”, Phys. Rev. B **90** (2014) 184420.

[bvi4] A. Aguado, A. Vega, A. Lebon, and B. von Issendorff, “Insulating or Metallic: Coexistence of Different Electronic Phases in Zinc Clusters”, Angew. Chem. Int. Ed. **54** (2015) 2111–2115.

[bvi5] K. Hirsch, V. Zamudio-Bayer, A. Langenberg, M. Niemeyer, B. Langbehn, T. Möller, A. Terasaki, B. von Issendorff, and J.T. Lau, “Magnetic Moments of Chromium-Doped Gold Clusters: The Anderson Impurity Model in Finite Systems”, Phys. Rev. Lett. **114** (2015) 087202.

[bvi6] C. Kasigkeit, K. Hirsch, A. Langenberg, T. Möller, J. Probst, J. Rittmann, M. Vogel, J. Wittich, V. Zamudio-Bayer, B. von Issendorff, and J. T. Lau, “Higher Ionization Energies from Sequential Vacuum-Ultraviolet Multiphoton Ionization of Size-Selected Silicon Cluster Cations”, J. Phys. Chem. C **119** (2015) 11148–11152.

[bvi7] C. Liu, B. Yang, E. Tyo, S. Seifert, J. DeBartolo, B. von Issendorff, P. Zapol, S. Vajda, and L. A. Curtiss, “Carbon Dioxide Conversion to Methanol over Size-Selected Cu4 Clusters at Low Pressures”, J. Am. Chem. Soc. **137** (2015) 8676–8679.

[bvi8] V. Zamudio-Bayer, K. Hirsch, A. Langenberg, M. Niemeyer, M. Vogel, A. Lawicki, A. Terasaki, J. T. Lau, and B. von Issendorff, “Maximum Spin Polarization in Chromium Dimer Cations as Demonstrated by X-ray Magnetic Circular Dichroism Spectroscopy”, Angew. Chem. Int. Ed. **54** (2015) 4498–4501.

[bvi9] V. Zamudio-Bayer, R. Lindblad, C. Bülow, G. Leistner, A. Terasaki, B. v. Issendorff, and J. T. Lau, “Electronic ground state of Ni_2^+”, J. Chem. Phys. **145** (2016) 194302.

[bvi10] S. T. Akin, V. Zamudio-Bayer, K. Duanmu, G. Leistner, K. Hirsch, C. Bülow, A. Lawicki, A. Terasaki, B. von Issendorff, D. G. Truhlar, J. T. Lau, and M. A. Duncan, “Size-Dependent Ligand Quenching of Ferromagnetism in Co3(benzene)n+ Clusters Studied with X-ray Magnetic Circular Dichroism Spectroscopy”, J. Phys. Chem. Lett. **7** (2016) 4568–4575.

Conference Talks

1. B. v. Issendorff, Water clusters: thermal behavior and electron solvation, ISSPIC XVII, Fukuoka (Japan), September 2014.

2. B. v. Issendorff, Water clusters: thermal behavior and electron solvation, Physical Chemistry Colloquium, ETH Zürich, October 2014.

3. B. v. Issendorff, Low temperature thermodynamics of water clusters studied by nanocalorimetry , APS march meeting, San Antonio (USA), March 2015.

4. B. v. Issendorff, Low temperature thermodynamics of water clusters studied by nanocalorimetry, ICPEAC XXIX, Toledo (Spain), July 2015.

5. B. v. Issendorff, Matter at the nanoscale: study of the structure and dynamics of clusters, Morino Lecture, Fukuoka (Japan) (followed by six talks in six other locations), August 2015.
6. B. v. Issendorff, The Complex Nonmetal-to-Metal Transition in Zinc Clusters, S3C, Davos (Switzerland), March 2016.
7. B. v. Issendorff, Photoelectron spectroscopy of simple and not so simple metal clusters, DEAMN 2016, Erice (Italy), July 2016.
8. B. v. Issendorff, Matter at the nanoscale: study of the structure and dynamics of clusters, Physics Colloquium Uni Heidelberg, Heidelberg, October 2016.
9. B. v. Issendorff, The electron carousel: angular distributions of photoelectron emitted from simple metal cluster anions, TAMC VIII, Beijing (China), September 2017.
10. B. v. Issendorff, The Complex Nonmetal-to-Metal Transition in Zinc Clusters, ISACC 2017, Varadero (Kuba), September 2017.

Kiepenheuer Institute for Solar Physics (KIS)

Publications

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1.4 PhD, Diploma and Master Theses

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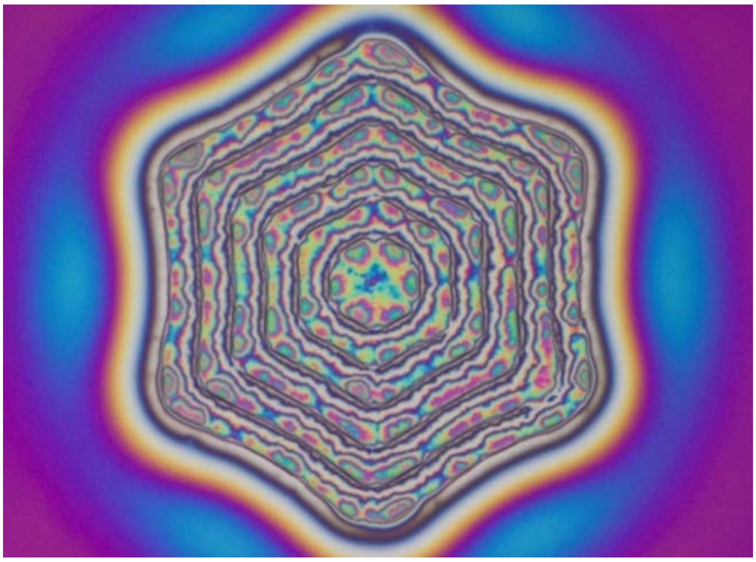
Chapter 2

Condensed Matter and Applied Physics



- **Experimental Polymer Physics**
  Prof. G. Reiter
- **Nanophysics and Molecular Nanomagnets**
  Prof. O. Waldmann
- **Functional Nano Systems**
  Prof. M. Moseler (PI and IWM),
  PD M. Walter
- **Statistical Physics of Soft Matter and Complex Systems**
  Prof. T. Schilling (successor Blumen)
- **Biomolecular Dynamics**
  Prof. G. Stock
- **Theoretical Condensed Matter Physics**
  Prof. M. Thoss (successor Grabert)
- **Dynamics in the Life Sciences**
  Prof. J. Timmer
  apl. Prof. T. Filk
- **Theoretical Applied Physics – Computational Physics**
  N.N.
- **Medical Physics (University Hospital)**
  Prof. M. Bock*
  Prof. J. Hennig*,
- **Bio and Nanophotonics (IMTEK)**
  Prof. A. Rohrbach*
- **Computational Neuroscience (Faculty of Biology)**
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- **Applied Solid State Physics (Fraunhofer IAF)**
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  apl. Prof. C. Elsässer,
- **Spectroscopy of Optical Materials (Fraunhofer IPM)**
  PD F. Kühnemann
- **Solar Energy Systems (Fraunhofer ISE)**
  N.N. (successor Weber)

* co-opted members

Chapter caption: Fascinating morphologies of polymer crystals.

2.1 Overview

Our research in the field of 'Condensed Matter and Applied Physics' explores classical and quantum physical phenomena, functional principles, and technological applications of systems which are built of a network of interacting nano- or microscale objects. The physical properties of the individual building blocks are typically well understood, as well as the short-range interactions between them; the targets of our research are the emerging complex structures, dynamics, transport and function.

The research area comprises seven groups located at the Institute of Physics, working on: Nanophysics and Molecular Magnetism (**O. Waldmann**), Theoretical Condensed Matter Physics (**M. Thoss**, successor of **H. Grabert**), Experimental Polymer Physics (**G. Reiter**), Functional Nanosystems (**M. Moseler**, **M. Walter**), Theoretical Physics of Soft Matter and Complex Systems (**T. Schilling**, successor of **A. Blumen**), Dynamic Processes in Life Sciences (**J. Timmer**), and Biomolecular Dynamics (**G. Stock**). In addition, there are three co-opted members of the Physics Institute, working on Bio- and Nanophotonics (**A. Rohrbach**, IMTEK), Medical Physics, (**J. Hennig**, **M. Bock**, Faculty of Medicine) and Neurobiology and Biophysics (**S. Rotter**, successor of **A. Aertsen**, Faculty of Biology) and three members from Frauenhofer Institutes, **J. Wagner** (IAF), **F. Kühnemann** (IPM) and **C. Elsässer** (IWM).

During the reporting period, G. Reiter and J. Timmer have each served as Dean of Studies.

In the frame of the new round of the German Excellence University Initiative, the University of Freiburg was invited to file applications for two Clusters of Excellence. Our research area is strongly represented in these clusters as well as in other collaborative, third party funded research structures. M. Moseler and G. Reiter are members of the cluster "Living, adaptive and energy-autonomous Material Systems" (livMatS). G. Stock and J. Timmer are members of the cluster "Center for Biological Signalling Studies (CIBSS). Reiter is the speaker of the International Research Training Group IRTG-1642 “Soft Matter Science: Concepts for the Design of Functional Materials” and principal investigator of the transregio collaborative research center SFB-TRR 141: “Biological Design and Integrative Structures – Analysis, Simulation and Implementation in Architectur”. J. Timmer is principal investigator of the trans regio collaborative research center TRR179: "Determinants and dynamics of elimination versus persistence of hepatitis virus infection" and member of the currently running Cluster of Excellence "Centre for Biological Signalling Studies" (BIOSS).

The systems we investigate in the Condensed Matter and Applied Physics research area embrace a large array of different building blocks, which range from magnetic metal ions over molecules, clusters, and polymers to biological entities such as proteins, viruses and cells. Correspondingly a large variety of interaction mechanisms exist, and the systems span all length scales from molecular to macroscopic. The research questions that arise naturally in this context concern the crossover from quantum to classical, and from microscopic to macroscopic. These questions are universal and thus tie our research activities on different physical building blocks into fruitful collaboration.

There is obvious overlap with the research of the

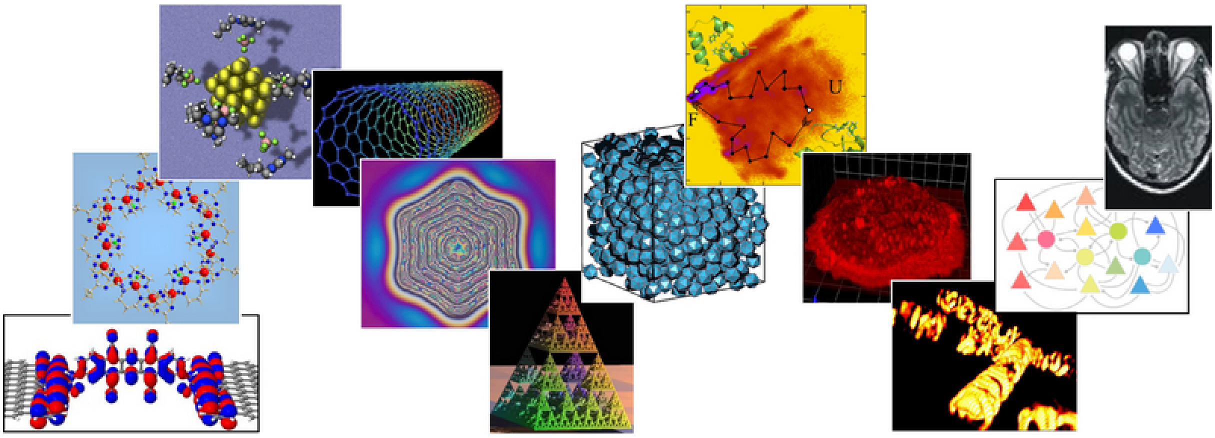

Figure 2.1: Sketch of the variety of condensed and soft matter materials investigated by the research groups in the Condensed Matter and Applied Physics area. They range from nanoscopic systems involving a few interacting units to macroscopic ensembles and networks.

colleagues in the research area of ”Atomic, Molecular and Optical Sciences”. In contrast to their work, however, our focus is on the understanding, tailoring and harnessing of the emerging complex quantum states and classical excitations, transport processes, novel functions, and information processing capabilities. These depend on the structures, topologies of the interaction pathways, and external fields or embedding environments. Figure 2.1 aims at sketching this richness in systems and materials investigated in the Condensed Matter and Applied Physics research area.

The various ongoing research activities have been arranged into the three sections ’Transport and Dynamics in Matter’, ’Functional Materials’, and ’Biological Systems’, with the understanding that a group’s research cannot always be strictly attributed to one or the other. The research activities presented in Section 2.2 primarily focus on advanced quantum mechanical phenomena in low-dimensional systems, such as complex quantum many-body states and excitations, quantum dynamics and transport as well as environmental effects such as dissipation, decoherence and relaxation in open systems. The systems and materials studied range from one and two dimensional carbon based materials, nano and micro structured semiconducting and optical materials, self-assembled monolayers and magnetic molecules to artificial and biological macromolecules and polymers.

The following Section 2.3 describes research activities, which are primarily devoted to the relation of the geometrical and electronic structure of the building blocks and their interactions under dimensionally restricted conditions (clusters, interfaces, films) with the function and macroscopic physical and chemical behavior of the material, such as self-assembly into higher-ordered structures, phase transitions, mechanical properties, catalysis, and light conversion and other properties of technological relevance. Materials-wise molecules, metal and metal-oxide nano clusters, supra-molecular architectures, polymer films, conducting polymers and silicon, as well as liquid crystals and soft composites are investigated.

Finally, Section 2.4 provides an overview of the research activities, which are primarily concerned with biological systems and model systems mimicking important biological interactions and functions. These groups investigate proteins and their interactions, biological cells, bio-mimetic systems and synthetic cell systems and ensembles of neurons and the brain. They focus on understanding the microscopic mechanisms and the statistical mechanics underlying these complex systems, their information processing and response, neuronal dynamics and coordinated activity.

The Condensed Matter and Applied Physics groups have achieved many outstanding research results in the past three years. Three findings shall exemplary be highlighted here:

Although it is well-known that fully fluorinated carbon materials are hydrophobic (despite the strong polarity of the C-F bond), the physical mechanism underlying this “polar hydrophobicity” was not clear. The group of Michael Moseler performed density functional calculations of water on fluorinated diamond surfaces and found a strong decay of the electric field such that the binding of the water dipole is strongly reduced [mos9]. A venerable article of Lennard-Jones (Trans. Faraday Soc. 1928) provides the mathematical explanation: the electric field of a dipole lattice decays exponentially and the decay is strong for the large dipole densities occurring in fluorinated carbon materials.

Allostery is the puzzling phenomenon of long-range communication between distant sites of protein, representing the elementary process of cell signaling. While a number of thermodynamic models have been proposed, the dynamic process of allosteric communication itself is still not well understood. Employing extensive nonequilibrium molecular dynamics simulations, the group of Gerhard Stock could draw a real-time picture of the way allostery works [stock8]. Mediated by the propagation of stress, allostery was found to trigger structural and dynamical changes in a nonlinear and nonlocal fashion, which gives rise to strongly nonexponential kinetics.

Singlet fission is a photophysical process in molecular materials, which involves the conversion of one singlet exciton into two triplet excitons. The ability to effectively implement singlet fission processes in solar cells could allow for more efficient harvesting of high-energy photons from the solar spectrum thus circumventing the Shockley–Queisser performance limit. To unravel the basic mechanisms of singlet fission, the Thoss group, in close collaboration with the experimental groups of D. Guldi, R. Tykwinski, and M. Wasielewski investigated the process of intramolecular singlet fission in conjugated and non-conjugated pentacene dimers [thoss8, thoss9]. Combining high-level electronic structure calculations, quantum dynamical simulations and time-resolved spectroscopy, it could be shown that the formation of the triplet pair state proceeds on an ultrafast timescale. Furthermore, it was found that the process is facilitated by indirect electronic coupling via charge transfer and quintet states as well as vibronic coupling.

2.2 Transport and Dynamics in Matter

2.2.1 Nanophysics and Molecular Nanomagnets

The **Nanophysics and Molecular Magnetism Group of Oliver Waldmann** investigates the spin excitations and magnetic relaxation dynamics in the so-called molecular nanomagnets. These magnetic materials consist of molecules containing magnetic metal ions and organic ligands. A representative example is shown in Fig. 2.2. The ligands play a threefold role: Via complex bonds they hold together the molecule in a well-defined geometry, such that all molecules in a macroscopic sample are structurally identical, and the structure is precisely known from x-ray crystallography. They also allow for magnetic exchange interactions between the magnetic metal ions in a molecule, such that these magnetic nanoclusters are essentially quantum many-body systems of a dozen or so of interacting spin centers. Lastly, the ligands act as "chicken fat" enclosing the molecule, which efficiently isolates a molecule magnetically and magnetic interactions between different molecules in a sample are negligibly small. These magnetic molecules hence do not exhibit any form or shape dispersion, their structures are precisely known, and magnetically they are well isolated from each other, and in this regard they are ideal model systems. These features make the molecular nanomagnets special among the class of magnetic nanoparticles.

In the Waldmann group the magnetic properties of these molecular nanomagnets are experimentally studied and numerically simulated from two different physical perspectives: On the one hand molecules in which the isotropic Heisenberg exchange is the dominant interaction term are regarded as experimental model systems for nanosized quantum many-spin systems and their low-energy spin excitations are studied. On the other hand the phenomenon of quantum tunneling of the magnetism and slow magnetic relaxation in molecular nanomagnets containing highly-anisotropic metal ions such as Co(II) and Lanthanides is investigated. Experimentally the group applies spectroscopic techniques such as inelastic neutron scattering and thermodynamic techniques such as in-house built micro Hall magnetometers and ac susceptometers.

Nano-sized quantum many-spin systems

Molecules with dominant isotropic Heisenberg exchange interactions between the molecule's metal ions are described by spin Hamiltonians similar to those found in the field of quantum spin systems, such as one-dimensional chains, ladders, and the many two-dimensional lattices (square, triangular, Kagome, etc.). They exhibit however two important differences: (i) The number of spin centers is limited to a dozen or so, and (ii) the spin lengths are typically 'large', i.e. $s \geq 3/2$, and it in fact turns out that these spin lengths are of more interest than the $s = 1/2$ quantum spin case. Ties to the physics observed in extended spin lattices or other fundamental models of physics exist.

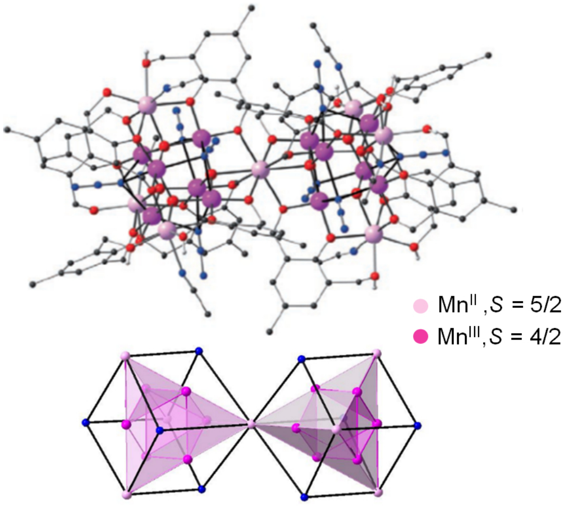

Figure 2.2: Top: Crystal structure of the Mn$_{19}$ molecule. The pink balls represent Mn(II) and Mn(III) metal ions, which carry a spin of $s = 5/2$ and $s = 2$, respectively. The other balls represent O, N, and C atoms; H atoms are omitted. Bottom: Sketch of the magnetic core. It can be considered a bi-supertetrahedron, where two supertetrahedra are fused at one corner. The corner and central positions are occupied by 7 Mn(II) ions, and the octahedral cores by 12 Mn(III) ions.

For instance, in the molecule Mn$_{19}$ a quantum magnon ladder could be experimentally observed for the first time. Mn$_{19}$ consists of seven Mn(II) spin-5/2 and twelve Mn(III) spin-2 metal ions (Fig. 2.2), which are ferromagnetically coupled such that a ground state with a huge total spin of $S = 83/2$ results. As is well known, the low-energy excitations in bulk ferromagnets can be described as spin waves, which essentially correspond to quantum harmonic oscillators with the magnons as the quanta of excitation. In bounded ferromagnetic spin clusters, such as Mn$_{19}$, the low-lying excitations can be described by the finite-size versions of the spin waves or magnons, which also correspond to quantum harmonic oscillators. However, usually the ladder of quantum states $E_n = \hbar\omega(n + 1/2)$ corresponding to one oscillator cannot be experimentally observed, since there are close-lying oscillators with $\omega' \approx \omega$. In contrast, as the Waldmann group discovered, the distinct exchange-coupling topology in Mn_{19} permits the existence of a well-separated low-energy magnon mode.

Inelastic neutron scattering experiments in the relevant energy range could be performed in cooperation with Powell's synthetic chemistry group (Karlsruhe, KIT), which revealed a cold, low-energy excitation at ca. 0.25 meV, see Fig. 2.3. Most importantly, the temperature dependence of its intensity is highly unusual for bounded spin clusters, but reminiscent of that of magnetic excitations in extended spin systems. A careful analysis of the Stokes and Anti-Stokes intensities revealed that their temperature dependencies are accurately described below ca. 8 K by the Bose-Einstein distribution, as expected for an isolated quantum harmonic oscillator, but unlike anything seen so far for bounded spin clusters. It is important to note that the neutron scattering intensity is a direct measure of the transition matrix elements, and that the experimental observation directly demonstrates the $\sqrt{n+1}$ and $\sqrt{n}$ dependence for the raising and lowering operators, thus representing a "smoking gun". The observation of the quantum magnon ladder in Mn_{19} is unique, and is possible only in the crossover regime between small and extended spin systems. As such it establishes a striking example of a mesoscopic phenomenon, which exists only in-between the microscopic and macroscopic limits.

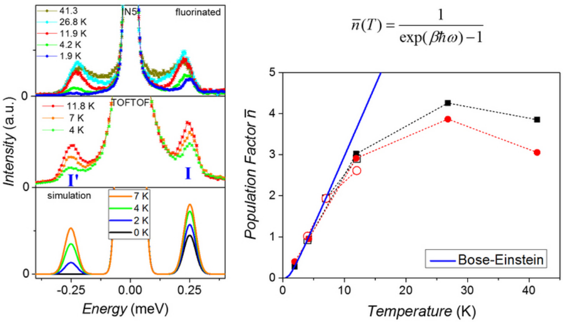

Figure 2.3: Left: Experimental inelastic neutron scattering intensities of Mn_{19} at small energies, as function of temperature. The results of two experiments are shown (top and middle panels), as well as numerical simulations (bottom panel). A prominent cold excitation is observed, labeled I on the Stokes side, and I' on the Anti-Stokes side. Right: Thermal population factor as function of temperature of the magnon states involved in the transitions I and I', as extracted from the experimental intensities of the Stokes and Anti-Stokes peaks (circles and squares). The low-temperature part, below ca. 8 K, can be well described by a Bose-Einstein distribution, which demonstrates the quantum magnon ladder in Mn_{19}.

Lanthanide-based single-molecule magnets

Molecules which contain highly-anisotropic metal ions may show single-molecule magnetism, i.e., slow-relaxation of the magnetization and magnetic hysteresis, below a blocking temperature of few Kelvins (the record is currently ca. 15 K). These systems can in principle be used as molecular data storage devices, which is obviously of considerable interest. A major stumbling block is however to raise the blocking temperature above room temperature. It is hence crucial to understand better the magnetic relaxation in these compounds.

The Waldmann group has recently, in cooperation with Evans's and Long's synthetic chemistry groups, made important progress by an inelastic neutron scattering study of the magnetic excitations in the single-molecule magnet $\mathrm{Tb}_2(\mu\text{-}\mathrm{N}_2^{3-})$, which is excelled by a world-record high blocking temperature of ca. 15 K [waldm3]. In the parent compound $\mathrm{Tb}_2(\mu\text{-}\mathrm{N}_2^{2-})$ two excitations were observed, at ca. 0.75 meV and 5.2 meV, which could be assigned to an exchange-based and a ligand-field based transition, respectively. With these results the magnetic model for $\mathrm{Tb}_2(\mu\text{-}\mathrm{N}_2^{3-})$ could be improved, and the nature of the excited states be clarified. Generally, inelastic neutron scattering experiments on Lanthanide-based molecular clusters are extremely difficult, because of the low magnetic scattering intensity, the large vibrational background scattering, the few lines to be observed, and the air-sensitivity in the case of $\mathrm{Tb}_2(\mu\text{-}\mathrm{N}_2^{3-})$. The work by the Waldmann group represents the most successful inelastic neutron scattering experiment on a poly-nuclear Lanthanide-based single-molecule magnet.

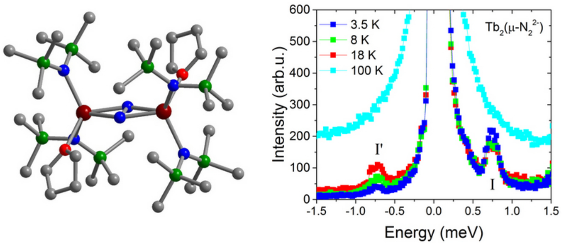

Figure 2.4: Left: Crystal structure of the parent compound $\mathrm{Tb}_2(\mu\text{-}\mathrm{N}_2^{2-})$. Tb(III) in dark red; the other balls represent N, O, and C atoms, H atoms were omitted. Inelastic neutron scattering intensity at various temperatures, showing the cold 0.75 meV exchange-based excitation.

2.2.2 Theoretical Condensed Matter Physics

Research in the **Theoretical Condensed Matter Physics Group of Michael Thoss** focuses on theory and simulation of nonequilibrium processes in many-body quantum systems, in particular nanostructures, surfaces, interfaces, and molecular systems. Theoretical and computational methods are being developed and used to understand fundamental aspects of dynamics and transport in complex quantum systems. More applied projects include the simulation of charge and energy transport as well as light-induced processes in the context of nanoscience and energy conversion, often in close collaboration with experimental groups from physics, chemistry and materials science.

M. Thoss joined the Institute of Physics at the University of Freiburg in October 2017. The main lines of research of the Thoss group include the topics discussed below. The specific projects reported have been carried out mostly at our previous institution, the University of Erlangen-Nürnberg.

Quantum transport in nanostructures

One of our main research activities concerns the theory and simulation of quantum transport in nanostructures. An example is charge transport in single molecule junctions, where single molecules are bound to metal or semiconductor electrodes. These systems combine the possibility to study fundamental aspects of nonequilibrium many-body quantum physics at the nanoscale with the perspective for technological applications in nanoelectronic devices. Employing a combination of first principles electronic structure methods and state-of-the-art transport theory, we have analyzed transport mechanisms in molecular junctions including electron-vibration and electron-electron interaction, quantum interference effects as well as fluctuations and noise phenomena [thoss1, thoss2]. Moreover, we have devised novel schemes for molecular nanoswitches based on proton transfer reactions [thoss3].

While most experiments on single-molecule junctions have employed metal electrodes, carbon-based materials represent another promising class of materials for electrodes. Graphene is of particular interest in this context, because it offers excellent electronic properties, especially high electron mobility, and, furthermore, may facilitate optical addressability of the nanocontact for optoelectronic applications. In a recent study together with the experimental group of H. Weber (University of Erlangen), we could show that the unique electronic properties of graphene strongly influence the transport in the nanojunctions [thoss4] (cf. Fig. 2.5). In particular, edge states in graphene electrodes with zigzag termination result in additional transport channels, which dominate transport at low voltages. Using the theory of local currents, electron pathways through the molecule-graphene junction were analyzed.

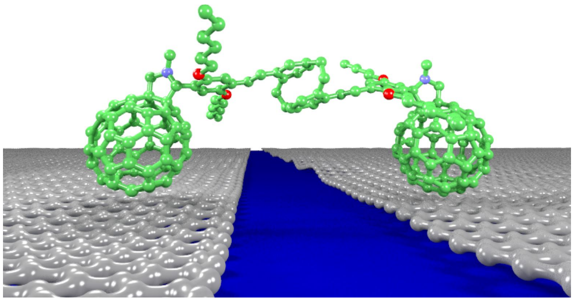

Figure 2.5: Schematic view of a C_{60}-endcapped molecule-graphene junction [thoss4].

In another line of research in this field, we have investigated charge transport in organic semiconductors [thoss5, thoss6]. Employing a novel multiscale methodology, which combines molecular dynamics simulations, electronic structure calculations and transport theory, we have analyzed electron transport in self-assembled monolayers (SAMs) of different types of molecules, which are used in novel organic field effect transistors (cf. Fig. 2.6). In collaboration with the experimental group of M. Halik and the theoretical group of T. Clark (University of Erlangen) it was shown that transport in these systems depends significantly on the morphology of the SAMs and is affected by static and dynamic disorder.

Light-induced processes

The availability of ultrashort laser pulses, which have recently reached the subfemtosecond time scale, allows studies of ultrafast processes in atoms, molecules and condensed matter in ‘real time’. Of primary interest in molecular systems and condensed matter is the unraveling of electronic and nuclear motion and their mutual correlation. Our theoretical work in this area concentrates on the simulation and analysis of time-dependent non-Born-Oppenheimer processes and their role in photoinduced charge and energy transfer processes in molecular materials. A focus of our work in the reporting period was the process of carrier multiplication by singlet-triplet fission in organic crystals, which holds promise to improve the efficiency of solar cells. Together with the experimental groups of D. Guldi (Universität Erlangen-Nürnberg), R. Tykwinski

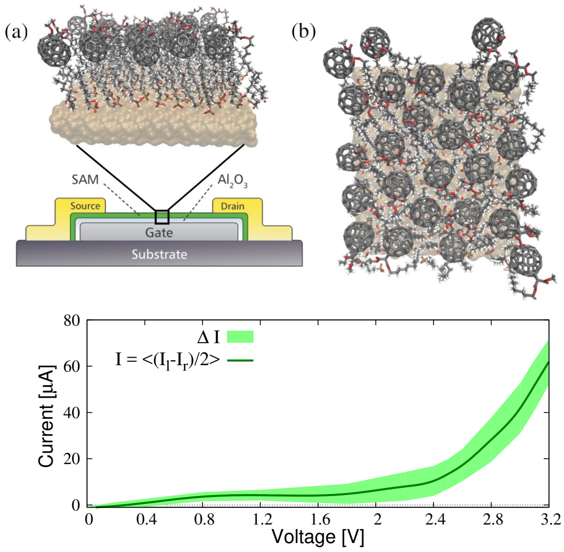

Figure 2.6: (a) Scheme of a C_{60}-based self-assembled monolayer field-effect transistor, (b) snapshot of the SAM (top view) (c) IV-characteristic of the SAM obtained from a time-dependent nonequilibrium Green's function method. The full line depicts the time-averaged current, while the shaded area represents the fluctuations. Adapted from [thoss5].

(University of Alberta, Canada), and M. Wasielewski (Northwestern University, USA) as well as the theory group of J. Neaton (UC Berkeley, USA), we studied the process of intramolecular singlet fission. The studies revealed the different mechanisms of singlet fission in conjugated and non-conjugated dimers and showed for the first time the importance of quintet states in the process [thoss7, thoss8, thoss9].

Fundamental aspects of quantum dynamics in many-body systems

In addition to first-principles simulations of specific systems, the Thoss group also investigates fundamental aspects of nonequilibrium quantum dynamics in many-body systems employing generic models such as the spin-boson model, Anderson-type impurity models as well as other many-body models with electron-electron and electron-phonon interaction. Recent studies in this area include the investigation of multistability and initial state dependence in quantum impurity problems as well as nonadiabatic effects [thoss1] (cf. Fig. 2.7) and noise phenomena in quantum transport.

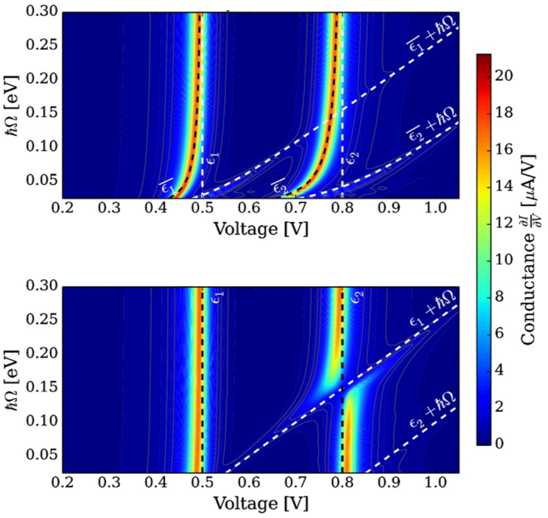

Figure 2.7: Conductance map for electron transport in molecular junctions obtained for models with adiabatic (upper panel) and nonadiabatic (lower panel) electronic-vibratinal coupling. In both plots, the conductance $\frac{\partial I}{\partial V}$ is plotted as a function of voltage V and and vibrational energy $\hbar\Omega$. The dashed lines indicate the positions of the unperturbed electronic resonances $\varepsilon_{1/2}$, the electronic resonances renormalized by the coupling to the vibrations $\bar{\varepsilon}_{1/2}$ as well as their respective vibrational satellites. Adapted from [thoss1]

Development of numerical methods for quantum dynamics in many-body systems

Theoretical studies of quantum dynamics in condensed matter or molecular systems require accurate methods capable of describing many-body quantum systems out of equilibrium. The range of methods developed and used in the Thoss group comprises quantum dynamical methods based on wave functions, density matrix theory and nonequilibrium Green's functions. Examples include the multilayer multiconguration time-dependent Hartree method (ML-MCTDH) [thoss10] and hierarchical quantum master equations (HQME) [thoss2]. Furthermore, semiclassical methods are being developed. These dynamical methods are combined with a first-principles description of the electronic structure using density functional theory (DFT) and wavefunction based approaches.

2.2.3 Biomolecular Dynamics

The **Biomolecular Dynamics Group of Gerhard Stock** is concerned with the theory and computation of structure, dynamics and function of biomolecules, driven by the ultimate goal of a truly microscopic understanding of the underlying physics. Because state-of-the-art molecular dynamics (MD) simulations and multidimensional experiments generate an enormous amount of data, a main objective is to derive simple “postsimulation models” that explain the essential dynamics of the process. The group provides a link between the molecular physics research and the biophysics/polymer research of the Institute and also connects to the Physical Chemistry groups the Chemistry department. Most of our research projects during the reporting period can be summarized in the following topics.

Free energy landscapes

Dimensionality reduction methods such as principal component analysis attempt to reduce the description of the highly correlated molecular motion of $3N$ atomic coordinates to some collective degrees of freedom q_i [stock10]. The resulting low-dimensional probability distribution $P(\{q_i\})$ can then be used to construct the free energy landscape $F = -k_{\mathrm{B}}TP(\{q_i\})$ of the process, which in a second step may be employed in a data-driven Langevin simulation to facilitate a detailed investigation of biomolecular dynamics in low dimensions [stock2]. Alternatively, one may partition the continuous MD trajectory in discrete metastable states and construct a Markov state model, which approximates the dynamics of the system by a memoryless jump process [stock7].

During the reporting period, several long-standing methodological endeavors have come to a successful end. For one, we have developed a density-based geometric clustering approach that provides a well-defined heuristic for the optimal bandwidth selection and is applicable to data with more than 10^7 frames [stock7]. Identifying well-defined microstates separated by local free energy barriers, the algorithm provides an essential improvement over commonly employed k-means-type methods. Second, by extending previous efforts to employ dihedral angles as collective coordinates, we have devised a dimensionality reduction method for high-dimensional circular data. The approach minimizes the periodicity-induced projection error, provides low-dimensional reaction coordinates and offers a direct interpretation of covariances and principal components [stock10].

The methods have be employed to study various biomoleculer processes of current interest, including folding [stock7], functional motion [stock1, stock9] and allosteric communication [stock8]. Moreover, they have been substantial in the development of a general strategy to identify reaction coordinates of protein functional dynamics. Adopting the hinge-bending motion of T4 lysozyme as a prominent example, we have tested prospective candidates for a reaction coordinate by studying the molecule’s response to external pulling along the coordinate, using targeted MD simulations. While trying to directly enforce the open-closed transition does not recover the two-state behavior of T4L, this transition is triggered by a locking mechanism, by which the side chain of Phe4 changes from a solvent-exposed to a hydrophobically-buried state. In extension of the usual two-state picture, we have proposed a four-state model of the functional motion of T4L, which describes a hierarchical coupling of the fast nanosecond opening-closing motion and the slow microsecond locking transition, see Figure 2.8.

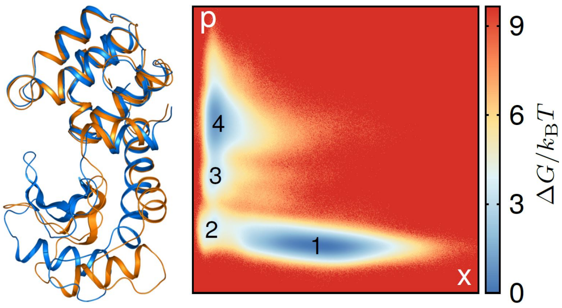

Figure 2.8: The hinge-bending motion of T4 lysozyme can be explained by a four-state model describing hierarchical coupling of fast opening-closing motion and slow locking transition.

Other recent methodological work in this area includes the derivation of a data driven Langevin equation that applies beyond the overdamped limit, which was shown to be an important feature for the modeling of conformational dynamics [stock2]. Based on a system-bath ansatz á la Zwanzig and on an “empirical valence bond”-type model, we have proposed a practical method to construct an analytically defined Langevin model to represent multidimensional free energy landscapes as well as an approximate description of the friction field [stock5]. The model can be used to investigate the dependence of the system on parameter changes and to predict the effect of site-selective mutations on the dynamics. We finally mention a recent idea using the Maximum Caliber approach to infer transition rates of networks from populations in continuous-time Markov processes [stock4].

Vibrational energy transport

The transport of vibrational energy in molecular systems plays an important role in the operation of mechanical and electronic machines. In order to avoid overheating, for example, molecular electronic devices as well as photoproteins need to dissipate excess energy on very short time and length scales. Computational studies of vibrational energy flow in biomolecules have to date mapped out transport pathways on a case by case basis. To provide a more general approach, we have derived scaling rules for vibrational energy transport in a globular protein, which are identified from extensive nonequilibrium molecular dynamics simulations of the vibrational energy flow in various proteins [stock6] We have parameterized a master equation based on inter-residue, residue-solvent and heater-residue energy transfer rates which closely reproduces the results of the all-atom simulations. From that fit two scaling rules emerge, one for energy transport along the protein backbone which relies on a diffusion model, and another for energy transport between tertiary contacts which is based on a harmonic model, see Figure 2.9. Currently the theory as well as nonequilibrium simulations are employed to model very recent transient infrared experiments on the energy transport in photoswitchable peptides and proteins (collaboration with P. Hamm, Zürich and J. Bredenbeck, Frankfurt).

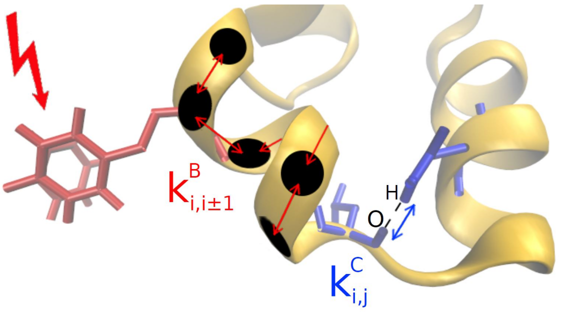

Figure 2.9: Following photoexcitation via a molecular photoswitch, the vibrational energy is transported though the protein along the backbone and via side-chain contacts. [stock6].

In a somewhat different line of research, we have employed extensive *ab initio* calculations and the time-propagation of a 6-dimensional nuclear Schrödinger equation to study the vibrational relaxation dynamics and resulting spectral signature of the OH stretch vibration of a hydrogen-bonded complex, $HCO_2^-\cdot H_2O$ [stock3]. Exploiting an adiabatic separation of timescales between the three intramolecular high-frequency modes of the water molecule and the three most important intermolecular low-frequency modes of the complex, we have identified a vibrational conical intersection seam that connects the OH stretch vibration to the HOH bend overtone. The conical intersection results in a coherent population transfer between the two states, the first step of which being ultrafast with 60 fs and irreversible.

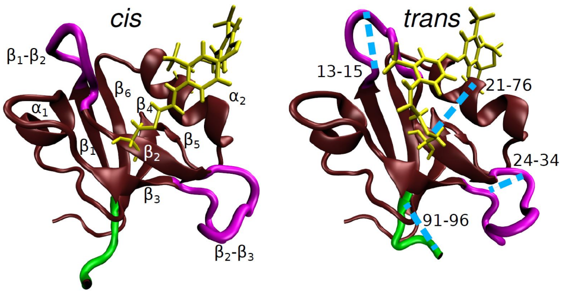

Figure 2.10: MD snapshots of PDZ2 in *cis* (left) and *trans* (right) equilibrium states. The blue lines in the right panel indicate selected Cα-distances which characterize the conformational transition following *cis*-*trans* photoisomerization of PDZ2. [stock8].

Nonequilibrium description of allosteric communication

Allostery represents a fundamental mechanism of biological regulation which is mediated via long-range communication between distant protein sites. While little is known about the underlying dynamical process, recent time-resolved infrared spectroscopy experiments on a photoswitchable PDZ domain (PDZ2S) have indicated that the allosteric transition occurs on multiple timescales (Figure 2.2.3). Employing extensive nonequilibrium MD simulations, we have developed a time-dependent picture of the allosteric communication in PDZ2S [stock8]. The simulations have revealed that allostery amounts to the propagation of structural and dynamical changes, that are genuinely nonlinear and can occur in a nonlocal fashion. We have constructed a dynamic network model that illustrates the hierarchy and exceeding structural heterogeneity of the process. In compelling agreement with experiment, three physically distinct phases of the time evolution have been identified, describing elastic response (≤ 0.1 ns), inelastic reorganization (~ 100 ns) and structural relaxation ($\geq 1\mu$s). Our work has shown a close analogy of the allosteric transition with downhill folding as well as lead to a different interpretation of allosteric pathways.

2.3 Functional Materials

2.3.1 Experimental Polymer Physics

Research of the **Experimental Polymer Physics Group by Günter Reiter** focusses on "Soft Matter", an essential link between (Macromolecular) Chemistry, Biology and Applied Sciences. Key questions concern the understanding and control of dynamics and structure formation processes in complex molecular systems and materials, inspired partially by processes found in nature.

Polymer physics represents a fundamental pillar in terms of basic and conceptual issues in an interdisciplinary approach of innovative materials research. Research of the Reiter group concentrates on questions dealing with properties of surfaces and interfaces, growth and structure formation processes, functional materials based on complex, nano-structured systems. Emphasis is on the study of basic molecular interactions, which control organization and structure formation.

The Experimental Polymer Physics group follows a "bottom-up" approach: molecular interactions and their control on a sub-nanometre scale determine the hierarchical organization of complex and functional (macro-) molecules over many length scales up to macroscopic lengths. These structures are made visible, the underlying ordering processes are identified and structure formation is varied and controlled by appropriate manipulation (external factors). Emphasis is intentionally placed on surface phenomena, because the corresponding (quasi-)two-dimensional systems allow for a set of experimental approaches and because these phenomena play a central role in materials research. The research of the group subdivides into three main themes, each illustrated here with one example:

Molecular interactions and structure formation

One of the main activities concerns the influence of structure formation on opto-electronic properties of conjugated polymers [reit8].

Crystallization allows to generate chains with highly planarised backbones, embedded in structures exhibiting long-range order. In the present example, we used spatially resolved optical spectroscopy to quantify differences in the degree of order of a bulky substituted poly (3-(2, 5-dioctylphenyl) thiophene) (PDOPT). In particular, we compared absorption and photoluminescence (PL) measurements from large spherulitic crystals and from the same region when rapidly recrystallized after melting.

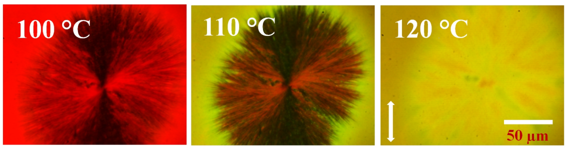

Figure 2.11: Photoluminescence micrographs from a spherulitic crystal grown at 100 ^{o}C for 50 hours, excited by light polarized in the direction indicated by the white arrow, during heating across the melting temperature.

In addition, we followed *in-situ* melting and recrystallization processes, i.e., transitions between ordered and disordered phases. A multi-peak analysis of absorption and PL spectra based on a modified Franck-Condon progression, showed changes in, e.g., the relative intensities of each peak, the excitonic bandwidth and the vibronic energy as a function of temperature. Most importantly, at the phase transition temperature, a clear change in the positions of the peaks (i.e., their wavelengths, corresponding to the energy of the emitted photons) could be detected.

Phase transitions in complex systems

For many years, the group studies processes of polymer crystallisation and the various resulting crystal morphologies, which are essential in deciding properties and performance of polymeric materials. Unlike small molecules, polymers have intrinsically slow dynamics due to their chain connectivity and their interpenetration with neighbouring chains.

In a systematic study [reit9], we have evidenced the impact of non-equilibrium conformational states (induced in isotactic polystyrene films through spin coating) on the crystallization kinetics of polymer films.

Trying to equilibrate such films at temperatures well above the equilibrium melting temperature of the polymer, showed striking changes crystal nucleation density and growth rate, which both decayed exponentially at an extraordinarily slow rate, in comparison with the expected characteristic relaxation time of isotactic polystyrene at equilibrium. These changes in rates were accompanied by changes in the morphology of crystals from spherulites (circular) to hexagons of rather uniform height to finally hexagons exhibiting periodic modulations in height.

Our observations clearly illustrate that the controlled relaxation of non-equilibrium states allows for a systematic tuning of morphology and crystallization kinetics of polymers.

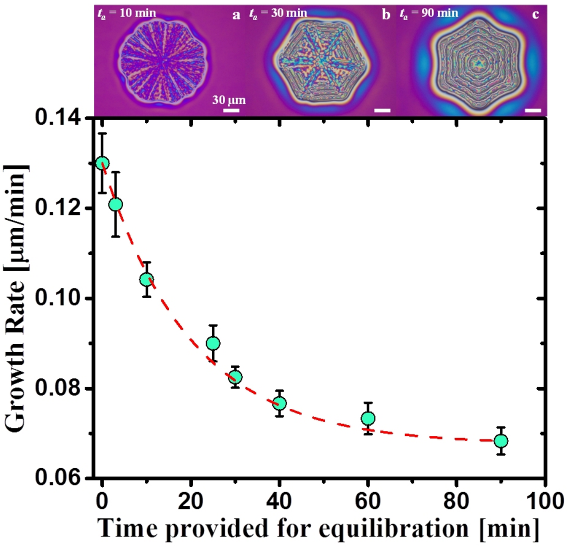

Figure 2.12: Growth rate of isotactic polystyrene crystals as a function of time (t_a) provided for equilibration in the molten state. Optical micropgraphs of the morphologies of crystals obtained after (a) t_a = 10 min, crystallization time (t_c) = 12 hr, (b) t_a = 30 min, t_c = 16 hr, and (c) t_a = 90 min, t_c = 20 hr. Isothermal crystallization was performed at 200 ^{o}C on sample which were annealed at 250 ^{o}C.

Polymers at interfaces and in thin films

Performance and properties of materials may strongly depend on processing conditions. This is particularly so for polymers, which often have relaxation times much longer than the processing times and therefore may adopt preparation dependent non-equilibrated molecular conformations that potentially cause novel properties. However, so far it was not possible to relate predictably and quantitatively processing steps and resulting properties of polymer films. We have demonstrated [reit10] that the behaviour of polymer films, probed through dewetting, can be tuned by controlling preparation pathways, defined through a dimensionless parameter $\wp$, which is the appropriate preparation time normalized with the characteristic relaxation time of the polymer. We revealed scaling relations between $\wp$ and the amount of preparation-induced residual stresses, the corresponding relaxation time, and the probability of film rupture.

Intriguingly, films of the same thickness exhibited hole nucleation densities and subsequent dewetting kinetics differing by up to an order of magnitude, indicating possibilities to adjust the desired properties of polymer films by preparing them in appropriate ways.

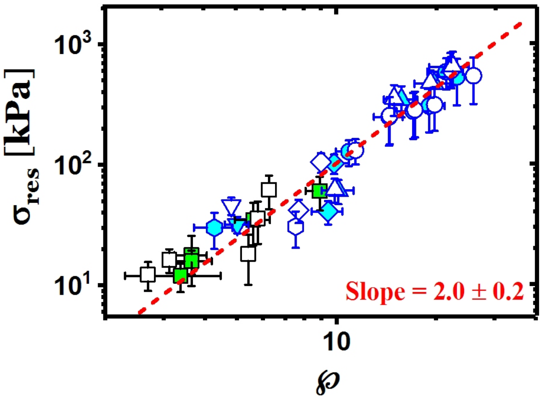

Figure 2.13: The characteristic preparation parameter $\wp$ influences the behaviour of polymer films: Double logarithmic representation of the residual stress σ_{res} as a function of $\wp$. The dashed line indicates the mean slope of 2.0 ± 0.2.

2.3.2 Theoretical Polymer Physics

In the last research period of the **Theoretical Polymer Physics Group of Alexander Blumen** at the University of Freiburg, we strengthened our international collaborations with scientific groups in Italy, Hungary, Russia, Brazil and France [blum1]–[blum10]. This was rendered possible by the outstanding involvement of Prof. Dr. Oliver Mülken and of Dr. Maxim Dolgushev [blum2]–[blum10]. In this way we continued our two main research directions, namely on the classical side investigating the dynamic properties of macromolecules, and on the quantum mechanical side studying in low far quantum transport is influenced by the topology of the underlying space.

As mentioned in our previous report, the problem of the cyclization of semiflexible polymers is particularly demanding, since the closing of branches to rings introduces restrictions which render the analytical treatment complex. On the other hand, the problem is of great experimental importance, since it determines the rate of intramolecular reactions between reactive groups attached to the same polymer. In the case of rings we have demonstrated that complex semiflexibility conditions (such as angular and dihedral restrictions) can be treated in the framework of a Gaussian formalism [blum3]. The cyclization problem of semiflexible chains can be handled using the general advanced first passage time methods developed by our French colleagues, as we have shown in a joint publication [blum5]. There we obtained explicit expressions for the cyclization time as a function of the capture radius, of the number of beads and of the positions of the reactive monomers in the chain. Our non-Markovian theory leads to results which agree with the numerical simulations, but which differ significantly from the classical Wilemski-Fixman forms. An extension of our approach for the case in which the flexible polymers experience hydrodynamic interactions in their embedding fluid was presented in [blum8].

In [blum7] we studied the kinetics of first contact between two monomers belonging to the same macromolecule. As underlying structures we considered three fractal families, namely on one hand Vicsek- and T-fractals, which are loop-less, and on the other dual-Sierpinski gaskets, i.e., fractals containing loops. We found a simple scaling relation for the mean first contact time between the monomers, which involves only their equilibrium distance and the spectral dimension of the macromolecule.

Further studies of classical dynamics from our group included encounters of particle pairs on branched structures [blum1], the behavior of semiflexible scale-free polymer networks [blum4] and the orientational mobility in macromolecules [blum6, blum10], a topic of much importance in NMR relaxation measurements.

On the side of quantum dynamics we made progress in the study of transport dynamics on Sierpinski fractals [blum2], where we analyzed the behavior of continuous-time quantum walks (CTQW) over Sierpinski gaskets and over Sierpinski carpets. While both fractal families show localization behavior, the gaskets show it to a much higher extent. Furthermore, distinct from the classical random walks, the spectral dimension does not fully determine the evolution of CTQW [blum2].

Furthermore, it turns out that sequentially grown complex quantum networks with loops show as limiting cases either a complete breakdown of transport for complete-graph substructures or optimal transport for ring-like substructures [blum9]. The key factors here are the special properties of the Hamiltonian of the network.

I like to remark, at the end of my employment at the University of Freiburg, that I view the fields of complex systems and of statistical physics to be as fascinating and lively as ever. I am thus extremely happy that Prof. Tanja Schilling was nominated to the chair I previously held, which is called now "Statistical Physics of Soft Matter and Complex Systems".

2.3.3 Statistical Physics of Soft Matter and Complex Systems

The **Statistical Physics of Soft Matter and Complex Systems Group of Tanja Schilling** has joined the Institute of Physics in April 2017. Therefore this report mainly covers activities that have been carried out at our previous institution, the university of Luxembourg.

The focus of our work is on theoretical physics and computer simulation of basic statistical mechanics models. We have long standing experience with Monte Carlo simulation as a means to predict equilibrium phase diagrams. Recently our interest has shifted to the modelling of non-equilibrium phenomena (in particular the dynamics of coarse-grained variables far from equilibrium). And we have added classical density functional theory to our portfolio of methods to predict equilibrium properties.

Coarse-graining out of equilibrium

In molecular dynamics simulations and single molecule experiments, observables are usually measured along dynamic trajectories and then averaged over an ensemble ("bundle") of trajectories. Under stationary conditions, the time-evolution of such averages is described by the generalized Langevin equation. In contrast, if the dynamics is not stationary, it is not a priori clear which form the equation of motion for an averaged observable has, and thus there are not yet any general coarse-graining procedures that could be used in multi-scale modeling approaches.

We have employed the formalism of time-dependent projection operators to derive the general equation of motion for a non-equilibrium trajectory-averaged observable as well as for its non-stationary auto-correlation function [schill8]. This piece of work lays the theoretical foundation to multi-scale modeling of non-equilibrium processes. We will apply it, in particular, to modelling of the crystallization process from an undercooled melt and of adsorption processes at surfaces.

Phase diagrams of soft matter systems

This branch of our work, in which we use Monte Carlo simulation to compute materials properties, is carried out in close collaboration with experimental physicists and chemical engineers who develop functional, soft materials. In the past three years, we had joint third party funding for several such collaborations: With Prof. J. Lagerwall (Luxembourg) we study the liquid crystalline properties of suspensions of cellulose nanocrystals. The aim of this project is to exploit cellulose as a sustainable material for optical applications [schill4, schill3]. With Prof. T. Kraus (Saarbrücken) we studied the agglomeration of binary colloidal mixtures in emulsions droplets. Here, the aim was to design functional nanoparticles with specific symmetries as building blocks in colloidal crystals and molecules [schill5, schill6] (for an example see fig, 2.14, which shows a micrograph from an experiment as well as a snapshot from a simulation, both of which had spontaneously produced the rather rare iscosahedral AB13 crystal phase). With Profs. Oettel and Schreiber (Tübingen) we study the formation of thin films of anisotropic particles with the aim to control the production of semiconducting organic films for transparent electrodes [schill7].

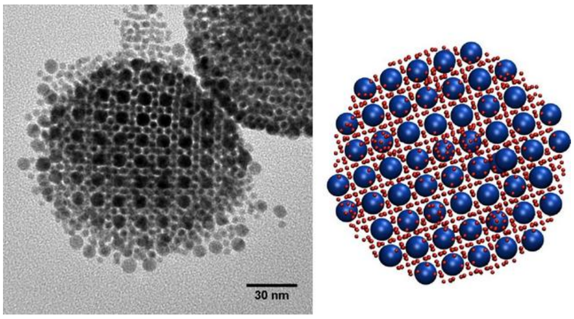

Figure 2.14: Experiment and simulation show the spontaneous formation of the rare icosahedral AB13 phase in a binary colloidal mixture [schill6]

Further, we worked with Prof. Sloutskin (Bar-Ilan University, Israel) on the dynamics of colloidal liquid crystals [schill2], and with Prof. Poulin (CRPP Bordeaux, France) on graphene as a filler in composites with very high dielectric constant [schill1]. This line of research, in which we feed theoretical results from basic statistical mechanics directly into applied materials research, will be continued in Freiburg. Currently, we prepare a joint DFG proposal with colleagues at the Institut für Werkstoffmechanik.

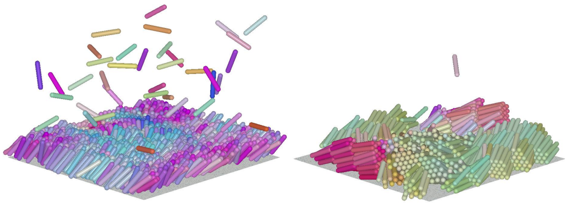

Figure 2.15: Simulation of the adsorption of rod-like molecules on a surface as a model for the growth of organic semiconducting films.

Density Functional Theory

Classical density functional theory (DFT) is a microscopic framework to describe classical many particle systems at non-zero temperature. In general, the framework is exact, but one needs to define an expression for the excess free energy that typically is an approximation. Very accurate functionals exist, in particular for hard spheres which represent an important model system for a whole class of colloidal systems of repulsive short-ranged interaction potentials.

Our recent work focused on charged hard spheres, i.e. the addition of electrostatics to the hard sphere functionals, in order to model the structure and packing effects in dense ionic systems [schill10]. Research on the fundamental mechanisms in these systems is important for the development and optimization of supercapacitors and related technologies for a sustainable treatment of water and energy. In a current collaboration with A. Lee (Cambridge), we use our theory to explain the structural properties of concentrated electrolytes. We will extend our theoretical framework to describe explicit dipolar solvents. This approach will allow us to study the capacitive effect of ionic solvation in electrolytes in contact with charged walls within a microscopical theory.

2.3.4 Functional Nanosystems

As a **member of the Physics Institute and the Fraunhofer IWM Michael Moseler** and his coworkers bridge the gap between fundamental and applied theoretical material physics. By modelling and understanding the basic mechanisms in materials and components the **Simulation and Modelling of Functional Nanosystem Group of Prof. Moseler** assists academic and industrial partners in research and development. The work of the group covers the classical molecular dynamics simulations of friction, lubrication, running-in and wear processes in carbon hard coatings [mos10, mos5, mos2], ceramics and metals [mos1, mos3]. Severe tribological loading of surfaces can trigger shear-induced non-equilibrium phase transformations [mos10, mos5, mos3] that are driven by mechano-chemical instead of thermo-chemical processes. The group develops multiscale models for the evolution of the resulting tribomaterials in complex tribosystems [mos6] as well as for friction and wear. Moseler and his coworkers also study the function of single components of tribosystems such as nanoparticles [mos5] under external loads. The classical molecular dynamics models are supplemented by tight-binding [mos10] and density functional calculations for tribochemical interactions of lubricants with tribological surfaces [mos4, mos9] as well as the mechanical, optical, magnetic and catalytic properties of nanoparticles and nanojunctions [mos8]. Further activities by the group are the ab-initio prediction of XPS spectra [mos7] to improve the accuracy of experimental materials characterisation (for nanoparticles and tribomaterials).

Friction regimes in water lubricated diamond (111): The role of interfacial ether groups and tribo-induced aromatic surface reconstructions

Exceptional mechanical properties, high chemical stability and thermal conductivity make diamond an ideal candidate for applications where a material has to withstand severe tribological conditions. Examples of such applications include the machining of rocks and non-ferrous materials, the mechanical polishing of diamond gems, and bearings that operate in highly abrasive environments. Facilitated by the advancement in growth and polishing techniques, the use of diamond films is spreading to disparate applications, like coatings for seals or microelectromechanical systems, where low friction is crucial. Despite the technological and scientific importance friction and wear mechanisms in diamond tribosystems are not completely understood.

Moseler and his colleagues performed large-scale quantum molecular dynamics of water-lubricated diamond (111) surfaces in sliding contact [mos10]. These simulations revealed multiple friction regimes (I-V in Fig. 2.16). While water starvation causes amorphization of the tribological interface (regime I), small traces of H_2O are sufficient to preserve crystallinity (regime II and III). This can result in high friction due to cold welding via ether groups (regime II) or in ultralow friction due to aromatic surface passivation triggered by tribo-induced Pandey reconstruction (regime III). At higher water coverage, Grotthuss-type diffusion and H_2O dissociation yield dense H/OH surface passivation leading to another ultralow friction regime (IV).

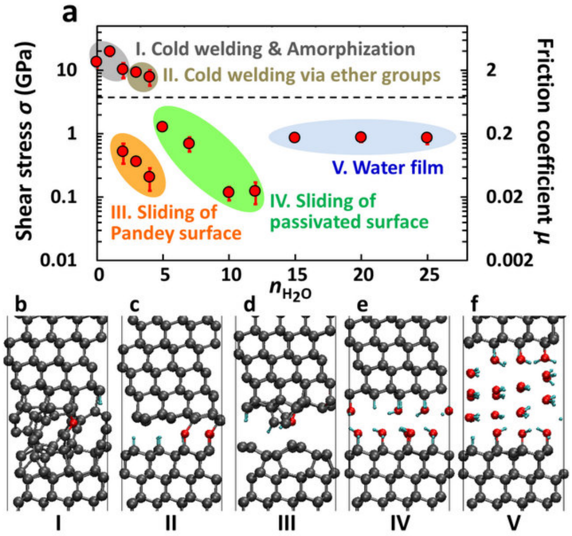

Figure 2.16: (a) Frictional shear stress σ and friction coefficient μ as a function of n_{H2O} for two initially non-reconstructed diamond (111) surfaces. Panels (b) to (f) show representative snapshots for Regime I-V at t = 0.1 ns (with n_{H2O} =1,3,2,10 and 25, respectively). Gray, red, and cyan spheres represent carbon, oxygen, and hydrogen atoms, respectively.

Fluorine-terminated diamond surfaces as dense dipole lattices: The electrostatic origin of polar hydrophobicity

Despite the pronounced polarity of C-F bonds, many fluorinated carbon compounds are hydrophobic - a controversial phenomenon known as ”polar hydrophobicity”. The group explored the underlying microscopic mechanisms by ab initio calculations of fluorinated and hydrogenated diamond (111) surfaces interacting with single water molecules [mos9]. Gradient- and van-der-Waals-corrected density functional theory simulations reveal that ”polar hydrophobicity” of the fully fluorinated surfaces is caused by a negligible surface/water electrostatic interac-

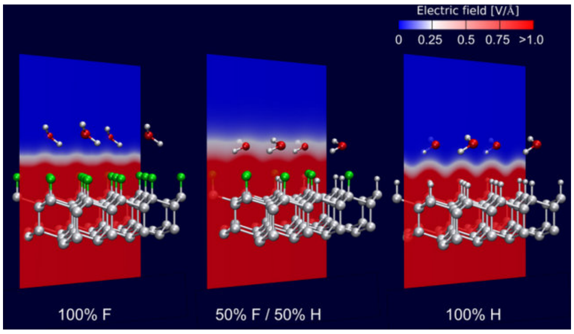

Figure 2.17: Near-surface electric field strength for the various investigated F/H-terminated C(111) diamond surfaces. Here we show the electric field strengths in two-dimensional cross-sections through the center of the O atom of the ad-sorbed H2O molecules, which are displayed in their optimized adsorption positions.

tion (Fig. 2.17). The densely packed C-F surface dipoles generate a short-range electric field that decays within the core repulsion zone of the surface and hence vanishes in regions accessible by adsorbates. As a result, water physisorption on fully F-terminated surfaces is weak (adsorption energies $E_{ad} < 0.1$ eV) and dominated by van-der-Waals interactions. Conversely, the near-surface electric field generated by loosely packed dipoles on mixed F/H-terminated surfaces has a considerably longer range, resulting in a stronger water physisorption ($E_{ad} > 0.2$ eV) that is dominated by electrostatic interactions. The suppression of electrostatic interactions also holds for perfluorinated molecular carbon compounds, thus explaining the prevalent hydrophobicity of fluorocarbons. In general, densely packed polar terminations do not always lead to short-range electric fields. For example, surfaces with substantial electron density spill-out give rise to electric fields with a much slower decay. However, electronic spill-out is limited in F/H-terminated carbon materials and therefore our ab initio results can be reproduced and rationalized by a simple classical point-charge model. Consequently, classical force fields can be used to study the wetting of F/H-terminated diamond revealing a pronounced correlation between adsorption energies of single H_2O molecules and contact angles of water droplets.

Coarse graining and localized plasticity between sliding nanocrystalline metals

Tribological shearing of polycrystalline metals typically leads to grain refinement at the sliding interface. Moseler and his group were able to show that nanocrystalline metals exhibit qualitatively different behavior. Using largescale atomistic simulations, they demonstrate that during sliding, contact interface nanocrystalline grains self-organize through extensive grain coarsening and lattice rotation until the optimal plastic slip orientation is established (Fig. 2.18). Subsequently, plastic deformation is frequently confined to localized nanoshear bands aligned with the shearing direction and emanating from voids and other defects in the vicinity of the sliding interface.

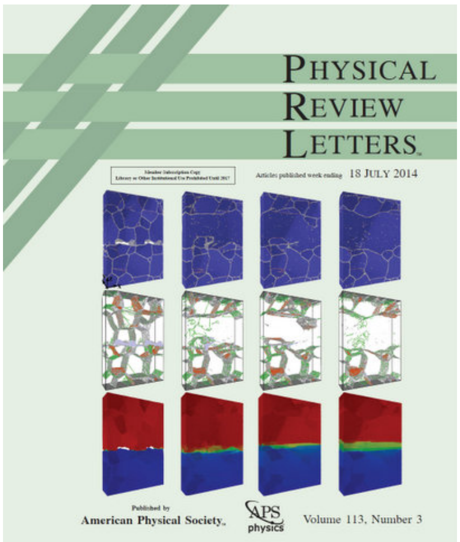
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Figure 2.18: Snapshots of the evolution of sliding contact between two nanocrystalline iron tribopartners. Each column presents the instantaneous state of the grain structure (top panel), the grain boundaries and dislocations (middle panel), and the corresponding sliding interface (bottom panel) at selected sliding times.

Spectroscopy and chemistry

The **Spectroscopy and Chemistry Subgroup of Michael Walter** is concerned with mostly chemistry related topics. Method development is central to the subgroup, which is reflected by the example of the simplified effective solvent model that was devised by us. The problem of the definition of the cavity that is formed by the solute inside of the solvent is solved by an effective potential for the solute molecules [walt2]. This approach gives a robust description of this debated quantity. It also gave a tool to directly obtain Hammett constants from density functional theory (DFT) calculations. These constants describe substituent properties in aromatic systems by assigning a single number. This approach furthermore allowed to investigate correlations between Hammett-constants on the example of spiropyran molecules [walt6, walt5].

The spiropyranes mechano-chromamtic, i.e. they change color on the response of external forces by

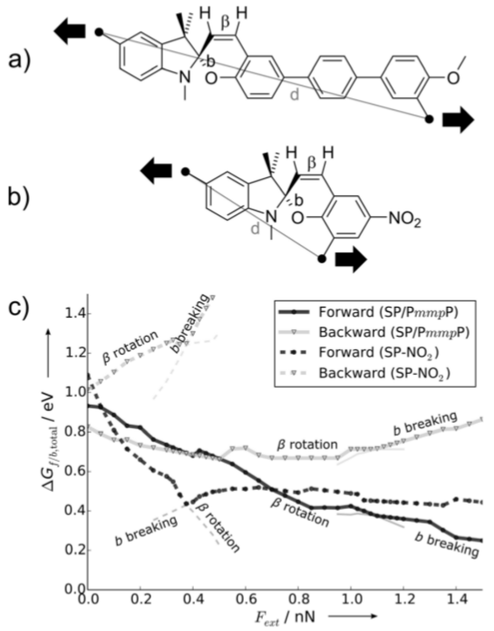

Figure 2.19: a+b)Structures of two spiropyran variants and c) the corresponding recation barriers depending on the external force F_{ext} [walt9]

cleavage of an internal bond. The reaction is thermally driven and the probability is dictated by the corresponding energy barriers that depend on the force applied [walt9] (see Fig. 2.19).

The development is based on an international cooperation in a state of the art DFT project that is able to reach the complete basis set limit. The latter was shown to be needed for a correct description of such simple systems like the chromium dimer, where we could show that removal of a single electron leads to a drastic change in the magnetic ground state [walt3].

We explained the properties of experimental observations in self organized cation-anion pairs on the gold 111 surface that adopt different shapes depending on the electro-chemical potential applied [walt1]. Switching the anion leads to dramatic changes in the molecular patterns due to steric effects or variations in the van der Waals interactions [walt8].

An important topic is the prediction of correct spectra, like photo-electrons from valence states to characterize triplet molecules [walt7], the correct prediction of absolute core state energies [mos7], or UV-Vis and vibrational spectra of iron-complexes [walt4].

2.3.5 Theoretical Materials Physics (Fraunhofer IWM)

The business unit **"Materials Design" at Fraunhofer IWM, headed by Christian Elsässer**, explains material behaviors and predicts material properties using computational and experimental methods based on solid-state physics and mechanics of materials. At the Institute of Physics, Christian Elsässer is Adjunct Professor for Physics, and he is Associated Member at the Freiburg Materials Research Centre (FMF) of the University of Freiburg. Our ambition is to design compositions and structures of materials for targeted properties and functions. We identify the effects of crystal defects and microstructures on the macroscopic behavior of materials. This enables the effective and efficient use of material and energy ressources in order to achieve long-term improvements to technical systems. Our theory group "Materials Modelling" investigates material behaviors and predicts material properties using theoretical and computational methods based on solid-state physics and materials science. Our task is to design material structures with targeted properties and functions. In the following the research work of our group are exemplified by some recent research topics. More information is provided on our webpages: `http://www.iwm.fraunhofer.de/en/services/materials-design.html`.

Searching for novel materials - reducing the dependence on critical raw materials

There is great demand in industry for designing novel materials, driven by strict technical challenges, economic concerns, or legal constraints. As a result, new materials must both have tailored physical properties and be compatible with established manufacture processes. Furthermore, they should be made of inexpensive raw materials and contain few - ideally zero - critical elements. Dependencies on fluctuating material prices and market monopolies should also be avoided. The design of novel materials in principle faces the need for expensive and tedious experimental synthesis series. At this point, a computational high-throughput screening approach is employed to speed up the development of novel materials. Advanced simulation methods and growing computer capacities enable a large number of structures and compositions to be virtually screened and predictions of their properties to be made. A wide variety of options can be tested systematically in an efficient manner. The basis for this is given by extensive theoretical material-property data. Data analysis tools exploit information in this database in order to adjust and extend the search directions. Materials with promising properties can subsequently be investigated in more depth and eventually synthesized experimentally. Our computational high-throughput techniques are suited to a large range of material classes. We employ screening methods for example to the search for permanent-magnet materials that contain less or no amounts of rare-earth elements [elsae1, elsae2].

NZP materials as solid-state electrolytes for lithium ion batteries

Ion-conducting solid-state electrolyte materials can significantly improve the operational safety of lithium ion batteries. Due to a three-dimensional channel network in the crystal structure, compounds derived from NaZr2(PO4)3 (NZP) are fast ionic conductors. Density functional theory and atomistic simulations are used to investigate Li-ion diffusion in relation to the NZP composition and Li stoichiometry in order to predict new NZP-type electrolytes for all-solid-state batteries (see Fig. 2.20) [elsae3, elsae4, elsae5].

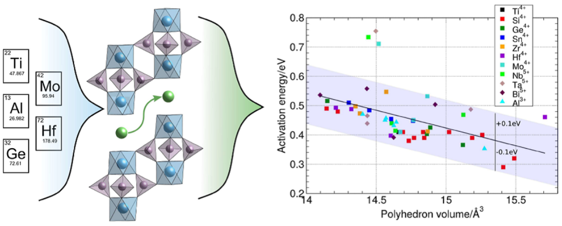

Figure 2.20: Schematic sketch of computational high-throughput screening procedure for metal-oxide compounds with NZP-type crystal structures and fast Li-ion conductance as inorganic electrolytes in all-solid-state Li-ion batteries (from ref. [elsae4]).

Optically transparent and electrically conducting oxides (TCOs)

Touchscreens are a common feature of smartphones, tablets or ticket machines. An important component in these screens is an oxide layer that is both optically transparent and electrically conducting. Such TCOs (transparent conducting oxides) are also used as solar-cell top contacts. We provide theoretical support to the development and optimization of TCOs by first-principles electronic-structure simulations at the atomic scale. This enables us to assess and predict the effect of (poly-) crystalline or amorphous structures and the effect of doping [elsae6, elsae7].

Precipitation of nitrides and penetration of hydrogen in metals

The efficiency of fossil-fuel power plants can be increased by the use of new heat and corrosion resistant steels that are able to withstand higher steam temperatures and pressures. Steels with a high chromium content can be made more resistant to fracture and creep by a microstructural design of Z-phase nitride precipitates. We investigate the formation of such nitrides in steels using a multi-scale approach that combines atomistic simulations with thermodynamic and kinetic modeling. This extends the understanding of reinforcing mechanisms and enables the prediction of material stability and failure [elsae8].

Hydrogen penetration into metals causes their mechanical stability to degrade – a phenomenon known as hydrogen embrittlement. This affects almost all metals and is therefore a cause of significant technical and economic damage. We investigate the adsorption and migration of hydrogen atoms in iron and nickel using quantum mechanics and atomistic computer simulations. The susceptibility of the metals to hydrogen embrittlement can be assessed from the thermodynamic, kinetic and mechanical properties determined in this manner [elsae9, elsae10].

2.3.6 Spectroscopy of Optical Materials (Fraunhofer IPM)

Central topic of the activities of the **research group headed by Frank Kühnemann** is the utilisation of nonlinear-optical frequency conversion for the development of (tunable) light sources and for infrared detection and spectroscopy. The properties of nonlinear optical crystals are a key parameter for the design of such frequency converters. As a result, the analysis of residual absorptions in optical materials is a second relevant field of activities in our group.

Infrared Detection via nonlinear optical frequency upconversion

The Mid-infrared wavelength region (MWIR; here, in particular, the 3–5 μm region) is of high importance for many analytical applications. Key factor for any implementation is the availability of suitable light sources and detectors. This holds especially for fast single-pixel detectors and for sensor arrays for imaging applications, which currently do require kryogenically cooled (< 70 K) InSb or HgCdTe detectors.

An alternative approach is the nonlinear optical frequency upconversion of mid-infrared radiation with the subsequent detection using standard silicon or GasAs-based detectors. Upconversion of 3–5 μm radiation with a 1064-nm laser yields sum frequency photons in the 780 to 880 nm range. Combining a sum frequency converter with a grating spectrometer with a detector array resulted in a system for the recording of 6500 spectra per second in the 3.7 to 4.7 μm range with 1.1 cm^{-1} resolution [kue7]. Measurements with blackbody sources between 100 and 1000 $^{\circ}$C allowed for an absolute intensity calibration and showed linearity over four orders of magnitude.

The high frame-rate of the spectrometer was used to monitor the evolution of gases during the ignition of an airbag gas generator through the recording of the infrared emission spectra of the gases with sub-millisecond time resolution (Fig. 2.21).

Mid-infrared detectors have temporal bandwidths well below 1 GHz, limiting the laser spectroscopic observation of fast processes and the application observation of heterodyning techniques. Upconversion from the mid-infrared to wavelengths below 1 μm allows one to use the much faster detectors based on Si or GaAs. Our setup combines the generation of MWIR pulses with 250 ps duration via seeded optical parametric generation with the subsequent upconversion detection of the MWIR pulses. The short pulse duration of the pump laser for down- and up conversion combined with the narrow spectral bandwidth of the upconversion process lead to an efficient suppression of thermal background signals. As a result the signal-to noise ratio exceeds the one achievable with mid-IR-only detection schemes [kue6].

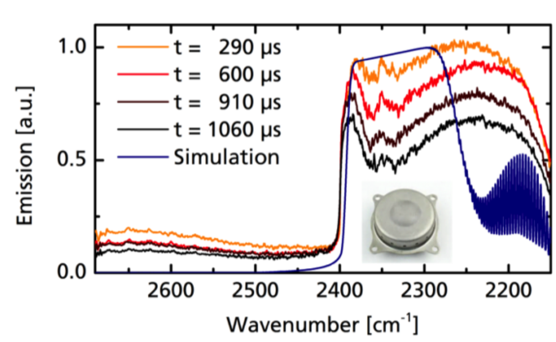

Figure 2.21: Time series of infrared emission spectra after the ignition of an airbag gas generator. Between 2400 and 2300 cm^{-1}, the absorption by cold(er) CO_2 is superimposed on the emission spectrum. Blue curve: To aid the orientation, the simulated emission spectrum of a gas at 700 K is added, containing 20% CO_2 and 10% CO at a total pressure of 10 bar. (from [kue7])

Absorption spectroscopy of transparent optical materials

High powers need high purities: The current development of high-power lasers results in a growing importance of the quality assessment of optical materials for high-power applications like material processing or nonlinear-optical frequency conversion. Material imperfections or impurities may lead to residual absorption. Under high laser intensities even absorption coefficients of 1000 ppm/cm or below may lead to local heating, resulting in component malfunction or even damage.

The primary method used at Fraunhofer IPM is Photothermal commonpath Interferometry(PCI) based on a pump-probe-technique: A strong continuous-wave (cw) pump beam is focusedinto the sample and heats it locally due to light absorption. The resulting local change of the refractive index in the sample causes refraction and diffraction effects on the crossing probe beam. This distortion is proportional to the absorption of the sample and can be measured by a lock-in technique. The detection limit depends on the laser power and can reach 1 ppm/cm in the bulk and below 1 ppm for surface coatings.

Combining the sensitive detection technique with tunable pump sources allows one to record absorption spectra rather than looking at the behavior at single isolated wavelengths, drastically enhancing the analytical capabilities. Building on our experience in nonlinear-optical frequency conversion, we use in-house developed optical parametric oscillators (OPO) as pump sources in the visible, near and middle infrared wavelength regions [kue3].

An important part of the establishment of new analytical methods is the understanding of the underlying effects, possible contributions to systematic errors and detection limits.

Due to the crossed-beam geometry of PCI, heating the sample by partial absorption of the pump laser induces anisotropies for the probe laser even in initially isotropic materials. Through combined experiments and simulations we could show the contribution of thermally induced strains and the elastooptic effect in glasses (BK7) and in uniaxial crystals (LiNbO3) [kue1].

The temperature dependence of the refractive index (thermo-optic coefficient) is the primary effect responsible for the formation of the thermal lens which is used in PCI. Reliable data for the thermooptic coefficients are important for the prediction of phase-matching conditions in nonlinear-optical frequency conversion as for OPOs. Using our OPO tunable in the visible and near infrared, we could perform measurements on LiNbO3 samples across a wide wavelength range and improve, in collaboration with colleagues from Cologne University the data base for LiNbO3. [kue4].

2.3.7 Applied Solid State Physics (Fraunhofer IAF)

Joachim Wagner is head of the Optoelectronics research unit at the Fraunhofer Institute for Applied Solid State Physics (Fraunhofer-Institut für Angewandte Festkörperphysik IAF). The IAF is one of the leading research institutions worldwide in the field of III-V compound semiconductors and diamond technology. We develop electronic and optoelectronic devices and integrated circuits as well as modules based on III-V semiconductors.
The key research topics are:

- Ultra-high frequency circuits for radar, communication and satellites
- Power electronics for mobile communications, radar and energy conversion
- Photodetectors for the infrared und ultraviolet spectral range
- Infrared semiconductor laser for sensor systems and medical applications
- Diamond technology for electronics and quantum sensing

The core competences of Fraunhofer IAF are simulation-aided design of electronic and optoelectronic devices and integrated microelectronic circuits, epitaxial growth of III/V-semiconductors and diamond, as well as front- and backside processing for single devices and integrated circuits including mounting and packaging. Further competences are in materials analysis, testing and characterization of devices and circuits up to 1.1 THz in the micro- and millimeter-wave domain as well as optical characterization from UV to the long-wave infrared.

Figure 2.22: Rapid-scanning quantum cascade laser in external cavity configuration employing a resonantly driven MEMS grating for wavelength-selective optical feedback.

Recent research highlights include the

- demonstration of a millimeter-wave (94 GHz) multiple-input-multiple-output (MIMO) staring array radar system,
- development of a compact rapid scanning mid-infrared (MIR) semiconductor laser (Fig. 2.22), based on a combination of quantum cascade laser (QCL) and optical MEMS technologies, enabling real-time MIR fingerprint spectroscopy,
- realization of a quantum sensor for magnetic fields based on a single nitrogen-vacancy (NV) defect center (Fig. 2.23) in epitaxially grown high purity single-crystalline diamond.

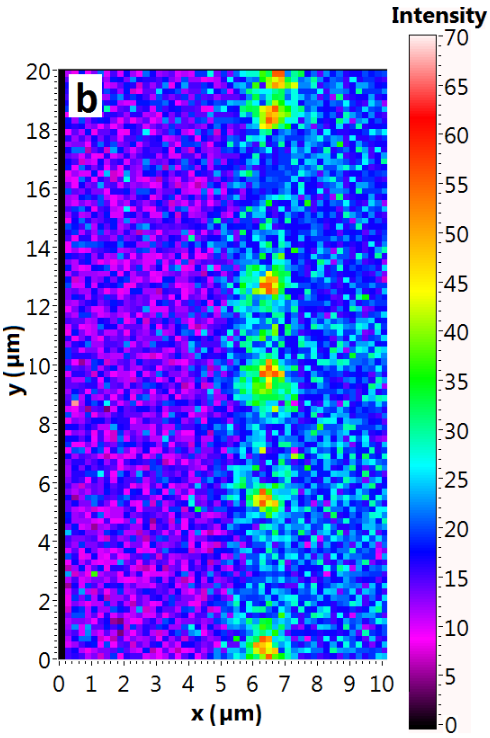

Figure 2.23: False-color 2D photoluminescence intensity map showing emission from isolated single NV defect centers in high-purity epitaxial diamond.

2.4 Biological Systems

2.4.1 Dynamics in the Life Sciences

The aim of the **Dynamic Processes in the Life Sciences Group of Jens Timmer** is to transfer the quantitative and predictive approach of physics to the life sciences. Especially, we aim to understand biological systems by mathematical modelling for cases where this is not possible by experimental techniques.

After Timmer's time at the Freiburg Institute for Advanced Studies (FRIAS) ended in October 2013, he had to take over his teaching duties again. As a consequence, the group was reduced from 40 members to 20 and is now mainly focusing on modelling of cellular signal transduction, i.e. the information processing of external stimuli by cells finally leading to altered gene expression and to cell fate decisions. To this aim, we develop mathematical methods for parameter estimation and uncertainty quantification in differential equations and apply them in close collaboration with experimental groups in biology and medicine.

Development of mathematical methods to model cell biological processes

A lot is known about the proteins involved in cellular signalling and their interaction, usually presented in ”pathway cartoons” which are qualitative, descriptive and static. To obtain quantitative, predictive insights into the dynamics of the pathways, the cartoons are translated into differential equations. These equations contain unknown parameters. Typically, not all proteins and their post-translational modifications can be measured. Moreover, different parts of the system often exhibit dynamics on quite different time scales. While the dynamics can be assumed to be deterministic, the measurements are noisy with a typical relative error of 10-20 %. Thus, we deal with modeling and parameter estimation in nonlinear, partially observed, stiff, sparse, noisy dynamical systems.

It has been observed that these kind of models are ”sloppy” meaning that the ratio of the largest to the smallest eigenvalue of the covariance matrix of the estimated parameters is very large, i.e. $> 10^6$. It has been argued that this renders parameter estimation in these models impossible. We were able to explain the reason for sloppiness by random matrix theory and provide a cure [timm1]. The fact that the model is only partially observable leads to structural non-identifiabilities, i.e. even for noise-free data, not all parameters can be estimated because a change in one parameter can be completely compensated by a change in other parameters. Analytical methods to identify this gauge symmetry were limited to very small systems. We developed a method based on Lie-group theory that can also deal with large systems [timm4]. Initial values of the dynamical systems are typically a part of the parameters to be estimated. This induces a consistency problem. If the system is in steady state before a stimulus, the dynamic parameters and the initial values are not independent, the former determine the latter. We were able to solve this problem in an efficient manner [timm5]. In applications, one is often interested to determine the differences between two cell types in terms of parameter values in their models, e.g. healthy and diseased, in order to infer efficient and cell-type specific intervention points for treatment. We developed a method based on L_1 regularisation to determine the minimal set of cell-specific parameters [timm6], see Fig. 2.24.

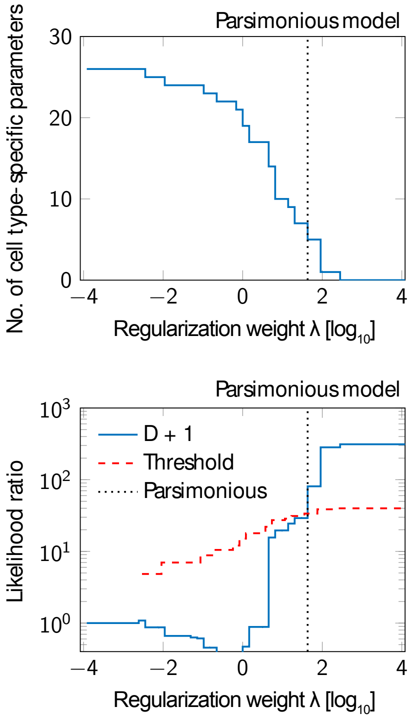

Figure 2.24: L_1 regularisation process to determine the minimum difference of two cell types. The regularisation strength λ is increased until a statistical threshold is reached.

If the parameters of a model can not be well determined by the given data but it is not possible to obtain measurements of additional players of the system, the model complexity has to be reduced. We developed a method for this task based on the profile likelihood [timm8], see Fig. 2.25.

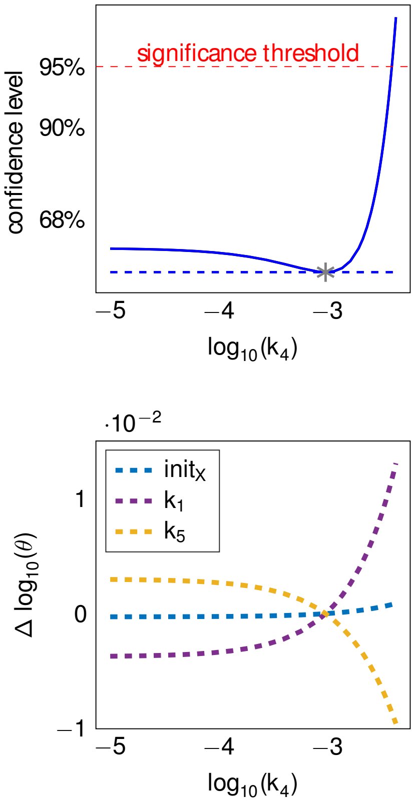

Figure 2.25: The profile likelihood of a certain parameter and the behavior of the other parameter is investigated for model reduction.

Applications

On the application side, we were able to disentangle the cross-talk between two signalling pathways stimulated by the Hepatocyte Growth Factor in collaboration with our main collaboration partner, Prof. U. Klingmüller from the German Cancer Research Institute in Heidelberg [timm3]. Also in collaboration with her we applied the L_1 regularisation approach to figure out the differences between healthy and cancer cells. Interestingly, due to the non-linearity of the systems, the most efficient points of interventions were not identical to the points in the networks that were identified as different [timm7]. For the differences between cell types described by differential equations

$$\dot{x} = f(x, p), \quad x(0) = x_0$$

there exists a hierarchy. In the simplest situation, the structure of $f(.)$ and kinetic parameters p are the same and only the initial values, i.e. the protein concentrations differ. One step further, also kinetic parameters might differ. In the most complex situation the structure $f(.,)$ differs for the cell types. Interestingly, also the latter two alternatives can be related back to biology because they also correspond to protein levels. For three cell types related to the blood building system we were able to show that differences in their cellular information can be captured by the first alternative [timm9].

In the frame of the German Excellence University Initiative, the group is member of the Cluster of Excellence Biological Signalling Studies (BIOSS). Here, we collaborated with Prof. P. Beyer from our Faculty for Biology. He had determined the crystal structure of a certain enzyme suggesting two possible modes of action. By experimental techniques it was not possible to decide with one takes place. We were able to answer this question based on a model of the dynamics of the process [timm10].

In a further BIOSS collaboration with Prof. W. Weber, Faculty for Biology, we used our modelling approach to optimise multiple optogenetic switches. We were able to design an orthogonal switch for three different wave lengths [timm2].

2.4.2 Bio- and Nano-Photonics (IMTEK)

The **Bio- and Nano-Photonics Group of Alexander Rohrbach** investigates novel techniques for optical microscopy and optical force based applications, which are used to investigate the physical properties of biological systems based on their nano-mechanics and thermal fluctuations.

Advanced optical measurement and manipulation technology developed in our lab enable experiments on the length scale down to a few nanometers and the timescale of a few microseconds. All experiments are supported and compared by mathematical modelling and computer simulations also developed in the group. The systems investigated can be separated into three classes: i) mesoscopic systems that do not contain biological matter, ii) bio-mimetic systems that contain biological materials and iii) biological systems such as cells and cell clusters.

Colloidal systems

The first class of systems subserves to identify and characterize physical forces that govern biological interactions. For example long range physical interactions control many short-ranged specific reactions between diffusing particles in biology, chemistry or soft matter physics. Indirect interactions such as hydrodynamic, electrostatic or plasmonic coupling between two particles, can reach unexpected interaction lengths and often control time-variant effects such as reactions kinetics or synchronization in biological processes. We have used line scanning optical and point-optical tweezers to trap two or more diffusing particles in a confined optical potential [rohrb6, rohrb4] to increase their collision rate. Using coherent light scattering of the trapping laser [rohrb9, rohrb6, rohrb4, rohrb3] we were able to track several particles in 3D with nanometer precision at 10 kHz-2 MHz. These results confirmed the hypothesis that inside living cells a dynamic change of the size of membrane compartments controls the collision rate between particles and thereby reaction efficiencies.

Bio-mimetic systems

The second class serves to identify and characterize physical processes based on statistical mechanics that are expected to play a decisive role in complex systems such as cells. In the last couple of years we have started to work on artificial bio-polymer networks, with colloidal anchor points held by an array of optical traps [rohrb9]. In this way momentum propagation on a broad temporal scale can be investigated depending on the meshwork symmetry. In addition we have worked on giant unilamellar vesicles (GUVs)

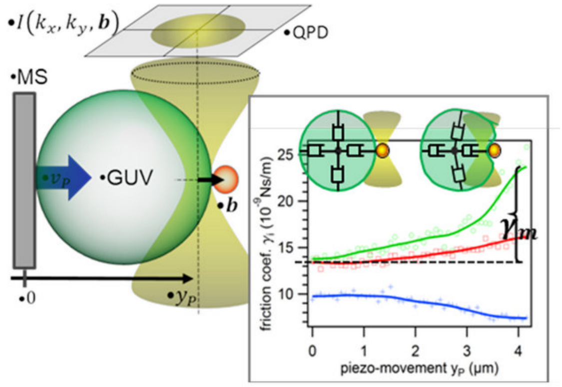

Figure 2.26: Optical force induced particle uptake into the artificial cell. Giant unilamellar vesicles (GUVs) are used to study statistical physics concepts relevant for phagocytosis, both in and out of equilibrium.

to study phagocytosis (see Fig. 2.26), where particle uptake into the artificial cell (GUV) is induced and measured with optical traps [rohrb1].

Cellular systems

The third class addresses simple cells such as bacteria or partial cellular systems such as cell protrusions. We developed a super-resolution total internal reflection fluorescence microscope based on structured illumination (TIRF-SIM) with 100nm spatial resolution, which was used to investigate the molecular motor driven dynamics of the cytoskeleton protein MReB inside rod-shaped bacteria (B. Subtilis) (see Fig. 2.27). Furthermore we investigated ultra-small, deformable, helical bacteria (S. Melliferum) which were oriented in object adapted optical traps. Fast shape changes of the bacterium based on protein chain switching inside the cell body were tracked with nanometer precision using scattered light, allowing to reveal smallest motions close to the thermal noise limit in 3D and at a KiloHertz. In another long-term project, we investigate the nano-mechanics at the periphery of macrophages, which use complex mechanism based on cytoskeleton reorganization and collaborative work of molecular motors [rohrb2]to uptake particles or bacteria either by thin cell protrusions or flat membranes. Using feedback controlled optical traps and 3D interferometric tracking in the MegaHertz range help to reveal the physical laws that influence phagocytosis [rohrb5]. The response of the cellular system can be read out on a broad temporal bandwidth (0.1 Hz to 100 Hz) with label free super-resolution microscopy based on rotating coherent scattering (ROCS) of blue laser light. Superior image contrast in resolution can be achieved even inside living cells by local destructive interferences of spherical waves emitted from adjacent scatterers in distances of only 140nm(see Fig. 2.28). In this way, unexpected dynamics of the living cells in the range of milliseconds could be detected and analyzed [rohrb8]. A system of much further complexity are clusters of thousands of cells, where cellular components are fluorescently labeled and scanned by holographically shaped, self-reconstructing illumination beams forming a light-sheet. In this way large 3-D image stacks can be recorded in a minimal time and at an optimal photon budget defined by the ratio of excitation light and fluorescence light [rohrb10, rohrb7].

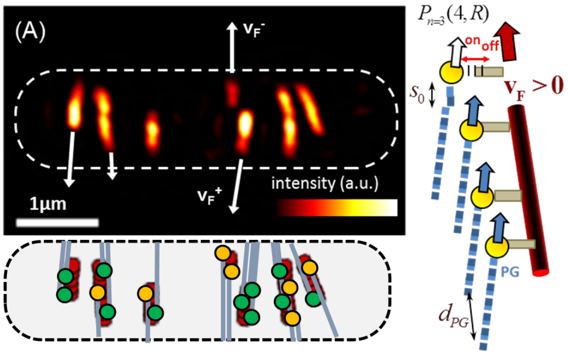

Figure 2.27: Coupled dynamics of the MreB-cytoskeleton in rod-shaped bacteria. MreB filaments - fluorescent in the superresolution image and as red filaments in the sketches - transported with complex dynamics inside the bacterium, thereby controlling the growth of cell wall strands (PG, gray-blue).

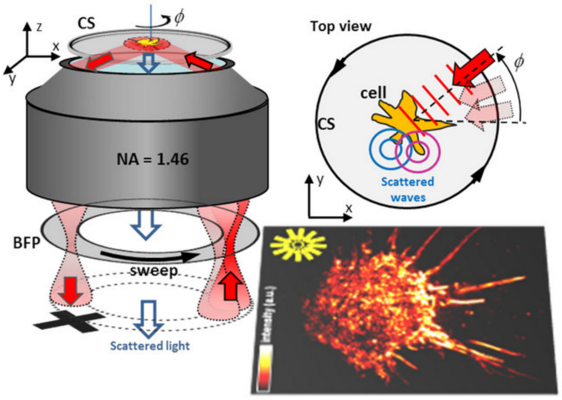

Figure 2.28: Rotating coherent scattering (ROCS) of blue laser light enables label-free super-resolution (at 140nm) of living cells at 100 Hz.

2.4.3 Computational Neuroscience (Faculty of Biology)

The **Computational Neuroscience Laboratory of Stefan Rotter** at the Bernstein Center Freiburg comprises a team of theoreticians from mathematics, physics, biology and various engineering sciences. We are interested in the relations between structure, dynamics and function of the neuronal networks of the brain, with a specific focus on the mammalian neocortex. Our work involves modeling and data analysis of (i) multi-scale neuronal network topology, (ii) spiking activity dynamics of recurrent networks, and (iii) biological function and dysfunction of neuronal networks. Mathematical (deterministic and stochastic) as well as computational methods (large-scale numerical simulations) are employed (see Fig. 2.29 for an example). The goal is to develop a theory of the brain which also supports a better understanding of the neuronal mechanisms underlying some brain diseases.

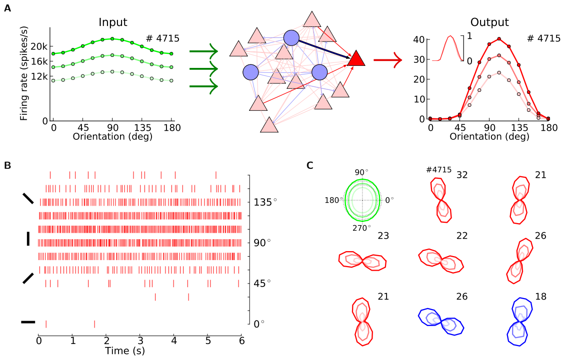

Figure 2.29: Emergence of contrast-invariant tuning curves of neurons in the primary visual cortex of mammals. Inhibition-dominated random networks dynamically process oriented visual stimuli in a meaningful way. They attenuate the homogeneous mode and amplify the tuned component of the input (Sadeh & Rotter, 2014 [rott1]).

Current research topics

- Computational neuroscience & brain theory
- Relations between structure, dynamics & function in neuronal networks
- Spiking activity dynamics & ensemble coding in recurrent networks
- Experience-dependent functional and structural plasticity in cortical networks
- Inference of network structure from multi-channel measurements

Techniques employed for research

- Stochastic modeling of neuronal activity (e.g. stochastic point processes)
- Stochastic modeling of neuronal networks (e.g. generalized random graphs)
- Advanced statistical data analysis (e.g. higher-order correlations)
- Large-scale numerical simulations

2.4.4 Medical Physics (University Hospital)

In biomedical imaging, the development of novel technologies together with the usage of new post-processing methods has enabled both anatomical as well as functional assessment of organ structure and disease detection. Medical physics is at the very heart of this research field with physicists developing new image acquisition methods, novel imaging hardware together with fast and efficient reconstruction and analysis programs. The **Medical Physics Groups of J. Hennig** (Department of Radiology) and **M. Bock** are developing new methods and technologies for magnetic resonance imaging (MRI) to apply them in basic science as well as preclinical and clinical studies. The research extends over all fields of MRI starting with MRI hardware (radio-frequency coils, gradients) to new image acquisition strategies (pulse sequences) and data processing both for image reconstruction (e.g., compressed sensing) and for clinical analysis (e.g., multimodal segmentation in tumor studies).The aim of these developments is to improve morphological, functional, metabolic, and physiologic assessment of biological and medical imaging on all spatial scales; therefore, activities range from cellular imaging (microMR) on cell ensembles and tissue preparations via small animal imaging for pre-clinical research to whole body MRI in volunteers and patients (Fig. 2.31). Key areas of applications are

- Neurology and Neuroscience
- Cancer
- Cardiovascular Imaging
- Metabolic Disease

Research highlights of the department include the development of an ultrafast technique for whole brain functional imaging (fMRI) at 10 fps, a method for continuous hyperpolarization, which increases the MR signal of specific marker molecules by a factor of several thousands, and metabolic imaging of the brain using the tracer ^{17}O.

Figure 2.30: Homebuilt matrix gradient coil for spatial encoding with 84 channels. Drawing(l), during construction (m), final coil (r).

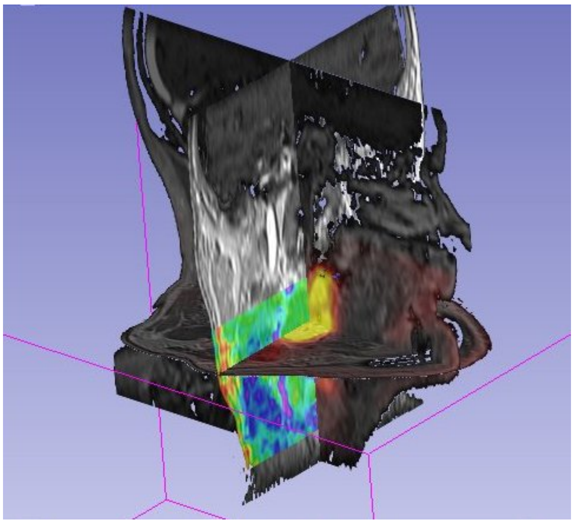

Figure 2.31: Image fusion of several imaging modalities (MRI, PET, CT) in a patient with a head and neck tumour to improve radiation therapy. Hypoxic areas of the tumour require higher radiation doses and are more prone to tumour recurrence – with a combination of F-MISO-PET and BOLD and diffusion MRI, these regions can be identified prior to therapy.

Figure 2.32: White matter fiber architecture of the human brain calculated from diffusion tensor imaging measurements in a normal subject.

2.5 Important Publications and Conference Talks

Group Blumen

Publications

[blum1] E. Agliari, A. Blumen, D. Cassi, Slow Encounters of Particle Pairs in Branched Structures, Phys. Rev. E 89 (2014) 052147.

[blum2] Z. Darázs, A. Anishchenko, T. Kiss, A. Blumen, O. Mülken, Transport Properties of Continuous-Time Quantum Walks on Sierpinski Fractals, Phys. Rev. E 90 (2014) 032113.

[blum3] M. Dolgushev, T. Guérin, A. Blumen, O. Bénichou, R. Voituriez, Gaussian Semiflexible Rings under Angular and Dihedral Restrictions, J. Chem. Phys. 141 (2014) 014901.

[blum4] M. Galiceanu, A. Reis, M. Dolgushev, Dynamics of Semiflexible Scale-Free Polymer Networks, J. Chem. Phys. 141 (2014) 144902.

[blum5] T. Guérin, M. Dolgushev, O. Bénichou, R. Voituriez, A. Blumen, Cyclization Kinetics of Gaussian Semiflexible Polymer Chains, Phys. Rev. E 90 (2014) 052601.

[blum6] D. Markelov, M. Dolgushev, YY. Gotlib, A. Blumen, NMR Relaxation of the Orientation of Single Segments in Semiflexible Dendrimers, J. Chem. Phys. 140 (2014) 244904.

[blum7] M. Dolgushev, T. Guérin, A. Blumen, O. Bénichou, R. Voituriez, Contact Kinetics in Fractal Macromolecules, Phys. Rev. Lett. 115 (2015) 208301.

[blum8] N. Levernier, M. Dolgushev, O. Bénichou, A. Blumen, T. Guérin, R. Voituriez, Non-Markovian Closure Kinetics in Flexible Polymers with Hydrodynamic Interactions, J. Chem. Phys. 143 (2015) 204108.

[blum9] N. Kulvelis, M. Dolgushev, O. Mülken, Universality at Breakdown of Quantum Transport on Complex Networks, Phys. Rev. Lett. 115 (2015) 120602

[blum10] M. Dolgushev, D. Markelov, F. Fürstenberg, T. Guérin, Local Orientational Mobility in Regular Hyperbranched Polymers, Phys. Rev. E 94 (2016) 012502

Conference Talks

1. A. Blumen, Exploring the Applications of Fractional Calculus: Hierarchically-Built-Polymers, in the ”International Conference on Statistical Physics”, July 7-11, 2014, Rhodes, Greece
2. M. Dolgushev, Branched and Loop-like Semiflexible Polymers, in the “International Conference on Molecules, Polymers and Material Physics” August 26-29, 2014, Manaus, Brazil
3. A. Blumen, From Continuous-Time Random Walks to Continuous-Time Quantum Walks, in “International Conference on Molecules, Polymers and Material Physics” August 26-29, 2014, Manaus, Brazil
4. A. Blumen, Dynamics in Complex Systems: Geometric and Topological Aspects, in the “2nd Dynamics Days, Central Asia” May 25-27, 2015, Khiva, Uzbekistan
5. A. Blumen, Dynamics in Complex Systems: Geometric and Topological Aspects in the “ 28th Marian Smoluchowki Symposium on Statistical Physics, September 14-17, 2015, Kraków, Poland
6. A. Blumen, Exploring the Applications of Fractional Calculus: Anomalous Diffusion of Hierarchically-Built-Polymers, in “XXXVI Dynamics Days”, June 6-10, 2016, Corfu, Greece

Group Elsässer

Publications

[elsae1] W. Körner, G. Krugel, and C. Elsässer, ”Theoretical screening of intermetallic ThMn12-type phases for new hard-magnetic compounds with low rare earth content”, Sci. Rep. 6, 24686, (2016).

[elsae2] T. A. Butcher, W. Körner, G. Krugel, and C. Elsässer, ”Dependence of magnetization and magnetocrystalline anisotropy on site distribution of alloying elements in RE-TM phases with ThMn12 structure”, J. Magn. Magn. Mater. 441, 1-5 (2017).

[elsae3] B. Ziebarth, M. Klinsmann, T. Eckl, and C. Elsässer, ”Lithium diffusion in the spinel phase Li4Ti5O12 and in the rocksalt phase Li7Ti5O12 of lithium titanate from first principles”, Phys. Rev. B 89 174301 (2014).

[elsae4] B. Lang, B. Ziebarth, and C. Elsässer, ”Lithium ion conduction in LiTi2(PO4)3 and related compounds based on the NASICON structure: a first-principles study”, Chem. Mater. 27, 5040-5048 (2015).

[elsae5] D. Mutter, D. Urban, and C. Elsässer, ”Systematic search for Lithium ion conducting compounds by screening of compositions combined with atomistic simulation”, MRS Advances 2, 483 (2017).

[elsae6] D. F. Urban, W. Körner, and C. Elsässer, ”Mechanisms for p-type behavior of ZnO, Zn1-xMgxO, and related oxide semiconductors”, Phys. Rev. B 94, 075140 (2016).

[elsae7] E. Rucavado, Q. Jeangros, D. F. Urban, J. Holovsky, Z. Remes, M. Duchamp, F. Landucci, R. Dunin-Borkowski, W. Körner, C. Elsässer, A. Hessler-Wyser, M. Morales-Masis, and C. Ballif, ”Enhancing the optoelectronic properties of amorphous zinc tin oxide by subgap defect passivation: a theoretical and experimental demonstration”, Phys. Rev. B 95, 245204 (2017).

[elsae8] D. F. Urban and C. Elsässer, ”Atomic defects and dopants in ternary Z-phase transition-metal nitrides CrMN with M=V, Nb, Ta investigated with density functional theory”, Phys. Rev. B 96, 104107 (2017).

[elsae9] D. Di Stefano, M. Mrovec, and C. Elsässer, ”First-principles investigation of quantum-mechanical effects on the diffusion of hydrogen in iron and nickel”, Phys. Rev. B 92, 224301 (2015).

[elsae10] D. Di Stefano, R. Nazarov, T. Hickel, J. Neugebauer, M. Mrovec, and C. Elsässer, ”First-principles investigation of hydrogen interaction with TiC precipitates in α-Fe”, Phys. Rev. B 93, 184108 (2016).

Conference Talks

1. C. Elsässer, Microscopic modelling of domains, defects, and dopants in perovskite ceramics, Seminar lecture, MPI for Solid State Research, Stuttgart, June 2014.
2. C. Elsässer, Atomic-scale modeling of the distribution and diffusion of Li ions in solid-state electrolyte materials, Sino-German Symposium on All-Solid-State Batteries, Karlsruhe, April 2015.
3. C. Elsässer, Search for substitutes of critical materials by multi-scale modeling and high-throughput Screening, MS&T 2015 Conference, Columbus (OH), USA, October 2015.
4. C. Elsässer, Search for substitutes of magnetic materials containing critical elements by high-throughput screening and multi-scale modeling, DPG Spring Meeting, Regensburg, March 2016.
5. C. Elsässer, Atomic-scale modeling of point defects, phase stability, and the formation of Z phases CrMN (M=V, Nb, Ta) in steel, International Workshop ADIS-2016, Ringberg Castle of the Max-Planck-Society, October 2016.
6. C. Elsässer, Search for substitutes of magnetic materials containing critical elements by high-throughput screening and multi-scale modeling approaches, MRS Fall Meeting 2016, Boston, USA, December 2016.
7. C. Elsässer, Search for substitutes of magnetic materials containing critical elements by high-throughput screening, EIC Expert Forum Materials and Technologies for Future Mobility, Darmstadt, December 2016.

8. C. Elsässer, Search for substitutes of magnetic materials containing critical elements by high-throughput screening and multi-scale modeling approaches, TMS Annual Meeting 2017, San Diego, USA, March 2017.
9. C. Elsässer, Search for substitutes of hard-magnetic materials containing less critical elements by computational high-throughput screening; Physics Theory Colloquium, University of Duisburg-Essen, April 2017.
10. C. Elsässer, Mechanisms for p-type conduction in ZnO, (Zn,Mg)O, and related oxide semiconductors, IUMRS-ICAM Conference 2017, Kyoto, Japan, August 2017.

Group Kühnemann

Publications

[kue1] St. Fieberg, B. Sturman, F. Kühnemann, K. Buse, "Strong polarization effects in photothermal common-path interferometry," Optics Letters, 39, pp.3880-3883 (2014)

[kue2] St. Fieberg, N. Waasem, F. Kühnemann, K. Buse, "Sensitive absorption measurements in bulk material and coatings using a photothermal and a photoacoustic spectrometer," Proceedings of the SPIE, vol 8964. Nonlinear Frequency Generation and Conversion. Materials, Devices, and Applications XIII , Paper 896410, 7 (2014).

[kue3] M. Leidinger, St. Fieberg, N. Waasem, F. Kühnemann, K. Buse, I. Breunig, "Comparative study on three highly sensitive absorption measurement techniques characterizing lithium niobate over its entire transparent spectral range," Optics Express 23, pp.21690-21705 (2015).

[kue4] St. Fieberg, L. Streit, J. Kiessling, P. Becker, L. Bohaty, F. Kühnemann, K. Buse, "Lithium niobate: Wavelength and temperature dependence of the thermo-optic coefficient in the visible and near infrared," Proceedings of the SPIE, vol 9347. Nonlinear frequency generation and conversion: materials, devices, and applications XIV, Paper 93471C, 9 (2015).

[kue5] A. Lambrecht; C. Bolwien; J. Herbst; F. Kühnemann; V. Sandfort; S. Wolf, "Neue Methoden der laserbasierten Gasanalytik", Chemie- Ingenieur- Technik 88, pp.746-755 (2016).

[kue6] S. Wolf, T. Trendle, J. Kießling, J. Herbst, K. Buse, F. Kühnemann, "Self-gated mid-infrared short pulse upconversion detection for gas sensing," Optics Express, 25, 24459 (2017).

[kue7] S. Wolf, J. Kießling, M. Kunz, G. Popko, K. Buse, F. Kühnemann, "Upconversion-enabled array spectrometer for the mid-infrared, featuring kilohertz spectra acquisition rates," Optics Express, 25, 14504 (2017).

Conference Talks

1. S. Wolf, J. Herbst, F. Kühnemann, Microscopic modelling of domains, defects, and dopants in perovskite ceramics, Seminar lecture, MPI for Solid State Research, Stuttgart, June 2014.
2. S. Wolf, J. Herbst, F. Kühnemann, Silicon-based MWIR Detection using Photon Upconversion, 8th International Conference on Advanced Vibrational Spectroscopy (ICAVS), Wien, 12.-17.7.2015
3. J. Herbst, S. Wolf, F. Kühnemann, and A. Lambrecht, Upconversion Detection for Mid-Infrared Gas Spectroscopy, Laser Applications to Chemical, Security and Environmental Analysis (LACSEA), 25.-28.7.2016
4. S. Wolf, J. Herbst, F. Kühnemann, and A. Lambrecht, Infrared Gas Spectroscopy with MWIR Upconversion Detection, Field Laser Applications in Industry and Research (FLAIR2016), Aix-Le-Bains, 12.-16.9.2016
5. M. Leidinger, J. Kiessling, S. Fieberg, N. Waasem, F. Kühnemann, I. Breunig, K. Buse, Absorption measurements in highly transparent optical materials using tunable sources: On calibration spectroscopy and cross-validation,XLVIII Annual Symposium on optical materials for high-power lasers. (SPIE Laser Damage 2016) Boulder, Colorado, 25.-28.9.2016, paper 10014-79

6. S. Wolf, J. Kießling, F. Kühnemann, M. Kunz, G. Popko, Fast MIR gas analysis for process monitoring using an MWIR-VNIR upconversion spectrometer,4th European Conference on Process Analytics and Control Technology, Potsdam, 12. Mai 2017.
7. F. Kühnemann, J.Kießling, M.Leidinger, Th. Best, E. Elbinger, Spectroscopy of the absorption in dielectric optical coatings, XLIX Annual Symposium on optical materials for high-power lasers. (SPIE Laser Damage 2017) Boulder, Colorado, 24.-27.9.2017, paper 10447-85

Group Moseler

Publications

[mos1] N. Beckmann, P. A. Romero, D. Linsler, M. Dienwiebel, U. Stolz, M. Moseler, P. Gumbsch, "Origins of folding instabilities on polycrystalline metal surfaces", Phys. Rev. Applied **2**, (2014) 064004.

[mos2] A. Klemenz, L. Pastewka, S. G. Balakrishna, A. Caron, R. Bennewitz, M. Moseler, "Atomic Scale Mechanisms of Friction Reduction and Wear Protection by Graphene", Nano Letters **14** (2014) 7145.

[mos3] P. A. Romero, T. T. Järvi, N. Beckmann, Matous Mrovec, M. Moseler, "Coarse graining and localized plasticity between sliding nanocrystalline metals", Phys. Rev. Lett. **113** (2014) 036101.

[mos4] M. Hassan, M. Walter, M. Moseler, "Polymer Interactions with Reduced Graphene Oxide: Van der Waals Binding Energies of Benzene on Defected Graphene", Phys. Chem. Chem. Phys. **16** (2014) 33.

[mos5] M. I. De Barros Bouchet, C. Matta, B. Vacher, J.M. Martin, J.C. von Lautz, T. Ma, L. Pastewka, J. Otschik, P. Gumbsch, M. Moseler, "Tribo-induced phase transformation of nanocrystalline diamond surfaces - combining energy-filtered transmission electron microscopy with atomistic simulations", Carbon **87** (2015) 317.

[mos6] J. von Lautz, L. Pastewka, P. Gumbsch, M. Moseler, "Molecular dynamic simulation of collision-induced third-body formation in hydrogen-free diamond-like carbon asperities", Tribo. Lett. **63** (2016) 26.

[mos7] M. Walter, M. Moseler, L. Pastewka, "Offset-corrected Δ-Kohn-Sham scheme for the semiempirical prediction of X-ray photoelectron spectra of molecules and solids", Phys. Rev. B **94** (2016) 041112(R).

[mos8] A.P. Singh, N. Kodan, B. R. Mehta, A. Held, L. Mayrhofer, M. Moseler, "Band Edge Engineering in an Oxide/Oxide Heterostructure Enhances Photoelectrochemical Performance through Improved Charge Transfer", ACS Catalysis **6** (2016) 5311.

[mos9] L. Mayrhofer, G. Moras, N. Mulakaluri, S. Rajagopalan, P.A. Stevens, M. Moseler, "Fluorine-terminated diamond surfaces as dense dipole lattices: the electrostatic origin of polar hydrophobicity", J. Am. Chem. Soc. **138** (2016) 4018.

[mos10] T. Kuwahara, G. Moras, M. Moseler, "Friction Regimes of Water-Lubricated Diamond (111): Role of Interfacial Ether Groups and Tribo Induced Aromatic Surface Reconstructions", Phys. Rev. Lett. **119** (2017) 096101.

Conference Talks

1. M. Moseler, Taming the Untamable - The Art and Science of Diamond Polishing, Cancun, Mexico, March 2014.
2. M. Moseler, Atomic scale modelling of third body formation and wear in hard carbon materials, Berkeley, California, October 2014.
3. M. Moseler, Atomic scale simulation as a numerical microscope to study material modification on tribologically loaded buried interfaces, Tokyo, Japan, June 2015.
4. M. Moseler, Atomic Scale Mechanisms of Friction Reduction and Wear Protection by Graphene, Aberdeen, UK August 2015.

5. M. Moseler, Atomistic Simulations of Tribo-induced Phase Transitions in Coatings, San Diego, USA April 2015.
6. M. Moseler, Atomic scale understanding of plowing friction and wear on simple metal surfaces, Istanbul, Turkey, June 2015.
7. M. Moseler, XPS spectra of free and supported Al cluster from density functional theory, Girona, Spain, July 2015.
8. M. Moseler, Tribo-induced mechanochemistry: lessons from atomic scale modelling, Chicago, USA, November 2016.
9. M. Moseler, Surface Passivation and Boundary Lubrication of Self-mated Carbon Surfaces: Friction Regimes of Water-Lubricated Diamond (111), Atlanta, USA, May 2017.
10. M. Moseler, Material complexity and atomic scale models in tribology, Bejing, China, September 2017.

Group Reiter

Publications

[reit1] Günter Reiter, “Some unique features of polymer crystallisation”, Chem. Soc. Rev. **43** (2014) 2055-65.

[reit2] Hui Zhang, Muhuo Yu, Bin Zhang, Renate Reiter, Maximilian Vielhauer, Rolf Mülhaupt, Jun Xu, Günter Reiter, “Correlating polymer crystals via self-induced nucleation”, Phys. Rev. Lett. **112** (2014) 237801.

[reit3] Bin Zhang, Jingbo Chen, Paul Freyberg, Renate Reiter, Rolf Mülhaupt, Jun Xu, Günter Reiter, “High Temperature Stability of Dewetting-Induced Thin Polyethylene Filaments”, Macromolecules **48** (2015) 1518-1523.

[reit4] Günter Reiter, “History Dependent Temporal Changes of Properties of Thin Polymer Films”, in: “Non-equilibrium Phenomena in Confined Soft Matter”, Ed. Simone Napolitano, Springer 2015.

[reit5] Sajedeh Motamen, Dominic Raithel, Richard Hildner, Khosrow Rahimi, Thibaut Jarrosson, Françoise Serein-Spirau, Laurent Simon, Günter Reiter, “Revealing Order and Disorder in Films and Single Crystals of a Thiophene-Based Oligomer by Optical Spectroscopy”, ACS Photonics **3** (2016) 2315–2323.

[reit6] Mithun Chowdhury, Xiaoyuan Sheng, Falko Ziebert, Arnold C.-M. Yang, Alessandro Sepe, Ullrich Steiner, Günter Reiter, “Intrinsic Stresses in Thin Glassy Polymer Films Revealed by Crack Formation”, Macromolecules **49** (2016) 9060-9067.

[reit7] Sivasurender Chandran, Günter Reiter, “Transient cooperative processes in dewetting polymer melts”, Phys. Rev. Lett. **116** (2016) 088301.

[reit8] Fanuel Keheze, Dominic Raithel, Tianyu Wu, Daniel Schiefer, Michael Sommer, Richard Hildner, Günter Reiter, “Signatures of Melting and Recrystallization of a Bulky Substituted Poly(thiophene) Identified by Optical Spectroscopy”, Macromolecules **50** (2017) 6829-6839.

[reit9] Purushottam Poudel, Sivasurender Chandran, Sumit Majumder and Günter Reiter, “Controlling Polymer Crystallization Kinetics by Sample History”, Macromol. Chem. Phys. **2017**, 1700315.

[reit10] Sivasurender Chandran, Rishab Handa, Marwa Kchaou, Samer Al Akhrass, Alexander Semenov, Günter Reiter, “Time Allowed for Equilibration Quantifies the Preparation Induced Non-equilibrium Behavior of Polymer Films”, ACS Macro Lett., **6** (2017) 1296-1300

Conference Talks

1. G. Reiter, European Polymer Congress, Dresden, June 2015

2. G. Reiter, Transient Cooperative Processes in Dewetting Crystallizable Polymer Melts, 12. Internationales Symposium für Polymerphysik, Guiyang, June 2016.
3. G. Reiter, International Conference ”Liquids @ Interfaces”, Paris, Oct. 2016
4. G. Reiter, Correlating Polymer Crystals via Self-Induced Nucleation, American Physical Society/APM Congress - March Meeting 2017, New Orleans, Mar 2017.
5. G. Reiter, Model Experiments for the Crystallization of Conjugated Polymers, International Discussion Meeting on Polymer Crystallization, Wittenberg, Sep. 2017.

Group Schilling

Publications

[schill1] J. Yuan et al.,”Graphene Liquid Crystal Retarded Percolation for New High-k Materials”, Nature Communications **6**, 8700 (2015)

[schill2] A. P. Cohen et al.,”Structural transition in a fluid of spheroids: a low-density vestige of jamming”, Phys. Rev. Letters **116**, 098001 (2016)

[schill3] C. Honorato Rios et al.,”Equilibrium Liquid Crystal Phase Diagrams and Detection of Kinetic Arrest in Cellulose Nanocrystal Suspensions”, Frontiers in Materials **3**, 21 (2016)

[schill4] J. R. Bruckner, et al.,”Enhancing Self-Assembly in Cellulose Nanocrystal Suspensions Using High-Permittivity Solvents” Langmuir **32** (38), pp 9854-9862, (2016)

[schill5] M. Mravlak et al.,”Structure diagram of binary Lennard-Jones clusters” J. Chem. Phys. **145**, 024302, (2016)

[schill6] T. Kister, et al, ”Pressure-controlled self-assembly of crystalline, Janus, and core-shell supraparticles” Nanoscale **8**, 13377-13384 (2016)

[schill7] M. Oettel et al.,”Monolayers of hard rods on planar substrates: I. Equilibrium” J. Chem. Phys. **145**, 074902, (2016) and M. Klopotek et al.,”Monolayers of hard rods on planar substrates. II. Growth” J. Chem. Phys. **146** 084903 (2017)

[schill8] H. Meyer, Th. Voigtmann, T. Schilling, ”On the non-stationary Generalized Langevin Equation”, J. Chem. Phys. **147**, 214110, Editor’s Pick (2017)

[schill9] H. Meyer, P. van der Schoot, T. Schilling, ”Percolation in suspensions of polydisperse hard rods : quasi-universality and finite-size effects” J. Chem. Phys. **143**, 044901 (2015)

[schill10] A. Härtel, ”Structure of electric double layers in capacitive systems and to what extent (classical) density functional theory describes it” J. Phys. Condens. Matter **29**, 423002 (2017)

Conference Talks

1. T. Schilling, ”Sampling Chess”, Brazilian Meeting on Simulational Physics, Natal, Brazil, August 2017
2. T. Schilling, ”On the crystallization process”, The 26th conference of the Condensed Matter Division of the European Physical Society, Groningen, The Netherlands, Sep. 9th, 2016
3. T. Schilling, ”Clearing out a maze”, 30th anniversary of Europhysics Letters, Groningen, The Netherlands, Sep. 7th, 2016
4. T. Schilling, ”The hungry walker and its anomalous diffusion”, Solvay workshop “Nonequilibrium and nonlinear phenomena in statistical mechanics”, Brussels, Belgium, 13th July, 2016

5. T. Schilling, ”Binary Lennard Jones Clusters”, SPC Symposium Physical Chemistry of Surfaces, Polymers and Colloids: present and future perspectives, Eindhoven, The Netherlands, June 3rd, 2016
6. T. Schilling, ”Percolation in colloidal model systems”, XXVII IUPAP Conference on Computational Physics CCP201, Guwahati, Assam, India, December 2015
7. T. Schilling, ”On Crystallization and Percolation”, “VIII Brazilian meeting on simulational physics”, Florianopolis, Brazil, August 2015
8. T. Schilling, ”Percolation Revisited”, Mainz Materials Simulation Days (MMSD), Mainz, Germany, June 2015
9. A. Kuhnhold, ”Motion of a nanoparticle in an unentangled polymer melt – passive and active microrheology”, 250th ACS National Meeting, Boston, USA, August 2015
10. A. Härtel, ”On the free energy functional for the primitive model of charged hard spheres”, 5th Tübinger DFT days, Tübingen, Germany, November 2017

Group Stock

Publications

[stock1] S. Buchenberg, N. Schaudinnus, and G. Stock, “Hierarchical biomolecular dynamics: Picosecond hydrogen bonding regulates micro-second conformational transitions”, J. Chem. Theory Comput. **11** (2015) 1330.

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[stock4] P. D. Dixit, A. Jain, G. Stock, and K. A. Dill, “Inferring Transition Rates of Networks from Populations in Continuous-Time Markov Processes”, J. Chem. Theory Comput. **11** (2015) 5464.

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[stock7] F. Sittel, and G. Stock, “Robust Density-Based Clustering To Identify Metastable Conformational States of Proteins”, J. Chem. Theory Comput. **12** (2016) 2426.

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[stock9] M. Ernst, S. Wolf, and G. Stock, “Identification and Validation of Reaction Coordinates Describing Protein Functional Motion: Hierarchical Dynamics of T4 Lysozyme”, J. Chem. Theory Comput. **13** (2017) 5076.

[stock10] Florian Sittel, T. Filk and G. Stock, ”Principal component analysis on a torus: Theory and application to protein dynamics”, J. Chem. Phys. **147**, in press (2017) .

Conference Talks

1. G. Stock, Energy and Signal Flow in Biomolecules, TSRC Workshop on Protein Dynamics, LesHouches, France, May 2014.
2. G. Stock, Molecular Dynamics Simulations of Biomolecules, ETH Zürich, Schweiz, October 2014.

3. G. Stock, Theory and Simulation of Functional Dynamics of Biomolecules, Greater Boston Area Theoretical Chemistry Lecture Series, Massachusetts Institute of Technology, Boston, USA, June 2016.
4. G. Stock, Energy and signal flow in biomolecules, Center of Computational Sciences, Boston University, Boston, USA, June 2016.
5. G. Stock, Energy and signal flow in biomolecules, Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, USA, June 2016.
6. G. Stock, Hierarchical dynamics of biomolecular processes, 8th Intern.Conference on Multiscale Materials Modeling, Dijon, France, October 2016.
7. G. Stock, Vibrational Conical Intersections as a Mechanism of Ultrafast Vibrational Relaxation, MPG-PKS, Dresden, June 2017.
8. G. Stock, Time-resolved description of protein allosteric communication, Allostery and molecular machines, The Royal Society, London, UK, June 2017.
9. G. Stock, Time-resolved description of protein allosteric communication, TSRC Workshop on Vibrational Dynamics, Telluride, USA, August 2017.
10. G. Stock, Time-resolved modelling of protein allosteric communication, Workshop: Computational approaches to investigation allostery, CECAM-HG-EPFL, Lausanne, Switzerland, November 2017.

Group Thoss

Publications

[thoss1] A. Erpenbeck, R. Härtle, and M. Thoss, “Effect of nonadiabatic electronic-vibrational interactions on the transport properties of single-molecule junctions”, Phys. Rev. B **91** (2015) 195418.

[thoss2] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, “Hierarchical quantum master equation approach to electronic-vibrational coupling in nonequilibrium transport through nanosystems”, Phys. Rev. B **94** (2016) 201407(R).

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[thoss5] S. Leitherer, C. M. Jäger, A. Krause, M. Halik, T. Clark, and M. Thoss, “Simulation of Charge Transport in Organic Semiconductors: A Time-Dependent Multiscale Method Based on Non-Equilibrium Green’s Functions”, Phys. Rev. Materials **1** (2017) 064601.

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[thoss7] P.B. Coto, S. Sharifzadeh, J.B. Neaton, and M. Thoss, “Low-Lying Electronic Excited States of Pentacene Oligomers: A Comparative Electronic Structure Study in the Context of Singlet Fission,” J. Chem. Theory Comput. **11** (2015) 147.

[thoss8] J. Zirzlmeier, D. Lehnherr, P.B. Coto, E.T. Chernick, R. Casillas, B.S. Basel, M. Thoss, R.R. Tykwinski, and D.M. Guldi, “Singlet fission in pentacene dimers,” Proc. Natl. Acad. Sci. USA **112** (2015) 5325.

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[thoss10] H. Wang and M. Thoss, “Employing an interaction picture to remove artificial correlations in multilayer multiconfiguration time-dependent Hartree simulations”, J. Chem. Phys. **145** (2016) 164105.

Conference Talks

1. M. Thoss, Quantum dynamics and transport in molecular systems using time-dependent multiconfiguration methods, International Workshop on Quantum and Classical Complexity, Bad Homburg, May 2014.
2. M. Thoss, Charge transport in molecular junctions: Vibronic effects and time-dependent phenomena, The Batsheva de Rothschild Seminar on Molecular Electronics 2015, Ma’ale Hachamisha, Israel, June 2015.
3. M. Thoss, Charge transport in molecular junctions: Vibrational effects and transient phenomena, International Workshop on Open Quantum Systems: Computational Methods, Hong Kong, December 2015.
4. M. Thoss, Quantum transport in molecular junctions: Vibrational effects and transient phenomena, International Workshop on Quantum Thermodynamics: Coherence, Transport, and Heat Engine Efficiency, MIT, Cambridge, USA, September 2015.
5. M. Thoss, Charge Transport in molecular junctions: Vibrational effects, density matrix theory, and graphene electrodes, International Workshop on Quantum Transport in Nanoscale Molecular Systems, Telluride, USA, August 2015.
6. M. Thoss, Simulation of electron transport in molecular junctions using multiconfiguration wavefunction and reduced density matrix methods, ACS-Meeting, San Diego, USA, March 2016.
7. M. Thoss, Quantum transport in molecular junctions: Vibrational effects and time-dependent phenomena, International Workshop on Classical and Quantum Non-equilibrium Dynamics, Tel Aviv, Israel, August 2016.
8. M. Thoss, Charge transport in molecular junctions: Vibrational effects, interference and decoherence, International Workshop on Interference Effects in the Transport Characteristics of Single Molecules and Molecular Quantum Dots, Dresden, April 2017.
9. M. Thoss, Charge transport in molecular junctions: Density matrix theory, vibrational effects,and proton transfer, International Workshop on Quantum Transport in Nanoscale Molecular Systems, Telluride, USA, July 2017.
10. M. Thoss, Nonequilibrium quantum dynamics using multiconfiguration wavefunction and reduced density matrix methods, CECAM-Workshop on Expeditious Methods in Electronic Structure Theory and Many Body Techniques, Tel Aviv, Israel, December 2017.

Group Timmer

Publications

[timm1] C. Tönsing, J. Timmer and C. Kreutz, “Cause and cure of sloppiness in ordinary differential equation models”, Phys. Rev. E **90** (2014) 023303

[timm2] K. Müller, R. Engesser, J. Timmer, M.D. Zurbriggen and W. Weber, “Orthogonal optogenetic triple-gene control in mammalian cells”, ACS Synthetic Biology **3** (2014) 796-801

[timm3] L.A. D’Alessandro, R. Samaga, T. Maiwald, S.-H. Rho, S. Bonefas, A. Raue, N. Iwamoto, A. Kienast, K. Waldow, R. Meyer, M. Schilling, J. Timmer, S. Klamt and U. Klingmüller, “Disentangling the complexity of HGF signaling by combining qualitative and quantitative modeling”, PLoS Computational Biology **11** (2015) e1004192

[timm4] B. Merkt, J. Timmer and D. Kaschek, “Higher-order Lie-symmetries in identifiability and predictability analysis of dynamic models”, Phys. Rev. E **92** (2015) 012920

[timm5] M. Rosenblatt, J. Timmer and D. Kaschek, “Customized steady-state constraints for parameter estimation in non-linear ordinary differential equation models”, Frontiers in Cell and Developmental Biology **4** (2016) 41

[timm6] B. Steiert, J. Timmer and C. Kreutz, “L_1 regularization facilitates detection of cell type-specific parameters in dynamical systems”, Bioinformatics, **32** (2016) i718-i726

[timm7] R. Merkle, B. Steiert, F. Salopiata, S. Depner, A. Raue, N. Iwamoto, M. Schelker, H. Hass, M. Wäsch, M. Böhm, O. Mücke, D.B. Lipka, C. Plass, W.D. Lehmann, C. Kreutz, J. Timmer, M. Schilling, U. Klingmüller, “Identification of cell type-specific differences in erythropoietin receptor signaling in primary erythroid and lung cancer cells”, PLoS Comp. Biology **12** (2016) e1005049

[timm8] T. Maiwald, H. Hass, B. Steiert, J. Vanlier, R. Engesser, A. Raue, F. Kipkeew, H.H. Bock, D. Kaschek, C. Kreutz and J. Timmer, “Driving the model to its limit: Profile likelihood based model reduction”, PLoS ONE **11** (2016) e0162366

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[timm10] J. Koschmieder, M. Fehling-Kaschek, P. Schaub, S. Ghisla, A. Brausemann, J. Timmer and P. Beyer, “Plant-type phytoene desaturase: Functional evaluation of structural implications”, PLoS ONE **12** (2017) e0187628

Conference Talks

1. J. Timmer, Profile likelihood and dynamical modeling, Conference on Statistical Inference and Nonlinear Dynamic Models, Banff, July 2014.
2. J. Timmer, One model to rule them all, Main Meeting Society for Experimental Biology, Pragues, July 2015.
3. J. Timmer, From *Science* to the Patients’ Bedside, Foundations of Systems Biology in Engineering, Boston, August 2015.
4. J. Timmer, Uncertainty Analysis in Systems Biology, Advanced Lecture Course on Systems Biology, Innsbruck, March 2016.
5. J. Timmer, A multi-scale model to improve anemia treatment in non-small cell lung carcinoma patients, Meeting of the ”Hinterzartener Kreis”, Como, March 2017.

Group Wagner

Publications

[wagn1] J. Däubler, T. Passow, R. Aidam, K. Köhler, L. Kirste, M. Kunzer, J. Wagner, ”Long wavelength emitting GaInN quantum wells on metamorphic GaInN buffer layers with enlarged in-plane lattice parameter”, Appl. Phys. Lett. 105, 111111 (2014).

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[wagn4] P. Holl, M. Rattunde, S. Adler, S. Kaspar, W. Bronner, A. Bächle, R. Aidam, J. Wagner, ”Recent advances in power scaling of GaSb-based semiconductor disk lasers”, IEEE J. Sel. Topics Quantum Electron. on Semiconductor Lasers 21, 1501012 (2015).

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Group Waldmann

Publications

[waldm1] K. S. Pedersen, L. Ungur, M. Sigrist, A. Sundt, M. Schau-Magnussen, V. Vieru, H. Mutka, S. Rols, H. Weihe, O. Waldmann, L. F. Chibotaru, J. Bendix, J. Dreiser, ”Modifying the properties of 4f single-ion magnets by peripheral ligand functionalisation”, Chem. Sci. **5** (2014) 1650-1660.

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Group Walter

Publications

[walt1] K. Cui, K. S. Mali, O. Ivasenko, D. Wu, X. Feng, M. Walter, K. Müllen, S. De Feyter, S. F. L. Mertens “Squeezing, then Stacking: from Breathing Pores to 3-Dimensional Ionic Self-Assembly under Electrochemical Control”, Angew. Chem. Int. Ed. **53**, (2014) 12951-12954.

[walt2] A. Held and M. Walter, “Simplified continuum solvent model with a smooth cavity based on volumetric data”, J. Chem. Phys. **141** (2014) 174108.

[walt3] R. Würdemann, H. H. Kristoffersen, M. Moseler, and M. Walter, “Density functional theory and chromium: Insights from the dimers”, J. Chem. Phys. **142** (2015) 124316.

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[walt5] L. Metzler, T. Reichenbach, O. Brügner, H. Komber, F. Lombeck, S. Müllers, R. Hanselmann, H. Hillebrecht, M. Walter, M. Sommer, “High Molecular Weight Mechanochromic Spiropyran Main Chain Copolymers via Reproducible Microwave-Assisted Suzuki Polycondensation ”, Polym. Chem. **6** (2015) 3694-3707.

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[walt7] O. Stauffert, R. Ghassemizadeh, M Walter, “Spectroscopic signatures of triplet states in acenes”, J. Phys. B **50** (2017) 154007.

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[walt9] F. Kempe, O. Brügner, H. Buchheit, S. N. Momm, F. Riehle, S. Hameury, M. Walter and M. Sommer, “Band Edge Engineering in an Oxide/Oxide Heterostructure Enhances Photoelectrochemical Performance through Improved Charge Transfer”, accepted by Angew. Chemie (2017) DOI: 10.1002/anie.201709142.

[walt10] T. Amann, A. Kailer, N. Oberle, K. Li, M. Walter, M. List, and J. Rühe, “Macroscopic Superlow Friction of Steel and Diamond-Like Carbon Lubricated with a Formanisotropic 1,3-Diketone”, ACS Omega **2** (2017) 8330-834.

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Publications

[hennig1] G. Schultz, D. Gallichan, M. Reisert, J. Hennig, M. Zaitsev, ”MR Image Reconstruction from Generalized Projections”, Magn. Reson. Med. 72 (2014) 546–557. doi:10.1002/mrm.24928.

[hennig2] J. Assländer, S.J. Glaser, J. Hennig, ”Spin echoes in the regime of weak dephasing”, Magn Reson Med. 75 (2016) 150–160. doi:10.1002/mrm.25579.

[hennig3] P. LeVan, S. Zhang, B. Knowles, M. Zaitsev, J. Hennig, ”EEG-fMRI Gradient Artifact Correction by Multiple Motion-Related Templates”, IEEE Trans Biomed Eng. 63 (2016) 2647–2653. doi:10.1109/TBME.2016.2593726.

[hennig4] A.E. Mechling, T. Arefin, H.-L. Lee, T. Bienert, M. Reisert, S. Ben Hamida, E. Darcq, A. Ehrlich, C. Gaveriaux-Ruff, M.J. Parent, P. Rosa-Neto, J. Hennig, D. von Elverfeldt, B.L. Kieffer, L.-A. Harsan, ”Deletion of the mu opioid receptor gene in mice reshapes the reward-aversion connectome”, Proc. Natl. Acad. Sci. U.S.A. 113 (2016) 11603–11608. doi:10.1073/pnas.1601640113.

[hennig5] A.B. Schmidt, D.L. Andrews, A. Rohrbach, C. Gohn-Kreuz, V.N. Shatokhin, V.G. Kiselev, J. Hennig, D. von Elverfeldt, J.-B. Hövener, ”Do twisted laser beams evoke nuclear hyperpolarization?”, J. Magn. Reson. 268 (2016) 58–67. doi:10.1016/j.jmr.2016.04.015.

[hennig6] N.S. Hübner, A.E. Mechling, H.-L. Lee, M. Reisert, T. Bienert, J. Hennig, D. von Elverfeldt, L.-A. Harsan, ”The connectomics of brain demyelination: Functional and structural patterns in the cuprizone mouse model”, NeuroImage. 146 (2017) 1–18. doi:10.1016/j.neuroimage.2016.11.008.

[hennig7] P. LeVan, B. Akin, J. Hennig, ”Fast imaging for mapping dynamic networks”, Neuroimage. (2017). doi:10.1016/j.neuroimage.2017.08.029.

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Conference Talks

1. J. Hennig, Basic Introduction into Magnetic Resonance Imaging and Spectroscopy, NSYSU Kaoushiung, Taiwan, März 2016
2. J. Hennig, New developments of MRI technology and applications. KMU Kaoshiung, Taiwan, März 2016

3. J. Hennig, New Insights and Results from Resting State fMRI. NCKU fMRI Center, Tainan, Taiwan, März 2016
4. J. Hennig, Which RF pulse should I choose for which function in my sequence? ESMRMB course Lectures of MR: RF-pulses, Krakow, Polen September 2016
5. J. Hennig, MR 4.0 – where will we go ? Chines Congress of Radiology. November 2016
6. J. Hennig, From Imaging Hardware of Tomorrow: My dream high-field MR scanner. iSi-Workshop New York, November 2016
7. J. Hennig, Introduction to MR Image Encoding and Reconstruction. NSYSU Kaoshiung, Taiwan, Januar 2017
8. J. Hennig, Technologies for life: Current trends and future developments in MRI. Symposium Recent Advances in MRI and MRS. AIIMS. Delhi. März 2017
9. J. Hennig, MR-Microscopy. Symposium TiSuMR. Southhampton, September 2017
10. J. Hennig, MRT: gestern - heute - morgen. Deutsche Gesellschaft für Neuroradiologie. Köln. Oktober 2017
11. J. Hennig, Phase Graphs. 34th Annual Meeting ESMRMB. Barcelona, Oktober 2017

Group Bock

Publications

[bock1] Borowiak R, Groebner J, Haas M, Hennig J, Bock M., ”Direct Cerebral and Cardiac 17O-MRI at 3 Tesla: Initial Results at Natural Abundance”, MAGMA 27(1):95-99 (2014).

[bock2] Ozen AC, Bock M, Atalar E., ”Active decoupling of RF coils using a transmit array system”, MAGMA 28(6):565-576 (2015).

[bock3] Reiss S, Bitzer A, Bock M., ”An optical setup for electric field measurements in MRI with high spatial resolution”, Physics In Medicine And Biology 60(11):4355-4370 (2015).

[bock4] Ozen AC, Ludwig U, Ohrstrom LM, Ruhli FJ, Bock M., ”Comparison of ultrashort echo time sequences for MRI of an ancient mummified human hand”, Magn Reson Med 75(2):701-708 (2016).

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[bock6] Strumia M, Reichardt W, Staszewski O, Heiland DH, Weyerbrock A, Mader I, Bock M., ”Glioma vessel abnormality quantification using time-of-flight MR angiography”, MAGMA 29(5):765-775 (2016).

[bock7] Kalis IM, Pilutti D, Krafft AJ, Hennig J, Bock M., ”Prospective MR image alignment between breath-holds: Application to renal BOLD MRI”, Magn Reson Med 77(4):1573-1582(2016).

[bock8] Kurzhunov D, Borowiak R, Hass H, Wagner P, Krafft AJ, Timmer J, Bock M., ”Quantification of oxygen metabolic rates in Human brain with dynamic 17 O MRI: Profile likelihood analysis”, Magn Reson Med (2017) (e-pub ahead of print)

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[bock10] Borowiak R, Reichardt W, Kurzhunov D, Schuch C, Leupold J, Krafft AJ, Reisert M, Lange T, Fischer E, Bock M., ”Initial investigation of glucose metabolism in mouse brain using enriched 17 O-glucose and dynamic 17 O-MRS”, NMR Biomed (2017).

Conference Talks

1. M. Bock, Quantitative Oxygen-17 MRI. Dreiländertagung der DGMP, ÖGMP und SGMP. Zürich 2014
2. M. Bock, Chemical Exchange Saturation Transfer (CEST) MRI: Physical Principles. Eur. Cong. for Radiology (ECR), Wien, 2015
3. M. Bock, Neue Sequenzen – nur eine Spielerei? Forum Neuroradiologicum, Mannheim, 2015.
4. M. Bock, MRI of the Prostate: Technical Considerations and Recent Advances. 7th Langendorff Congress, Freiburg, 2017
5. M. Bock, ^{17}O MRI: From Basic Principles to Tissue Oxygenation. Ann. Meet. of the Int. Soc. for Magnetic Resonance in Medicine, Oahu, Hawaii 2017

Group Rohrbach

Publications

[rohrb1] A. Meinel, B. Tränkle, W. Römer, and A. Rohrbach, ”Induced phagocytic particle uptake into a giant unilamellar vesicle”, Soft Matter 10 3667-3678 (2014).

[rohrb2] F. Kohler, and A. Rohrbach, ”Synchronization of elastically coupled processive molecular motors and regulation of cargo transport”, Phys Rev E, **91**, 012701 (2014).

[rohrb3] L. Friedrich, and A. Rohrbach, ”Surface imaging beyond the diffraction limit with optically trapped spheres”, Nature Nanotechnology, **10**, 1064-1069, (2015).

[rohrb4] M. Blattmann, A. Rohrbach, ”Plasmonic coupling dynamics of silver nanoparticles in an optical trap”, Nano Letters, **15** 7816-7821 (2015).

[rohrb5] F. Jünger, F. Kohler, A. Meinel, T. Meyer, R. Nitschke, B. Erhard, A. Rohrbach, ”Measuring local viscosities near plasma membranes of living cells with photonic force microscopy”, Biophys. J. 109(5), 869-882 (2015).

[rohrb6] B. Tränkle, D. Ruh, and A. Rohrbach, ”Interaction Probability of Two Diffusing Particles: Contact Times And Influence Of Nearby Surfaces”, Soft Matter, **12**, 2729-2736 (2016).

[rohrb7] T. Meinert, O. Tietz, K. Palme, A. Rohrbach, ”Separation of ballistic and diffusive fluorescence photons in confocal Light-Sheet Microscopy of Arabidopsis roots” Scientific Reports **6**, 30378 (2016).

[rohrb8] F. Jünger, P. Olshausen, A. Rohrbach, ”Fast, label-free super-resolution live-cell imaging using rotating coherent scattering (ROCS) microscopy”, Scientific Reports **6**, 30393, (2016).

[rohrb9] M. D. Koch, N. Schneider, P. Nick, A. Rohrbach, ”Single microtubules and small networks become significantly stiffer on short time-scales upon mechanical stimulation”, Scientific Reports **7**, 4229 (2017).

[rohrb10] C. Gohn-Kreuz, and A. Rohrbach, ”Generation of light-needles in scattering media using self-reconstructing beams and the STED-principle”, Optica **4**, 1134-1142 (2017)

Group Rotter

Publications

[rott1] S. Sadeh, S. Cardanobile, S. Rotter, ”Mean-field analysis of orientation selectivity in inhibition-dominated networks of spiking neurons”, *SpringerPlus* 3(1): 148 (2014).

[rott2] F. Lagzi, S. Rotter, ”A Markov model for the temporal dynamics of balanced random networks of finite size”, *Frontiers of Computational Neuroscience* 8: 142 (2014).

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2.6 PhD, Diploma and Master Theses

Group Blumen

PhD Theses

1. Piet Schijven, Quantum Stochastic Walks - A Model for Coherent and Incoherent Transport on Networks, October 2014, `https://freidok.uni-freiburg.de/data/9762`
2. Florian Fürstenberg, Struktur und Dynamik hyperverzweigter Polymere: Über Dendrimere und Vicsek-Fraktale, January 2015. `https://freidok.uni-freiburg.de/data/9957`
3. Julian Helfferich, Glass dynamics in the continuous-time random walk framework, January 2015, `https://freidok.uni-freiburg.de/data/9985`

Diploma/Master Theses

1. Chi-Hung Wenig, Quantum Walks on Quasicrystals, April 2014.
2. Marco Tabarelli, Transport Efficiency of Quantum Stochastic Walks on Complex Networks, March 2015.
3. Nikolaj Kulvelis, Quantum Dynamic Universality of Complex Trees in the Hyper-Branching Limit, September 2015.

Group Elsässer

PhD Theses

1. Benedikt Ziebarth, Interactions between metallic impurities and extended defects in silicon from first-principles, 2015.
   `https://freidok.uni-freiburg.de/data/10590`
2. Davide Di Stefano, First-principles investigation of hydrogen interaction with metals, 2016.
   `https://freidok.uni-freiburg.de/data/11338`

Diploma/Master Theses

1. Lukas Elflein, DFT investigations of anisotropic magnetic and crystalline properties of rare-earth-free intermetallic phases, 2017.

Group Kühnemann

PhD Theses

1. Stephan Fieberg, Analyse thermooptischer Effekte zur Absorptionsmessung, Universität Freiburg, 2014.
2. Sebastian Wolf, Infrarotmesstechnik und -Spektroskopie durch nichtlinear-optische Hochkonversion, Universität Freiburg, 2017.

Diploma/Master Theses

1. Tina Preisinger, Spektrale Charakterisierung eines nichtlinear-optischen Frequenzhochkonverters, Universität Freiburg, 2015.
2. Tobias Trendle, Hocheffiziente gepulste Aufwärtskonversion von mittelinfrarotem Licht, Universität Freiburg, 2016.

Group Moseler

PhD Theses

1. N. Beckmann, ”Atomistische Simulation tribologischer Elementarprozesse bei nanokristallinen Übergangsmetallen”, 2015.
2. A. Klemenz, ”Atomistische Simulation der Materialmodifikation durch die Kohlenstoffallotrope Graphen und Kohlenstoffnanoröhren”, 2015.
3. A. Peguiron, ”Atomistic Simulations of Silica by Sequential and Concurrent Multiscale Coupling”, 2015.

Diploma/Master Theses

1. R. Leute, ”Ab initio phonon and electronic structure calculations for SiSn hot carrier solar cell absorbers”, 2017.
2. T. Reichenbach, ”Theoretical modelling of the Co2 hydrogenation to methanol in ZnO/Cu”, 2016.
3. C. Bentler, ”Molekulardynamische Untersuchung von Deformationsverhalten und Tribologie von AlSiCu-Legierungen”, 2014.

Group Reiter

PhD Theses

1. Bin Zhang, Investigation of Structure Formation and Reorganization of Polymer Crystals, 2014.
   `https://freidok.uni-freiburg.de/data/9635`
2. Hui Zhang, Pattern Formation on Single Crystals of Isotatic Polystyrene in Thin Film, 2014.
   `https://freidok.uni-freiburg.de/data/9798`
3. Paul Freyberg, Triangular Dewetting by Symmetry Breaking in Blends of Stiff and Flexible Polymers, 2015.
   `https://freidok.uni-freiburg.de/data/9976`
4. John O. Agumba, Formation and Optical Characterization of Single Crystals of Poly(3-Hexylthiophene) (P3HT), a Model Conjugated Polymer, 2016.
   `https://freidok.uni-freiburg.de/data/10598`
5. Rainhard Machatschek, Large area crystal surfaces of precisely sidebranched polyethylenes: Preparation, surface order and functionalization, 2016.
   `https://freidok.uni-freiburg.de/data/11069`
6. Sajedeh Sadat Motamen, Crystallization and Resulting Optical Properties of Thiophene-Based Oligomers, 2016.
   `http://d-nb.info/1118630130`
7. Asad Jamal, Self-assembled Nanotubes and Nanoribbons of Aromatic Diamide-esters, 2016.
   `https://freidok.uni-freiburg.de/data/11172`
8. Fallou Fall, Self-Assembly and Polymerization of Diacetylene Molecules on Epitaxial Graphene, 2017.

Diploma/Master Theses

1. Angelika Beinert, Der Einfluss der Additivformulierung auf die mechanischen Eigenschaften von Poly(ethylen-co-vinylacetat) in der Photovoltaik, 2014
2. Sven Renkert, Electron transport measurement on organic nanocrystals, 2014.
3. Max Bergau, Effects of catalyst layer thickness in PEM fuel cells, 2015.

4. Zhexiong Yang, Membrane Organization upon Interaction with Bacterial Proteins, 2016.
5. Rishab Handa, Role of Preparation Pathways and Tacticity on the Non-Equilibrium Dynamics of Polystyrene Films, 2016.
6. Emna Khechine, Probing the Elasticity of Langmuir Polymer Films of High Molecular Weight Poly (γ-benzyl-L-glutamate), 2016.
7. Adrian Linn, Manipulating the dewetting dynamics of polymer films by creating non-equilibrium conformational states at the interface, 2017.

Group Schilling

In the past three years, three Master theses and one PhD thesis were completed in our group. Two of the Master theses won the award for the best Master thesis in physics in Luxembourg (in 2017 and 2016). As we have just moved to Freiburg and have not yet defended a thesis here, we do not list the theses of the past three years in detail.

Group Stock

PhD Theses

1. N. Schaudinnus, ”Stochastic modeling of biomolecular systems using the data-driven Langevin equation”, 2015. `http://www.freidok.uni-freiburg.de/volltexte/10391/`
2. L. Cheng, ”Modeling protein dynamics in solution effects of Ligand binding and crowding”, 2015. `http://www.freidok.uni-freiburg.de/volltexte/10493/`
3. S. Buchenberg, ”Energy and Signal Transport in Proteins: A Molecular Dynamics Simulation Study”, 2016. `http://www.freidok.uni-freiburg.de/volltexte/8283/`

Diploma/Master Theses

1. J. Bartz, ”Linear response description of allosteric transitions in PDZ2 domains”, 2014.
2. B. Lickert, ”Modeling biomolecular dynamics by using a Langevin framework”, 2016.

Group Thoss

In the past four years, three Master theses and one PhD thesis were completed in our group. Since these thesis were completed before our group joined the University of Freiburg, the details are not listed here.

Group Timmer

PhD Theses

1. Daniel Kaschek: Application of Statistical Inference, Lagrangian Mechanics and Dynamic Modeling in the Observation and Identification of Cell Biological Processes, 2014.
2. Malenka Mader: Time-Resolved Multivariate Analysis of Dynamic Processes with Application to Neurological Data, 2014.
3. Wolfgang Mader: Reconstruction of complex systems from data, 2014.

4. Bernhard Steiert: Dynamical modeling and data analysis of information processing by biological systems, 2016.
5. Helge Hass: Quantifying cell biology: Mechanistic dynamic modeling of receptor crosstalk, 2017.
6. Raphael Engesser: Mechanistic Modeling for the Construction and Optimization of Synthetic Biological Systems, 2017.

Diploma/Master Theses

1. Benjamin Merkt: An Application of Lie Group Theory to Identifiablity Analysis of Differential Equation Models, 2014.
2. Carolin Arand: Identifiability of Models of Effective Brain Connectivity, 2014.
3. Hagen Klett: Optimal Experimental Design to improve the Identifiability of a Model for the Inflammatory Response in the Hypothalamus ensuing Heat Stroke, 2014.
4. Lena Maetani Appel: An adaptative integration method for the calculation of the profile likelihood in dynamical systems, 2014.
5. Marcus Rosenblatt: Unified Parameter Estimation in Non-autonomous Dynamical Systems with Applications to Cell Signaling, 2014.
6. Patrick Metzger: Dynamic modeling with imprecise measurement times, 2014.
7. Daniel Lill: Approximating Riemann Normal Coordinates with applications to non-linear least squares, 2016.
8. Lukas Refisch: Impact of parameter transformations on model calibration and model-based personalized anemia treatment, 2017.
9. Svenja Kemmer: Dynamic modeling of the MAP Kinase signaling network in breast cancer cell and its interplay with therapeutic antibodies, 2017.
10. Timo Schweiger: The Performance of Constrained Optimization for Ordinary Differential Equation Models, 2017.

Group Wagner

PhD Theses

1. Bastian Galler, Ladungsträger-Rekombination und -Transport in InGaN-basierenden Leuchtdioden, 2014.
2. Peter Holl, Halbleiter-Scheibenlaser und ihre Integration in anwendungsspezifische Resonatoren, 2017.

Diploma/Master Theses

1. Steffen Adler, Infrarot-Halbleiterscheibenlaser: Einfluss und Optimierung des resonatorinternen Wärmespreizers, 2014.
2. Verena Blattmann, Untersuchung von Fernfeldeigenschaften und Modenstruktur von Quantenkaskadenlasern im externen Resonator, 2014.
3. Markus Reisacher, Verbesserung der Lichtextraktionseffizienz von UV-Dünnschicht-LEDs durch nasschemische Oberflächenstrukturierung, 2014.
4. Karl Jacob, Untersuchung der Eigenrauschmechanismen metamorpher Feldeffekttransistoren mit hoher Elektronenbeweglichkeit (HEMT) zwischen 5GHz und 25 GHz bei 15 K, 2014.
5. Lukas Stolch, Etablierung einer Messtechnik zur quantitativen Gain-Bestimmung von Avalanche-Photodioden, 2016.

6. Lukas Götz, Charakterisierung einer Serie von GaInAs/AlInAs-Avalanche-Dioden im Geiger-Modus, 2017.
7. Chiara Lindner, Spektrale Eigenschaften von GaSb-basierten Halbleiter-Scheibenlasern, 2017.

Group Walter

PhD Theses

1. Alexander Held, ”Beschreibung geladener Systeme in verschiedenen Umgebungen mit den Methoden der Dichtefunktionaltheorie”, 2015.
2. Rolf Würdemann, ”Berechnung optischer Spektren und Grundzustandseigenschaften neutraler und geladener Moleküle mittels Dichtefunktionaltheorie”, 2016.

Diploma/Master Theses

1. Oliver Brügner, ”Substituent Effects in Photochromatic Spiropyrans”, 2015.

Group Hennig

PhD Theses

1. Hans Weber, Novel Encoding Strategies in Magnetic Resonance Imaging, Januar 2014.
2. Jakob Assländer, Static Field Inhomogeneities in Magnetic Resonance Encephalography: Effects and Mitigation, April 2014.
3. Denis Kokorin, Magnetic Resonance Imaging With Spatially-Selective Pulses Using Multiple Transmission Channels, Juli 2014.
4. Elias Kellner, Quantitative Bestimmung der zerebralen Durchblutung mittels Dynamischer Suszeptibilitätskontrast-magnetresonanztomographie, April 2016.
5. Alexander Ruh Mesoscopic structure through the prism of transverse relaxation, Dezember 2016.
6. Rebecca Ramb, k-t-sub-Nyquist sampled Parallel Echo Planar Imaging in MRI, Mai 2016.
7. Waltraud Buchenberg Development of experimental methods to measure temperature fields and velocity fields in fluid flows using Magnetic Resonance Imaging, November 2016.
8. Ursula Nemer Analyse und Verbesserung der quantitativen PET-Bildgebung. Juni 2017.
9. Marius Menza, Accelerated, High Spatial And Temporal Resolution Phase Contrast Techniques For Functional Analysis Of The Myocardium, Juni 2017.
10. Sebastian Bär: Evaluierung der bSSFP-Sequenz für die hyperpolarisierte Magnetresonanztomographie, Januar 2017.

Diploma/Master Theses

1. Stephan Knecht. Spin order transfer from parahydrogen and orthodeuterium: a simulation study, 2014.
2. Andreas Schmidt. Nuclear hyperpolarization using twisted light beams at low magnetic fields, 2014.
3. Moritz Braig: Analyzing myocardial motion: Optimized phase contrast sequence for cryogenic coils, 2014.

4. Stephan Berner. Simulations of parahydrogen spin order transfer for X-nuclei hyperpolarization, 2015.
5. Christoph Müller. Fast MRI Methods for Metabolite Mapping, 2015.
6. Anna Lena Cremer. Optimization and Characterization of a PASADENA Polarizer, 2015.
7. Philipp Amrein. Inductively coupled intraoral receiving coils for dental MRI, 2017.

Group Bock

PhD Theses

1. Ali Caglar Özen (KIT / Uni Karlsruhe): Novel MRI Technologies for Structural and Functional Imaging of Tissues with Ultra-short T2 Values, January 2017.
2. Dmitry Kurzhunov: Novel Reconstruction and Quantification Methods for Oxygen-17 Magnetic Resonance Imaging at Clinical Field Strengths, September 2017.
3. Robert Borowiak: Neue Methoden zur Untersuchung metabolischer Prozesse mittels spektroskopischer und bildgebender 17O-Kernspinresonanz, September 2017.
4. Inge Manuela Kalis: Zeitaufgelöste BOLD Magnetresonanztomographie der Nieren mit prospektiver Bewegungskorrektur, October 2017.

Diploma/Master Theses

1. Robert Schall: Messung der arteriellen Inputfunktion für die Perfusionsquantifizierung mit aktiven Kathetern, 2014.
2. Simon Reiss: Elektro-optische E-Feld-Messungen in klinischen Magnetresonanztomographen, 2014.
3. Katharina Schleicher: Suszeptibilitätsartefakte eines MR-sicheren Führungsdrahts in radial abgetasteten Bildern, 2016.
4. Philipp Wagner: Application of referenceless temperature measurements for MR-guided thermal interventions, 2016.
5. Timo Abels: Dynamische MR-Bildgebung der Stimmlippenoszillation im Submillisekunden-Bereich, 2017.

Group Rohrbach

PhD Theses

1. Benjamin Landenberger: Sortieren und Manipulieren von biologischen Objekten mit optischen Fallen und interferometrischem Tracking, 2015.
2. Matthias Koch: Biomechanics of prokaryotic & eukaryotic cytoskeletal model systems probed by time-multiplexed optical tweezers, 2015.
3. Felix Jünger: Messung zellulärer Reaktionen bei mechanischen Stimuli mittels photonischer Kraftmikroskopie und kohärenter Lichtstreuung, 2016.
4. Cristian Gohn-Kreuz: Mikroskopie mit selbst-rekonstruierenden Strahlen unter Ausnutzung des STED-Prinzips, 2017.
5. Tobias Meinert: Optimierungsstrategien zur computerholographischen Beleuchtung und zur Abbildung streuender Objekte in der Lichtscheibenmikroskopie mit Bessel-Strahlen, 2017.

Diploma/Master Theses

1. Benjamin Alexander Gutwein: Licht-Scheiben-Mikroskopie mit gescannten Bessel-Strahlen, rückgekoppelte Anpassung der Beleuchtung in einer Glaskapillare, 2014.
2. Peter Piechulla: Untersuchungen zur plasmonischen Kopplung optisch gefangener Nano-partikel, 2014.
3. Sandra Ulrich: Kontraststeigerung in der Fluoreszenzmikroskopie durch linear modulierte Objekt-Beleuchtung, 2014.
4. Thomas Gerrer: Super-resolution by total internal reflection fluorescence structured illumination microscopy, 2014.
5. Kuntz Iris: Messungen zur induzierten Phagozytose von Latexkugeln in J774 Makrophagen mit Photonischer Kraftmikroskopie, 2016.
6. Anjan Bhat Kashekodi: A micro machined light-sheet illumination system implemented in a conventional microscope, 2017.
7. Gerardo González-Cerdas: Interferometric Light-Sheet Microscopy with Scanned Continuous-Wave Laser Beams, 2017.
8. Mark Skamrahl: Dissecting the surfing-like particle transport along adherent macrophage filopodia, 2017.
9. Md. Mahmud Salek: Rotating Coherent Scattering (ROCS) Microscopy with adaptive zeroth order blocking, 2017.

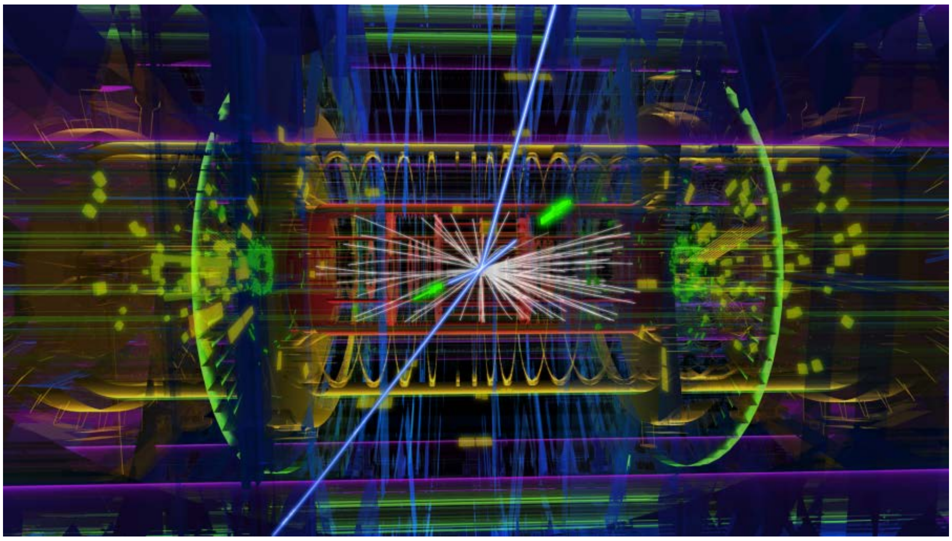
Group Rotter

Diploma/Master Theses (submitted to the Institute of Physics)

1. Leonidas Richter, ”Modeling contextual modulations in functional recurrent networks”, 2014.
2. Friedrich Schüßler, ”An analytical theory for spiking neurons driven by colored noise”, 2017.

Chapter 3

Particles, Fields and Cosmos



- **Experimental Particle Physics**
  Prof. B. Heinemannn (PI and DESY)
- **Experimental Particle Physics**
  Prof. G. Herten,
  apl. Prof. U. Landgraf
- **Experimental Particle Physics**
  Prof. K. Jakobs,
  Dr. C. Weiser (Interim Professor),
  Hon.-Prof. P. Jenni
- **Experimental Particle Physics**
  Prof. M. Schumacher
- **Experimental Astroparticle Physics**
  Prof. M. Schumann (successor Königsmann)
  apl. Prof. H. Fischer
- **Theory of Particle Physics and Quantum Field Theory**
  Prof. S. Dittmaier
- **Quantum Fields and Particle Phenomenology**
  Prof. H. Ita,
  visiting Prof. F. Febres Cordero
- **Elementary Particle Phenomenology**
  Prof. J. van der Bij

Chapter caption: View of a candidate event for the production of a Higgs boson decaying via two Z bosons into two electrons and two muons in the ATLAS experiment.

3.1 Overview

Particle Physics in Freiburg has a long tradition and is one of the major research areas of the Institute of Physics. Over the past decades groups from Freiburg have participated very actively in the experimental research programme at the European Centre for Particle Physics, CERN in Geneva/Switzerland, at DESY in Hamburg and at the US research laboratory Fermilab. In 2016, the Particle Physics area of the Institute extended to Astroparticle Physics with participation in experiments at the Gran Sasso Laboratory (LNGS) in Assergi/Italy.

Today's experimental activities are focused on CERN with participation in the ATLAS experiment at the LHC with groups led by **B. Heinemann, G. Herten, K. Jakobs** and **M. Schumacher**, in the COMPASS experiment with the group of **H. Fischer** (former group of K. Königsmann). The group of **M. Schumann** participates in the XENON and DARWIN experiments (at LNGS) and in CAST (at CERN). The permanent faculty members **H. Fischer, U. Landgraf, U. Parzefall, C. Weiser and S. Zimmermann** contribute in leading roles to these experiments. Since 2013 **P. Jenni** works as a Honorary Professor at our institute. He led the ATLAS Collaboration as spokesperson from 1995 to 2009 and had a leading role during the initialization and realization of the experiment. The experimental activities are accompanied by strong activities in theory led by **S. Dittmaier, H. Ita** and **J. van der Bij**. In 2014 **F. Febres Cordero** joined the theory groups for five years, funded by a Sofja Kovalevskaja Award of the Alexander von Humboldt foundation. Their groups cover a wide area in the field of fundamental forces acting between elementary particles, including strong and electroweak interactions as described by the Standard Model of particle physics and extensions thereof.

The Freiburg Institute of Physics has been among the founding institutes of the ATLAS collaboration and right from the beginning has contributed significantly to studies of the detector concept and physics performance as well as to research and development activities in the area of silicon tracking and muon detectors. During the years 2001 to 2006 important detector elements of the silicon-based tracking detector (SCT, K. Jakobs) and of the muon precision chambers (MDT, G. Herten) were built at the Institute. In parallel the group was involved in leading roles in the investigation of the physics potential of the ATLAS experiment in the areas of Higgs-boson physics and searches for supersymmetry. Since the start of the LHC the group (M. Schumacher) operates a so-called ATLAS Tier-2 Grid-centre for high performance computing. Today the total of about 50 physicists from the University of Freiburg constitutes one of the largest groups in the world-wide ATLAS collaboration. They contribute to the operation of the ATLAS detector at CERN, to the operation of the twelve Tier-2 centres around the German Tier-1 centre *GridKa*, to the analysis of the data as well as to detector and computing research and development for the upgrade of the ATLAS experiment towards the High-Luminosity LHC (HL-LHC). After the discovery of the Higgs boson in 2012, precision studies of the Higgs boson and of electroweak symmetry breaking are still in the focus of present and future particle collider physics, including the HL-LHC phase. Having already played a significant role in the Higgs-boson discovery, the Freiburg ATLAS groups will further pursue this direction of research emphatically. Since spring 2017 K. Jakobs is spokesperson of the ATLAS experiment, while C. Weiser acts as his substitute in all affairs concerning the Jakobs group at the Physics Institute. Beate Heinemann joined Freiburg in August 2016 and was Deputy Spokesperson of the ATLAS collaboration until February 2017.

The COMPASS (COmmon Muon and Proton Apparatus for Structure and Spectroscopy) experiment at CERN studies the spin-structure of hadrons to improve our understanding of QCD in the non-perturbative regime. The Freiburg group (H. Fischer) develops data acquisition electronics and contributes to data analysis.

The activities in Astroparticle Physics (M. Schumann, H. Fischer) are focusing on the direct search for dark matter and the development of low-background detectors for rare event searches. The XENON1T experiment, filled with 2 tons of liquid xenon as dark matter target, is currently the world's most sensitive running detector searching for dark matter in form of weakly interacting massive particles (WIMPs). The Freiburg group is responsible for the data acquisition system, coordinates the design of the central time projection chamber (TPC), and is currently leading the data analysis efforts. These key responsibilities are kept for the upgrade phase XENONnT, which will triple the sensitive target mass. Furthermore, the group very actively contributes within the DARWIN collaboration which envisages the ultimate liquid-xenon based dark matter detector being limited by irreducible neutrino backgrounds only. Within the ERC-funded project ULTIMATE important R&D work is performed towards this detector and towards improving liquid xenon-based low-background detectors. The group also participates in the CAST experiment at CERN, searching for dark matter in form of ultra-light axions which could be emitted by the Sun.

In the theory area, special emphasis is directed to the phenomenology in collider experiments, most notably at the LHC, and to the corresponding precision calculations required by experiments, which include strong and electroweak quantum corrections. Among other things, the theory group made substantial contributions to predictions used in Higgs-boson analyses by the LHC experiments and worked out important precision calculations for the production of electroweak gauge bosons for present and future LHC data analyses. Technically, both traditional Feynman-diagram-based methods as well as modern unitarity-based techniques for many-particle processes are further developed at the "next-to-leading-order" (NLO) and "next-to-next-to-leading-order" (NNLO) levels and applied in cutting-edge calculations where existing techniques are not sufficient. Conceptually, also more fundamental aspects of quantum field theory are analysed, such as the structure of infrared singularities or the perturbative description of unstable particles. Besides the activity directly related to LHC physics, theoretical research is intensified at the interface between particle physics and cosmology. The theory group is integrated in important international activities. Examples are the *LHC Higgs Cross Section Working Group* (where S. Dittmaier was theory co-chair from 2010 to 2012 and is member of its Theory Advisory Committee since 2016, M. Schumacher was experimental co-chair from 2014 to 2016) and the *LHC Electroweak Working Group* (where S. Dittmaier acts as theory contact since 2017). A further example, where both experimental and theoretical physicists are involved, was the EU Training Network *HiggsTools* which was active from 2014 to 2017.

The Freiburg particle-physics groups have also strong involvements in detector physics and are members of important Research and Development (R&D) Collaborations. Studies on future silicon-based tracking detectors and on micro-pattern gaseous muon detectors are performed within the RD50 (K. Jakobs, U. Parzefall; *Radiation hard semiconductor devices for very high luminosity colliders*) and RD51 collaborations (G. Herten, U. Landgraf, and S. Zimmermann; *Development of micro-pattern gas detector technologies*), respectively. Further research projects on the application of semiconductor detectors, e.g. in medical diagnosis or in radiation surveillance, are carried out in collaboration with the *Freiburg Material Research Centre (FMF)*, partly within the EU project *REWARD (Real time wide-area radiation surveillance) 2011–2014*. Digitisation and trigger electronics are being developed (H. Fischer) for the COMPASS experiment. This concerns high-speed and high-resolution transient recorders, time-to-digital converters and trigger processors, all programmable to adapt to different applications. The astroparticle physics group (M. Schumann) works on R&D to build detectors with a very low background from natural radioactivity. To identify suitable detector materials and components, the group operates one of the world's most sensitive low-background gamma spectrometers in the Vue-des-Alpes tunnel in the Swiss Jura mountains. New computing models for data-intensive analyses on heterogeneous compute resources are developed in the context of the World Wide LHC computing Grid (WLCG), the Virtual Open Science Collaboration Environment (VICE) collaborative project of the state of Baden-Württemberg and ATLAS FSP-103 (M. Schumacher).

The activities in the ATLAS experiment, as well as the particle theory groups, are embedded in a *Collaborative Research Centre* of the German Ministry for Education and Research (BMBF Forschungsschwerpunkt FSP-103 ATLAS), where 13 German universities, the Deutsche Elektronen Synchrotron (DESY) and the Max-Planck-Institute for Physics in Munich (MPP), collaborate. During the previous funding period (2012–2015) the University of Freiburg had the lead in this centre with Karl Jakobs as spokesperson and National contact physicist in the ATLAS experiment. In addition, both the experimental and theoretical groups are involved in the Helmholtz Alliance *Physics at the Terascale* (since 2007), a national research network comprising 18 universities, two Helmholtz Centres (DESY and KIT) and the MPP. The XENON activities are supported by the German Ministry for Education and Research (BMBF) and the R&D towards DARWIN by the consolidator grant *ULTIMATE* of the European Research Council (ERC).

Particle physicists from Freiburg are also very visible in the German high-energy physics community. G. Herten was the chair of the particle physics section within the German Physical Society (DPG) from 2013–2015, M. Schumacher is one of the representatives of experimental particle physics in the German committee for Particle Physics (KET) since 2015, member of the GridKa Overview Board since 2011 and KET representative in the newly formed working group of the BMBF "Digitale Agenda für Erforschung von Universum und Materie" since 2017, and S. Dittmaier is a member of the committee of valuation experts for the above mentioned BMBF FSP.

Finally, two Freiburg physicists were awarded very prestigious prices: K. Jakobs was awarded the Stern-Gerlach-Medal, the highest distinction in experimental physics in Germany, of the German Physical Society in 2015 and P. Jenni was awarded the W.H.K. Panofsky Prize of the American Physical Society in 2017.

To offer an excellent education and research environment for PhD students and to foster closer collaboration between theory and experiment, the particle physics groups have successfully established the Research Training Group 2044 *Mass and Symmetries after the Discovery of the Higgs particle at the LHC* (2014–2019), funded by the Deutsche Forschungsgemeinschaft (DFG). This programme is extremely successful and has attracted students from other German universities and from abroad—in both theory and experiment—to carry out their research and to obtain their PhD in Freiburg. The topics covered within the school span the entire range of activities on theory, data analysis and detector R&D.

The future activities of particle physics in Freiburg are directed towards further precision studies of the Higgs boson, the investigation of rare electroweak processes (such as vector-boson scattering), and the search for physics beyond the Standard Model. These efforts are being complemented and expanded by the direct search for the dark matter particle using ultra-sensitive instruments filled with liquid xenon. The successful cooperation between experiment and theory within RTG 2044, for which an application for a prolongation will be submitted in 2018.

3.2 ATLAS Data Analysis

Since the startup of data-taking in 2009 the groups from Freiburg have been involved in the operation of the ATLAS detector in the areas of the silicon tracking and muon detector systems and in Grid computing. Right from the beginning they have participated significantly in the analysis of the proton-proton collision data. The focus of the analysis activities lay on the search for and investigation of the Higgs boson and the search for new particles in particular supersymmetric particles and in the measurement of Standard Model processes. In parallel, they have always been engaged in the important study groups on the detector performance, i.e. in the reconstruction and identification of tau leptons, in the tagging of b-quarks, in the reconstruction of electrons and the development of the embedding technique. In addition, they have contributed to important detector simulation projects. Scientists from Freiburg have held and hold leading and visible roles in the collaboration, e.g. spokesperson, run coordinator, collaboration board chair and co-convenors of performance, data preparation and physics groups.

3.2.1 Standard Model Processes

Measuring important Standard Model (SM) processes allows precise tests of theoretical predictions. Our groups have been mainly involved in analyses with W or Z bosons, where aspects of both the electroweak and strong interaction can be tested. The understanding of these processes is also essential for analyses e.g. in the Higgs-boson sector or searches for new particles, where these processes are a source of background.

Production cross-sections of W und Z bosons are very sensitive to higher orders in theoretical calculations and parton density functions (PDF). Using the large number of W and Z bosons in the dataset of the year 2011, differential cross sections have been measured for several kinematic variables [jak7]. Fig. 3.1 shows the differential cross section $d\sigma/d|\eta_\ell|$ for the decay $W^- \to \ell^- \bar{\nu}_\ell$ where our group has made major contriubutions to the $W \to e\nu$ channel.

The production of W bosons has also been studied in events where a jet originating from the fragmentation of a charm quark is present. This process is mainly initiated by a strange see-quark in the proton and thus provides important information on the s-quark PDF.

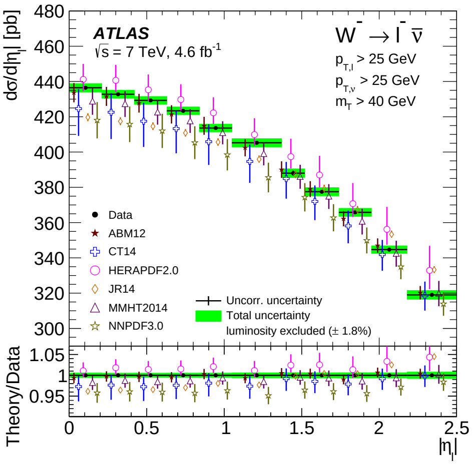


Figure 3.1: The differential cross section $d\sigma/d|\eta_\ell|$ for the decay $W^- \to \ell^- \bar{\nu}_\ell$ compared to theoretical predictions using different sets of parton density functions.

The analysis of processes with multiple vector bosons in the final state is particularly important to investigate the coupling structure of vector bosons, if e.g. so-called *anomalous couplings* are present. These processes also constitute a major background source in Higgs-boson measurements, e.g. WW production is an irreducible background for decays $H \to WW^*$. We have analysed the production of W-boson pairs in the final states $\ell\nu\ell\nu$, where both W bosons decay leptonically, and $\ell\nu qq$, where one of the W bosons decays into quarks fragmenting into jets. The channel $WW \to \ell\nu\ell\nu$ was first analysed selecting events without additional hadronic jets in order to suppress background from top-quark production [jak6], leading to an increased dependency on theoretical predictions for the production of additional jets. In a subsequent analysis, the phase space of the measurement was thus extended including events with one hadronic jet. The combination of both measurements allowed a significant reduction of the uncertainty of the WW production cross-section, as can be seen in Fig. 3.2.

The channel $WW/Z \to \ell\nu qq$ has also been analysed and published. A major challenge was the determination of the background from the copious production of W bosons with additional jets. Our group was leading the analysis where both jets from the hadronic W-boson decay are reconstructed as separated jets, consituting the largest farction of the total cross section.

Out group is also involved in the investigation of WW final states where both W bosons have the same electric charge, to isolate the process of *Vector Boson Scattering*, which plays an important role in the electroweak symmetry breaking.

From a measurement of the forward-backward asymmetry in the reaction $pp \to Z/\gamma^* \to \ell^+\ell^-$, with ℓ

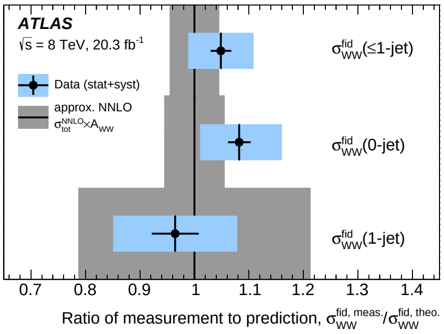


Figure 3.2: The ratios of the measured WW production cross-sections and the corresponding theoretical prediction for events with no, exactly one or up to one hadronic jet.

being electrons or muons, the the effective weak mixing angle can be extracted [citeAad:2015uau]. The results are based on the full set of data collected in 2011 in pp collisions at the LHC at $\sqrt{s} = 7$ TeV, corresponding to an integrated luminosity of 4.8 fb^{-1}. The measured asymmetry values are found to be in agreement with the corresponding Standard Model predictions. The combination of the muon and electron channels yields a value of the effective weak mixing angle which agrees with the other measurements of the weak mixing angle as shown in Fig. 3.3.

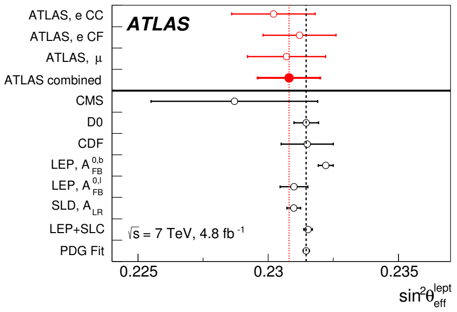


Figure 3.3: Measurements of the effective weak mixing angle.

3.2.2 Higgs boson physics

Since the start of data taking the groups of Profs. Jakobs and Schumacher have contributed significantly to the searches for the Higgs boson of the SM and for Higgs bosons in its supersymmetric extension (MSSM) in various decay modes and to the discovery of a Higgs boson in July 2012 in particular via the search for the decay $H \to WW$ (Group Jakobs). After this milestone discovery the most important question is, whether electroweak symmetry breaking proceeds as predicted by the SM or whether an extended Higgs sector is realised in nature. In order to answer this question several routes can be taken: (a) precise investigation of the observed Higgs boson with a mass of 125 GeV in order to find deviations in production cross sections or decay branching ratios predicted by the SM model; (b) search for violation of symmetries conserved in the SM, additional coupling structures in the context of Effective Field Theories (EFT) and exotic decay modes forbidden in the SM; and (c) search for additional heavy Higgs bosons predicted in many extensions of the SM e.g. the MSSM.

As the Higgs boson was discovered via bosonic decay modes $H \to \gamma\gamma, \to WW \to \ell\nu\ell\nu, \to ZZ \to 4\ell$ an important step was to establish evidence for the major fermioninc decay modes $H \to \tau\tau$ and $H \to bb$.

Investigation of SM decay modes

$H \to \tau\tau$ (Jakobs and Schumacher)

The final analysis of the Run 1 data collected in 2011 and 2012 at center-of-mass energies of 7 and 8 Tev with leading contributions from the Freiburg groups used multivariate techniques and yielded evidence for the decay into a pair of tau leptons (4.5 standard deviations, see Fig. 3.4) and determined the production rate to be consistent with the SM prediction $\mu = \sigma/\sigma_{SM} = 1.43^{+0.43}_{-0.37}$ [schumach4]. The analyses using data collected in 2015/16 at $\sqrt{s}$ = 13 TeV is ongoing and aims to yield observation and more precise determination of the tau lepton Yukawa coupling. The Freiburg team is responsible for the optimisation of the event selection using multivariate techniques in the $\tau_{lep}\tau_{lep}$ and $\tau_{lep}\tau_{had}$ decays, for the estimation of the major background from $Z + jet$ production and from jets misidentified as leptons or hadronically decaying tau leptons. The statistical interpretation and combination of the findings and the evaluation of theory uncertainties is conducted by members from our groups. Results are expected to be published until summer 2018. Studies how to measure differential and fiducial cross sections, which allow setting limits on the parameters in EFT have started.

$H \to b\bar{b}$ (Jakobs)

The observation of this decay is of particular importance as it yields the dominant contribution to the total width. The search utilises the associated production with a weak gauge boson and its subsequent leptonic decay W/ZH with $W \to \ell\nu, Z \to \ell\ell\ (\ell = e, \mu)$

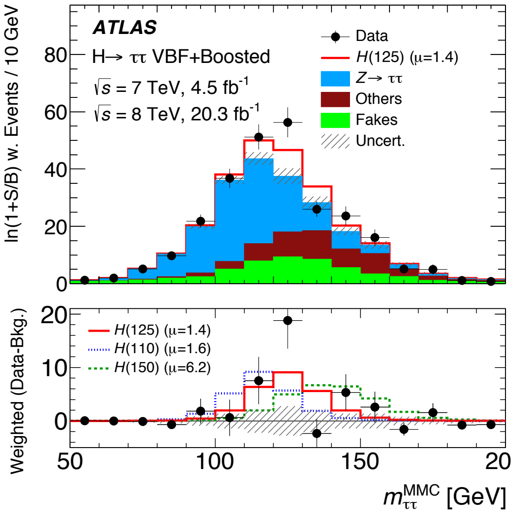


Figure 3.4: The invariant di-tau-mass distribution in the $H \rightarrow \tau\tau$ search for events selected in Run 1 data.

and $Z \rightarrow \nu\bar{\nu}$. Our group has a long-standing experience in these channels.Our contributions include the estimation of systematic uncertainties for the dominant background processes from $W+Jet$- and $t\bar{t}$ production. The combination of the Run 1 results with the findings based on 2015/16 data yields evidence for the decay with a significance of 3.6 standard deviations and a measurement of the production rate of $\mu = \sigma/\sigma_{SM} = 0.90 \pm 0.18(\text{stat.})^{+0.21}_{-0.19}(\text{syst.})$ consistent with the SM prediction [jak8]. The invariant mass of the identified b-jets in selected Run 2 events is shown in Fig. 3.5 after subtraction all background except those from di-boson production.

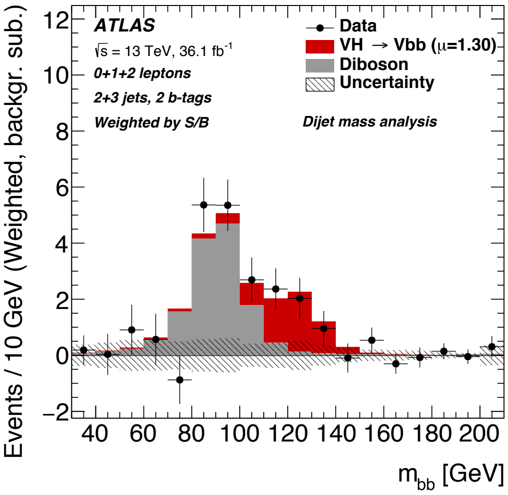


Figure 3.5: The invariant di-b-jet-mass distribution in the$H \rightarrow b\bar{b}$ search after subtracting all backgrounds except from di-boson production.

$H \rightarrow WW$ (Jakobs)

The analysis of the $H \rightarrow WW$ decay was continued with Run 2 data at $\sqrt{s}$ = 13 TeV for both gluon fusion and vector boson fusion production. The selection was optimized and the determination of dominant background processes was performed. The group also contributed to the statistical interpretation of the results. Preliminary results based on 2015 data collected until spring 2016 were published showing no deviation from the SM. The production rates normalized to the SM prediction in vector boson fusion and VH production were determined to be $\mu_{VBF} = 1.7+1.1-0.9$ and $\mu_{VH} = 3.2+4.4-4.2$, respectively. It is expected that final results based on the full 2015/16 data including the gluon fusion production mode set will be published in spring 2018.

Parameter estimation in SM and EFT

The results of all investigated decay channels including our contributions described above were combined to extract in a global fit the coupling modifiers κ with respect to the SM prediction. The combined results from ATLAS and CMS Run 1 data are shown in Fig. 3.6 [schumach7]. The measurements agree with the SM prediction and show the expected scaling of the coupling to the different particles with their mass.

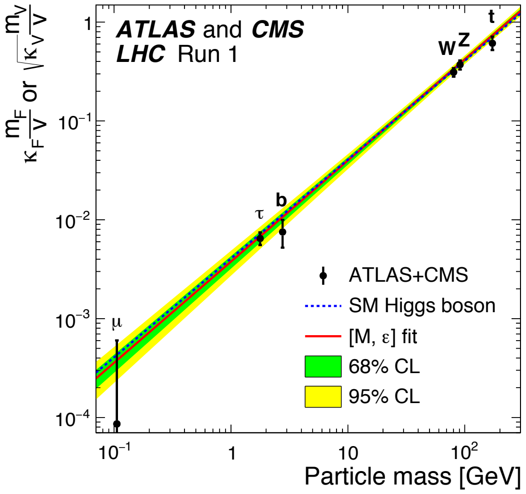


Figure 3.6: The measured leading order scaled coupling modifiers of the Higgs boson to other particles as a function of the particle's mass from a combined fit to ATLAS and CMS Run 1 data.

The Jakobs group was also involved in the first combination of measurements of differential cross sections from $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ \rightarrow 4\ell$ decays with 2015/16 data.

Both groups contributed to the modelling of signal prediction in EFT via the development of novel morphing and reweighting techniques.

Search for violation of symmetries (Schumacher)

Searches for the violation of CP-invariance in Higgs boson production and for lepton flavour violating (LFV) Higgs boson decays have been performed based on 8 TeV data.

CP-violation is a necessary ingredient to explain the observed baryon asymmetry of the universe. The magnitude of the observed CP-violation parametrised by the CKM-matrix however is to small to yield the observed asymmetry. The first test of CP-invariance in Higgs boson production has been performed by our group. The method of the Optimal Observable was developed and applied to the 8 TeV data set utilizing the $H \to \tau\tau$ decay mode. The complete analysis from event selection to statistical interpretation was conducted in Freiburg. No hints for new CP-violation were observed and most stringent limits on a CP-violating parameter in the context of an EFT were derived, which are tighter by a factor of five than the bounds obtained from $H \to WW/ZZ$ [schumach8].

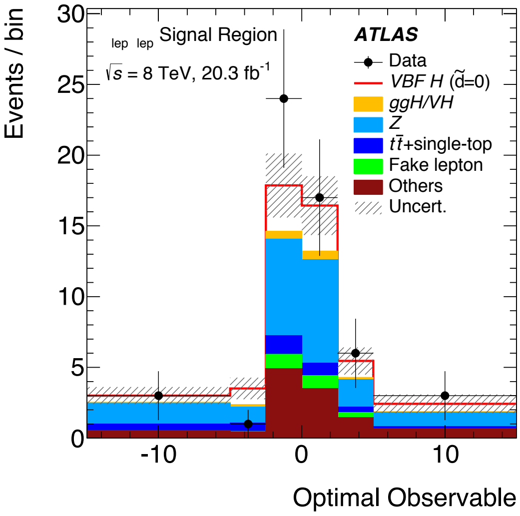


Figure 3.7: Distribution of the optimal CP-odd observable in selected events in the $H \to \tau_{lep}\tau_{lep}$ channel. CP-violation would manifest itself in an asymmetric distribution and non vanishing mean value.

LFV was observed in the form of neutrino-oscillations in the neutral lepton sector. LFV in the charged lepton sector is predicted in many extensions of the SM (e.g. supersymmetric one, Two-Higgs-Doublet Models etc.) and can be searched for e.g. in Higgs boson decays. We contributed to the search for $H \to \tau e$ and $H \to \tau\mu$ in the $e\mu 2\nu$ final state via the development of multivariate selection and new mass reconstruction techniques. The special characteristic of the analysis is the completely data-driven approach for estimating all background contributions. No hints for LFV have been observed and limits on the branching ratios of approximately 1% were extracted, improving indirectly obtained limits by almost one order of magnitude [schumach9].

Search for additional Higgs bosons (Jakobs)

The increased center of mass energy of the LHC in Run 2 extends the mass reach in the search for additional Higgs bosons and other resonances. Several searches have been performed in the group of Prof. Jakobs.

In the $WW \to \ell\nu\ell\nu$ final state searches have been performed in the mass range from 200 GeV to 2 TeV yielding no significant deviation from the Standard model expectation. Limits on production cross-section times branching ratio have been derived for various assumption in the total width and the results have been interpreted in various models e.g. a two-Higgs- doublet model, a heavy vector triplet model, a warped extra dimensions model, in the Georgi–Machacek model and a model with heavy tensor particle coupling only to gauge bosons. The results based on data collected in 2015 and 2016 have been published recently.

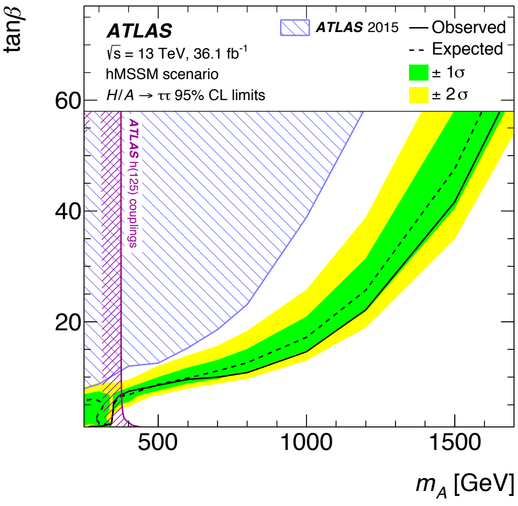


Figure 3.8: Excluded parameter space in the $\tan\beta - vs - M_A$-plance of the MSSM from the search for $H \to \tau\tau$.

A search for heavy neutral Higgs bosons of the Minimal Supersymmetric Model (MSSM) $H/A \to \tau\tau$ has been conducted in the mass range of 0.2 - 2.25 TeV. No hints for the production of additional Higgs bosons are observed in the data collected in 2015 and 2016 and limits on cross-section times branching ratio and on the parameter space of the MSSM in several benchmark scenarios were derived as shown in Fig. 3.8.

The ZH final states with decays $Z \to l^+l^-, \nu\bar{\nu}$ and $h \to bb$ has been untilised to search for a heavy pseudoscalar Higgs boson A via $A \to ZH$ and for heavy gauge bosons via $W'/Z' \to W/Zh$. In order to cover a wide mass range the analyses have been split up in two topologies where the b-jets were either reconstructed as two separate jets or as one broad jet The Freiburg group was leading the analyses in the 2 lepton channel ($A \to ZH$, $Z \to \ell\ell$) and statistical interpretation and contributed to the $W \to \ell\nu$ analysis. The data collected in 2015 and 2016 show no compelling excess and hence new limits in Two-Higgs-Doublett-Modells and a Heavy-Vector-Triplet-Modells were derived and published.

The groups plan to continue the above activities and to itensify the research in the measurement of differential and fiducial cross sections and their interpretation in the framework of EFT and pseudo-observables.

3.2.3 Search for new Particles

With the discovery of the Higgs Boson the last missing particle of the Standard Model has been found. This success has transformed the research in particle physics into a new era, because there is no clear theoretical guidance anymore which experiments might have the highest potential to discover new laws of nature, new particles and new effects. Although many theoretical models exist to describe known facts like neutrino masses or dark matter, an experimental hint is still lacking to single out classes of models which have higher chances to describe nature than others. Experiments at the LHC have a high potential to provide such experimental hints, because they allow experiments with proton-proton collisions of the highest man-made center of mass energies and at the same time, especially after the luminosity upgrade, with unprecedented collision rates. New high-mass particles could be produced, processes with small cross-sections could be observed or small deviations from Standard Model prediction could point to new effects.

Besides the study of the mechanism for electroweak symmetry breaking, a second focus in the data analysis with the ATLAS experiment is therefore the search for new particles with an emphasis on supersymmetric particles (groups of G. Herten and K. Jakobs). Supersymmetry (SUSY) is a promising extension of the Standard Model, which tries to resolve the hierarchy problem by introducing supersymmetric partners (e.g. $\tilde{\chi}_1^0$, $\tilde{g}$, $\tilde{q}$, $\tilde{b}$, $\tilde{t}$) of the known bosons and fermions and which can provide a natural particle candidate for dark matter in the universe. The predicted mass range for the new particles coincides with the energy reach of the LHC and therefore searches for supersymmetric partners are among the important goals of the LHC experiments. SUSY theories contain a large number of free parameters, which result into a wide spectrum of possible mass combinations. The implication for experiments at the LHC is to perform searches which are sensitive to many different parameter choices. Supersymmetry has such a rich phenomenological spectrum of different final states that these experimental searches test at the same time many other theories beyond the Standard Model.

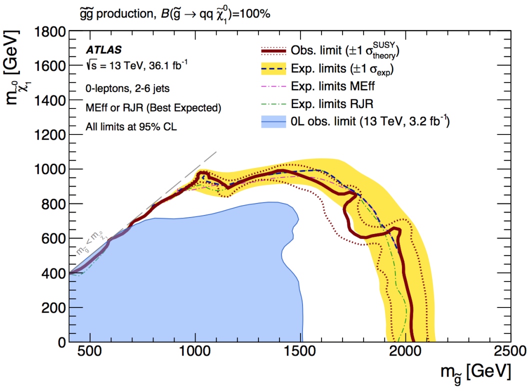


Figure 3.9: Exclusion limits for direct production of gluino pairs ($\tilde{g}$) with a direct decay into two light flavoured quarks and a neutralino ($\tilde{\chi}_1^0$).

In Freiburg we concentrate our research on searches for gluinos ($\tilde{g}$) and 1^{st}- and 2^{nd}-generation squarks $\tilde{q}$ as well as specific searches for 3^{rd}-generation sbottom and stop quarks ($\tilde{b}$, $\tilde{t}$). These searches are motivated by the fact that cross-sections for pair-production of these particles are large at the LHC and that models like natural SUSY prefer light stop and gluino masses, which could be accessible at the LHC.

The first strategy uses inclusive searches based on a generic signature with leptons, jets and missing transverse momentum, which is expected due to the escaping lightest neutralino $\tilde{\chi}_1^0$ (the dark matter candidate). This strategy offers the best sensitivity for a wide spectrum of SUSY models, especially for the search of gluinos and squarks of the 1^{st}- and 2^{nd}- generation, which are copiously produced at the LHC via the strong interaction. Because of the large cross sections, masses in the TeV range and above can be explored. The Freiburg group made important contributions over many years to the analyses of events with jets and missing transverse energy [[hert10], [hert7]] and with additionally two leptons with the same electric charge [[hert9],[hert5],[hert1]]. The challenge in all analyses is to optimise the detection efficiencies for new particle production and to reject the corresponding background from Standard Model processes. Most background contributions, especially those involving many jets, have to be determined directly from data using control regions. So far, no significant excess of events has been observed compared to the Standard Model expectation. Therefore the measurements are expressed as 95% confidence level (CL) exclusion contours.

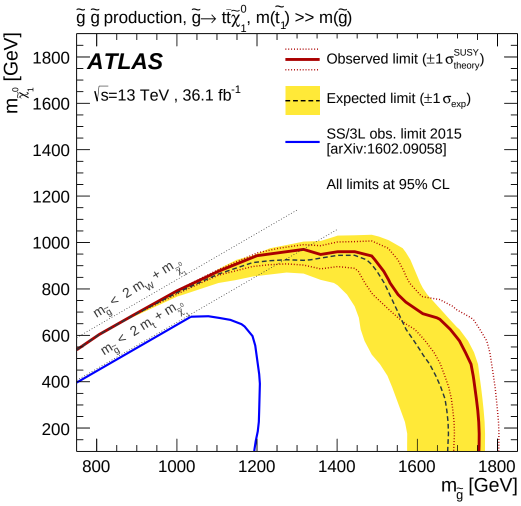


Figure 3.10: Observed and expected exclusion limits on the $\tilde{g}$ and $\tilde{\chi}_1^0$ masses for a model with gluino decays via a virtual stop.

As an example, Fig. 3.9 shows the published ATLAS result for the event category with jets and missing transverse momentum [[hert10]] based on data corresponding to an integrated luminosity of 36.1 fb^{-1} collected at a centre-of-mass energy of 13 TeV. The red line shows the 95% exclusion limit in the $(m_{\tilde{g}},\ m_{\tilde{\chi}_1^0})$- mass plane. In the model considered, gluino masses up to 2000 GeV and neutralino masses up to 950 GeV, respectively, are excluded. This analysis alone excludes many SUSY models, which have been proposed before the start of the LHC. A complementary analysis uses final stated with two leptons of the same electric charge (same-sign leptons) or three leptons. The advantage of this analysis is that the Standard Model background is very small and that it provides sensitivity in so called compressed mass regions (small mass differences between SUSY particles) and processes with small cross-sections, e.g. electro-weak production of SUSY particles. Fig. 3.10 shows as example the limits in a simplified SUSY model where gluinos decay via a heavy, virtual stop quark leading to same-sign leptons of three leptons in the final state [[hert9]]. The same final state can be used to obtain limits in a model where the gluinos decay via heavy charginos and neutralinos, see Fig. 3.11.

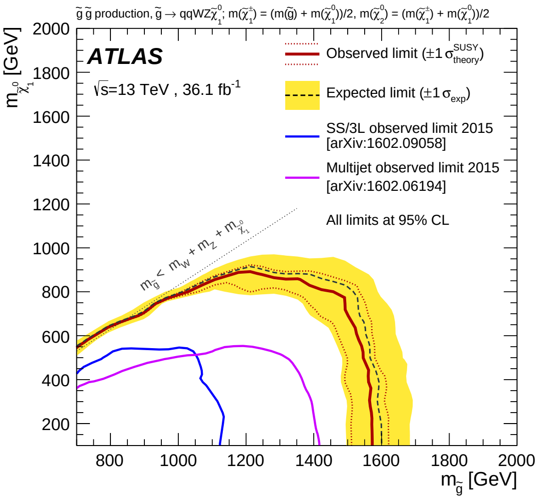


Figure 3.11: Observed and expected exclusion limits on the $\tilde{g}$ and $\tilde{\chi}_1^0$ masses for a model with gluino decays via virtual chargino and neutralino.

With stringent constraints on the masses of first and second generation squarks and gluinos, as well as considerations of squark mixing and the stability of the Higgs mass, a strong focus is put on searches for direct production of third generation squarks. Production cross sections are typically more than one order of magnitude smaller than for e.g. gluino production, but the presence of bottom quarks in the final state allows additional suppression of backgrounds, where specific Freiburg expertise in b-tagging is utilized. Results based on the full data of LHC Run-1 have been published in 2015, including a summary of all ATLAS SUSY searches reinterpreted in the context of the phenomenological minimal supersymmetric Standard Model[jak5].

Depending on the mass spectrum of SUSY particles a large number of final states has to be considered, with Freiburg contributing significantly to the ATLAS searches in fully hadronic final states as well as final states with one charged lepton. As an example a summary of recent results for one class of scenarios is shown in Fig. 3.12. For light neutralinos, top squarks with masses lower than 960 GeV are excluded in the context of the simplified models used.

Results with the full data sets of 2015 and 2016, corresponding to an integrated luminosity of 36 fb^{-1} at a centre-of-mass energy of 13 TeV, have been

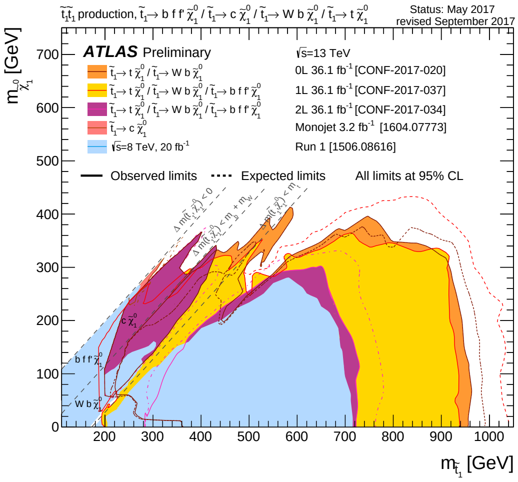


Figure 3.12: Constraints on the masses of top squarks and neutralinos in simplified models by the ATLAS experiment. Freiburg contributed significantly to the orange and yellow contours, which amount to the majority of the new phase space covered since Run-1 results (light blue).

published in September 2017 for fully hadronic final states [jak5] and in November 2017 for one electron or muon in the final state. In addition to simplified models, both publications include interpretations in new classes of SUSY models motivated by up to date phenomenological constraints, e.g. the Dark Matter density from cosmological models. The analysis in the 1-lepton final state also includes an interpretation of results in the context of generic models of Dark Matter. A dedicated search for the case of tau leptons in the final state has made first results with Run-2 data public in summer 2016, with a journal publication planned for early 2018.

The current SUSY activities in Freiburg and in the ATLAS collaboration in general concentrate on further improving selection and reconstruction algorithms, aiming at a publication of final Run-2 results for the above mentioned analyses in 2019. Together with this optimization of techniques the increase in integrated luminosity from 36 fb$^{-}1$ to an estimated 120 fb$^{-}1$ is expected to increase the sensitivity to physics beyond the Standard Model significantly beyond current results. In addition model studies and scans are ongoing to identify scenarios which might not be sufficiently covered by current analyses.

3.2.4 Detector performance

The Freiburg groups have contributed in many aspects to the so-called *Combined Performance Groups* in ATLAS, dealing with the reconstruction and identification of basic detector signatures which are essential for any physics analysis performed in ATLAS. Our focus was on the development and calibration of algorithms for the reconstruction and identification of physics objects like electrons, muons, τ leptons, b-quark jets. These activities have lead to several publications. In addition, we have been active in the area of software development. The major contributions are briefly summarized in the following:

Reconstruction and identification of electrons: The so-called *tag-and-probe* method for very clean $Z \rightarrow e^+e^-$ and $W \rightarrow e\nu$ events has been used to measure the reconstruction and identification efficiencies for electrons. The probabilities to assign the wrong charge to electrons have also been determined, because this constitutes an important background component for analyses with multiple electrons with the same charge in the final state.

Reconstruction and identification of τ leptons: The efficiencies to reconstruct and identify hadronically decaying τ leptons have been determined using a tag-and-probe method for $Z \rightarrow \tau^+\tau^-$ events. The topology of $t\bar{t}$ events has been exploited to measure the efficiencies at the level of the trigger, being responsible for an efficient recording of events with τ leptons in the final state. The so-called *embedding* method has been used to extrapolate kinematic properties of well reconstructable $Z \rightarrow \mu^+\mu^-$ to $Z \rightarrow \tau^+\tau^-$ events in the $H \rightarrow \tau^+\tau^-$ analysis.

Identification of b-quark jets: Our group has made numerous contributions to the identification of b-quark jets, called *b-tagging*, e.g. the development of highly performant b-tagging algorithms, the measurement of their identification efficiencies using novel methods and event topologies, and the adaption and optimization of the algorithms for the Run 2 data taking period of the LHC.

Software development: We have developed central analysis software that is used by many analysis groups. Furthermore, we have been involved in the definition of the data formats for Run 2 of the LHC to ensure an efficient analysis of the increased data volume.

3.3 ATLAS Detector Development

The ATLAS groups (G. Herten and K. Jakobs) have made significant contributions to the construction of the ATLAS detector, mainly for the muon system and the silicon strip detector. In view of the planned luminosity upgrades at the LHC a number of detector components need to be replaced with higher performing sensors in order to cope with the increased particle rate. In the first step, the New Small Wheel (NSW) muon detector will be installed during the long shutdown in 2019-2020. Presently a major production effort is ongoing in Freiburg to construct these components. In parallel, a large-scale R&D activity and intensive prototyping is underway in the silicon detector domain to develop an entirely new silicon strip detector system for the High Luminosity LHC upgrade which is planned in 2024.

3.3.1 Semiconductor Particle Detectors

Silicon detectors have by now become the gold standard technology at the center of virtually all major particle physics detector systems. The development has started from compact detectors, with an ongoing evolution that has lead to ever larger, faster and more complex silicon detector systems. In addition, the conditions have become far more stringent, including harsh radiation environments, and strict requirements on low-mass, robustness and cost.

The group of K. Jakobs has fifteen years' experience in the development and production of silicon particle detectors and associated fast and radiation-tolerant readout electronics. Significant contributions were made to the construction of the current ATLAS silicon strip system, and continue into the provision of ongoing expert support for it, both during data-taking and maintenance periods.

Based on the vast silicon experience, the group is now concentrating its efforts on R&D into silicon strip sensors for extreme radiation environments, including studies on 6-inch and 8-inch sized sensors and prototyping for the LHC High-Luminosity upgrade [jak9]. In the R&D domain, we are working on detectors in a 3D-configuration, where read-out electrodes are placed orthogonal to the silicon surface and facilitate the collection of signal charges after heavy irradiation. Another R&D topic are novel silicon sensors where the wafers were enriched with Nitrogen. These *Nitrostrip* sensors, manufactured and evaluated in the framework of the CERN RD50 collaboration, are compared to sensors realized in several standard technologies in various stages of irradiation.

In the last two years, the prototyping work centered around construction of realistic front-end electronic boards and modules, assembled in our clean-rooms from front-end electronics and sensors [jak10]. In 2018, this will evolve into production of pre-series modules in preparation for a larger-scale series production of around 1000 modules. These modules will then be in-house integrated into larger-scale structures, which in turn will be installed in the ATLAS experiment. In Figure 3.13, the first full-size ATLAS End-Cap module, using a 6-inch Hamamatsu sensor co-developed here and front-end electronic boards designed and populated in our electronics workshop, and successfully evaluated in a beam test at DESY Hamburg, is shown.

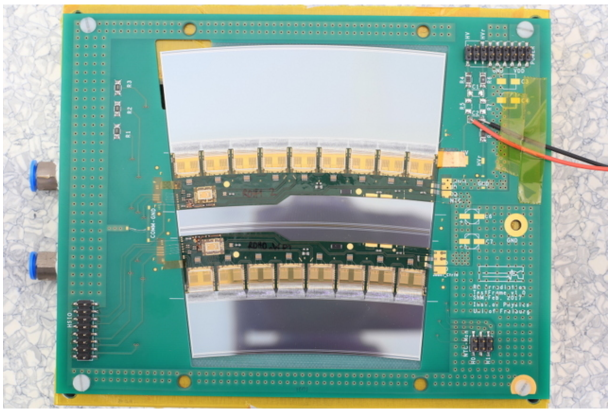


Figure 3.13: The first full-size ATLAS End-Cap module, built in our clean-rooms from components designed, co-developed and produced in Freiburg.

In a separate R&D effort that is performed as part of a long-standing cooperation with the Freiburg Materials Research Center *Freiburger Materialforschungszentrum* (FMF), we are investigating high-Z semiconductor detectors made from among others Cadmium-Zink-Telluride (CZT). Our CZT-detectors are successfully employed to convert and detect high-energy photons in gamma photography, computer tomography or radiation-monitoring applications.

3.3.2 Muon Detectors

In the second long-shutdown (LS2) of LHC in 2019-2020, the ATLAS collaboration intends to improved the forward muon system with the aim to achieve the same muon trigger and reconstruction performance as today but with a luminosity in the range of $2-3\times10^{34}$ cm^{-2}s^{-1}. The plan is to replace the current Muon Small-Wheel with a New Small Wheel (NSW), using improved detectors for precision tracking and momentum measurement and dedicated trigger detectors. The Freiburg ATLAS muon group is strongly involved in several areas of this effort: Stephanie Zimmermann is the project leader of the NSW project; new Micromegas (MM) detectors are developed in Freiburg; MM chamber construction in Germany is in preparation in collaboration with the Universities of Mainz, München and Würzburg; alignment bars for the overall alignment of the NSW with respect to the rest of the muon system will be constructed and calibrated in Freiburg; the detector control system (DCS) will be improved and the NSW will be integrated.

Micromegas (an abbreviation for micro mesh gaseous structure) detectors have been used since the mid 1990's, for example in the COMPASS experiment. The development effort in ATLAS has lead to a significant improvement in the spark protection by adding a layer of resistive strips on top of a thin insulator directly above the readout electrode. The readout electrode is no longer directly exposed to the charge created in the amplification region, instead the signals are capacitively coupled to it. By adding this protection some fraction of the signal height is lost, but the chamber can be operated at higher gas gain and thus have spark intensities reduced by about three orders of magnitude. The required position resolution below 100 μm has been achieved in test beams with large chambers. The present effort is fully concentrated on producing the chambers, testing their performance in test beams, to assemble the wheels and install them into the ATLAS cavern in the 2019-2020 shutdown. Fig. 3.14 shows the prototype of an SM2 module producced in Germany, being tested at CERN.

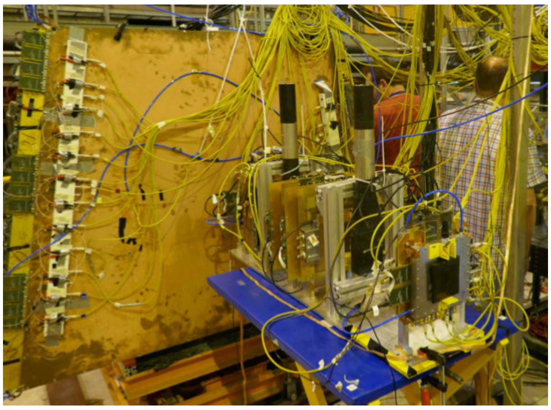


Figure 3.14: Performance test of a prototype of the SM2 MicroMegas chamber in a test beam at CERN.

3.4 Astroparticle Physics

A new experimental astroparticle physics group was established in fall 2016, with the move of Prof. Marc Schumann to Freiburg. The group's research focus is on the direct detection of particle dark matter using ultra-sensitive low-background experiments. There is plenty of indirect evidence that the vast majority of the energy density in the Universe is dark. About 25% of the energy density, outnumbering ordinary matter by a factor 5, is due to dark matter, a yet undetected form of matter which is responsible for the creation of large-scale structures in the Universe.

The main activity of the group is the search for dark matter in the form of weakly interacting massive particles (WIMPs), as predicted by various theories beyond the Standard Model, e.g., supersymmetry (SUSY). WIMPs could be produced thermally in the early Universe following the big bang. To achive the required exposure to find the elusive WIMP, massive detectors filled with ultra-pure liquid xenon (LXe) are used for the search. These instruments are built and operated within the international XENON and DARWIN collaborations and provide sensitivities complementary to WIMP searches at LHC. The group is also involved in the search for axions and other exotic particles with the CAST experiment at CERN. Axions are alternative dark matter particles to the WIMP and are mainly motivated by the strong CP-problem.

3.4.1 The XENON Programme

The XENON collaboration designs, builds and operates massive detectors to search for WIMPs. These detectors are installed in the Italian Gran Sasso underground laboratory (LNGS) and are based on the principle of a liquid xenon-filled dual-phase time projection chamber (TPC). Xenon is an excellent scintillator: the scintillation light from a particle interaction in the TPC is recorded together with the ionization signal (which is converted to proportional scintillation light in the xenon gas phase above the liquid target) by means of sensitive photomultipliers. The combination of both signals allows the reconstruction of the event vertex, multiplicity, energy and the nature of the incident particle: WIMPs (and neutrons) are expected to interact with the xenon nucleus (inducing nuclear recoils), while the overabundant backgrounds from β- and γ-radiation interact primarily with the atomic electrons (electronic recoils).

The largest and most sensitive dark matter detector to-date is XENON1T (see Fig. 3.15), which is acquiring high-quality science data at LNGS since fall 2016. The design, construction and assembly of the inner TPC was coordinated and organized by members of the Freiburg group. The group is also responsible for the readout of the 248 photomultipliers recording the light and charge signals: a virtually trigger-less, asynchronous data acquisition (DAQ) system was developed to achieve the lowest possible trigger threshold and is continuously maintained by Freiburg. In dark matter mode, the system records about 500 GB/day at zero deadtime. The data bandwidth can be scaled by increasing the level of parallelization of the system.

Figure 3.15: Construction of the XENON1T TPC.

A first dark matter search using 34.2 live days of data showed no excess above the expected background and led to the most stringent exclusion limit on spin-independent WIMP-nucleon scattering cross sections σ_{si} above WIMP masses $m_\chi > 10\,\text{GeV}/c^2$, see Fig. 3.16. The electronic recoil background level of $1.9(3) \times 10^{-4}$ events/(kg×day×keV) is the lowest ever achieved in a dark matter detector [schumann10]. The Freiburg group led the detector performance team for this analysis. The second science run is still ongoing as of today. A researcher from Freiburg serves as analysis coordinator for this run, coordinating a total of more than 50 scientists from all participating XENON institutions. The main Freiburg contributions are data quality and the modelling of anomalous background contributions.

XENON1T will explore cross sections $\sigma_{si} < 2 \times 10^{-47}\,\text{cm}^2$ at $m_\chi \sim 40\,\text{GeV}/c^2$ with an exposure of $2\,\text{t} \times \text{y}$. The next instrument of the XENON program, XENONnT, will feature a larger LXe target mass of 6.0 t, a factor 10 lower background (mainly due to a reduction of ^{222}Rn) and is expected to increase the WIMP sensitivity by a factor 10 with respect to XENON1T [schumann3]. The new instrument is currently being designed and constructed: Freiburg is contributing the DAQ system, which will be based on the one developed for XENON1T, but extended to read out about twice the number of channels. The group is also heavily involved in the design of the TPC, contributing to the overall coordination of the project, Geant4-based Monte Carlo simulations to estimate backgrounds from construction materials, and to the material selection using the group's spectrometer GeMSE [schumann4]. Some TPC components will be machined in Freiburg. A first science run with XENONnT is planned to start by mid 2019.

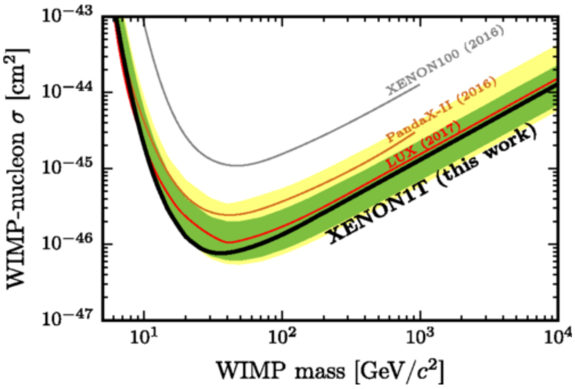


Figure 3.16: First result of the XENON1T experiment on spin-independent WIMP-nucleon scattering cross sections.

XENON100, the predecessor to XENON1T with a target mass of 62 kg, could rule out the DAMA/Libra modulation signal as being due to electronic recoils based on a dataset acquired over four years [schumann7]. In addition, the Freiburg group presented the world's first search for signals from magnetic inelastic dark matter was published. This model predicts a unique delayed coincidence signature from WIMPs inelastically scattering off Xenon nuclei. This allows for a virtually background-free search region. No event was observed and the best-fit points to explain the DAMA/Libra claim are excluded by by 3.3σ and 9.3σ [schumann8].

3.4.2 DARWIN: The ultimate Detector

The experimentally accessible space for WIMP-nucleon interactions will eventually be limited by irreducible backgrounds induced by coherent neutrino-nucleus scattering (CNNS) processes. These will produce single-scatter nuclear recoils which are indistringuishable from WIMP signals. At low m_χ, solar ^{8}B neutrinos dominate the CNNS signals while while atmospheric neutrinos take over for larger masses, see dashed line in Fig. 3.17. The DARWIN collaboration aims at realizing the ultimate detector, capable to explore the parameter space down to the neutrino floor [schumann5]. Members of the Freiburg group have shown that a dual-phase LXe TPC with a target mass of 40 t and a 100 times reduced background compared to current standards is necessary to achieve this goal [schumann1].

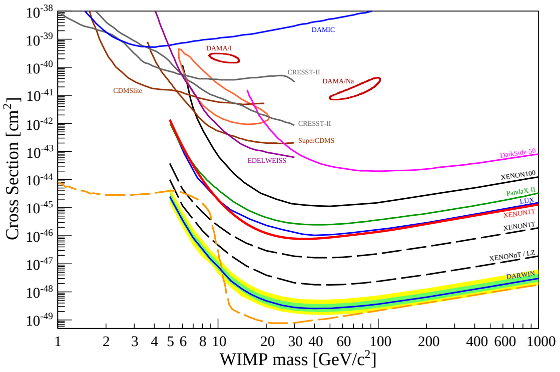


Figure 3.17: The expected sensitivity of the DARWIN detector will cover the entire experimentally accessible parameter space, which will eventually be limited by coherent neutrino-nucleus interactions (dashed orange line).

With linear dimensions of $\sim$2.6 m, this detector will be considerably larger compared to current instruments. At this point, it is also unclear how the required background level can be achieved. These questions are studied in Freiburg within the ERC-funded project ULTIMATE, mainly focusing on the (currently dominating) background from daughters of the noble gas ^{222}Rn, which is constantly emanated from all detector surfaces, and on (α,n)-induced neutrons from the detector materials. R&D on these topics, as well as on alternative ways to generate the charge signal in very large TPCs and on the mechanical challenged to build TPCs with a diameter of 2.6 m, is being pursued on a small-scale LXe detector platform in the laboratory in Freiburg. This platform allows the study of selected aspects and prototypes. A new platform with significantly larger dimensions is currently being planned to extend the studies to the scale relevant for DARWIN.

The group's low-background HPGe spectrometer GeMSE, operated in the Vue-des-Alpes underground laboratory in the Swiss Jura mountains, is used to identify materials with a very low intrinsic radioactive background [schumann4]. GeMSE consists of a 2 kg HPGe crystal in a low-background shielding, featuring a background of <250 events/day above 100 keV. Information on materials feeds directly into Monte Carlo-based sensitivity studies: the low-background, low-threshold detector DARWIN is not only sensitive to WIMP dark matter, but also to low-energy solar neutrinos (pp, ^{7}Be), CNNS, supernova neutrinos, axions and axion-like particles and other rare nuclear processes, the most prominent being the neutrino-less double beta-decay of ^{136}Xe, which has a high natural abundance of 8.9% in natural xenon [schumann5].

3.4.3 CAST: Searching for Axions

The CAST (CERN Axion Solar Telescope) experiment uses a LHC test magnet to search for axions which might constantly be emitted from the Sun. In certain ranges of the parameter space, these particles could solve the strong CP-problem and also make up the dark matter density. They would be converted to detectable X-ray photons via the Primakoff-effect in the 9 T field of the magnet. While the Freiburg group made large contributions in the initial phase of the experiment, due to the lack of funding, the involvement in the past years was reduced to data analysis and to the search for Chamaeleons in the KWISP setup. Nevertheless, Freiburg remains an important active player in the project.

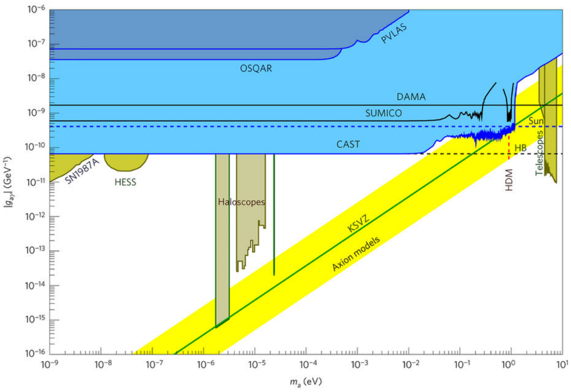


Figure 3.18: The exclusion limit from the CAST experiment searching for solar axions cover a large fraction of the parameter space and reaches into the QCD-axion region.

The latest CAST results in the search for solar axions are shown in Fig. 3.18: no excess of events have been observed while tracking the Sun with the magnet and a world leading limit of $g_{a\gamma} < 0.66 \times 10^{-10}$ GeV^{-1} (95% C.L.) on the axion-photon coupling was obtained for masses $m_a \lesssim 0.02$ eV [schumann9]. The Sun tracking capabilities of the experiment allow the search for other new particles as well, even without using the magnet for axion-photon conversion. Chamaeleons are posulated spin-0 particles which couple to matter weaker than gravity. Such particles are expected to have an effective mass which depends on the local energy density. The KWISP setup at CAST aims at detecting Chamaeleons emitted from the Sun with a ultra-sensitive opto-mechanical force sensor; the constant Chamaeleon flux is being time-modulated my means of a mechanical chopper. Members of the Freiburg group are heavily involved in this experiment. They also study whether gravitational lensing effects of solar system bodies could enhance a signal from a stream of dark matter axions.

3.5 COMPASS

COMPASS-II at CERN's SPS (Super Proton Synchrotron) tests chiral perturbation theory, measures transverse-momentum-dependent parton distributions in polarized Drell-Yan reactions and determines generalised parton distributions (GPD) in the exclusive processes of deeply virtual Compton scattering (DVCS) and hard exclusive meson production (HEMP). Semi-inclusive deep inelastic scattering, which allows for extractions of quark and gluon helicity structure functions, complements the COMPASS-II physics programme. Understanding the hadron structure is interesting per se and also indispensable for exploring the limits of the Standard Model: the overall precision of LHC measurements depends on the precise knowledge of parton distribution functions.

The Freiburg group focuses on exclusive measurements with naturally polarized muon beams to resolve the transverse structure of the nucleon. Muons of 160 GeV/c scatter off a liquid hydrogen target, which is surrounded by a target time of flight (tToF) system and an open field two-stage spectrometer, to detect and identify charged and neutral particles.

Deeply virtual Compton scattering, $\gamma^* p \to \gamma p$, is the production of a single real photon γ through the absorption of a virtual photon γ^* by a proton p whereas in HEMP processes the final state photon is replaced by a π^0 or heavier meson. Both, DVCS and HEMP, combine features of the elastic process and such of the inelastic processes. In a certain kinematic domain DVCS allows access to correlations between transverse-position and longitudinal-momentum distributions of the partons in the proton, where longitudinal and transverse refer to the direction of motion of the initial proton facing the virtual photon. Therefore, measurements of DVCS provides information on the momentum dissected 3D-structure of the proton by probing the transverse extension of the parton density in the experimentally accessible region of longitudinal parton momentum.

The sum of the pure DVCS cross sections obtained by measurements with μ^+ and μ^- beams of opposite respective polarizations can be studied as a function of the four-momentum transfer between the initial and the final state proton. The slope B of the $|t|$-dependence can be converted into an average transverse size of the proton, $\sqrt{\langle r_\perp^2 \rangle} = (0.60 \pm 0.04_{\text{stat}} \,{}^{+\,0.01}_{-\,0.02}|_{\text{sys}})$ fm. For this measurement, the average virtuality of the photon mediating the interaction is $\langle Q^2 \rangle = 1.8\,(\text{GeV/c})^2$. The average value of the Bjorken variable is $\langle x_{Bj} \rangle = 0.056$, i.e.,in a kinematic region that probes ranges between the low-x_{Bj} domain dominated by gluons and the valence-quark domain of $x_{Bj} \geq 0.1$.

Fig. 3.19 shows a compilation of all existing results on the slope B of the differential DVCS cross section, or equivalently on the average transverse proton size $\langle r_\perp^2 \rangle$. The results of the HERA experiments (H1, ZEUS) were obtained at higher virtuality compared to the COMPASS-II measurement and need for rigorous interpretation evolution in Q^2. The COMPASS-II measurement probes $\langle r_\perp^2 \rangle$ at $x_{Bj}/2 \approx 0.03$, i.e., in a region that is dominated by sea quarks, the HERA-measurements have probed it in the gluon-dominated region.

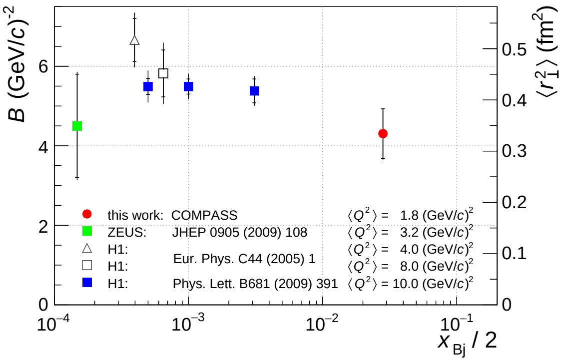


Figure 3.19: Measurements of the transverse size of the nucleon. The inner (outer) error bars illustrate the statistical (statistical+systematic) uncertainties.

Single exclusive π^0 production was also studied, extracting for the first time the total cross section and differential cross sections at large virtuality and small four-momentum transfer of the proton. Significant discrepancies to predicted cross sections were observed, emphasizing the importance of chiral-odd GPDs.

The main contributions of the Freiburg group are listed in the following: Development and construction of the readout and trigger system for the tToF system; Major contributions to the construction and commissioning of the tToF; Calibration of the tToF, data quality and detector performance studies; Development of a new detailed GEANT4 based description of COMPASS-II; Significant contributions to a new event generator for exclusive photon and meson final states; Key player in the reconstruction and analysis of exclusive reactions.

Two years of data taking have just been completed to conclude on a possible shrinkage of the proton in the transition region from sea to valence quarks. The analysis of these data will improve statistical and systematic uncertainties and allow for a conclusive answer.

3.6 Theory

The theory groups (S. Dittmaier, H. Ita and J. van der Bij) have directed special emphasis to particle phenomenology in collider experiments, such as the LHC, and to precision predictions required by the experiments. Furthermore, research of the group van der Bij also encompasses models of modified gravity and quantum gravity as well as their application to cosmology.

In the recent years the groups have made important contributions to the phenomenology of electroweak symmetry breaking, Higgs physics and the precision physics including electroweak gauge bosons. Furthermore, the groups have a strong expertise in formal research in perturbative quantum field theory and have contributed pioneering results in precision computations including the electroweak and the strong interactions.

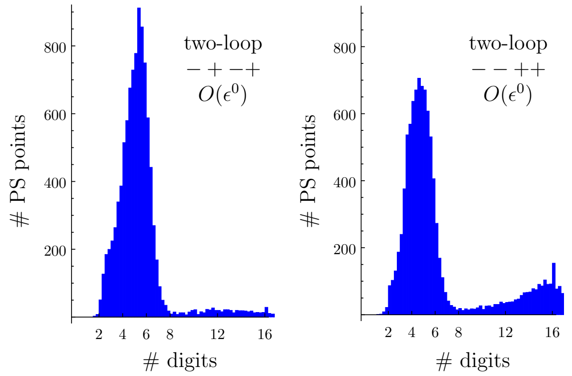


Figure 3.20: The numerical unitarity method yields precise numerical results for two-loop four-gluon process [ditt10] pointing towards an automatable approach for NNLO precision predictions in QCD. It is shown that results with more than two correct digits are correctly obtained when sampling phase-space (PS) points.

3.6.1 Concepts and Techniques in Perturbative Quantum Field Theory

The calculation of higher-order corrections in relativistic quantum field theory is notoriously complicated. Already the evaluation of the lowest orders in perturbation theory in predictions for particle scattering can become arbitrarily complicated if the numbers of produced particles increases in the final state. While full lowest-order (tree-level) predictions with up to 10 final-state particles are possible with modern, automated Monte Carlo generators since about 10 to 20 years, predictions at NLO (one-loop level) became possible in the last 5 to 10 years for the production of 4 to 7 particles in the final state. depending on the level of complexity of the process. The groups of Profs. Dittmaier and Ita contributed to this development—often called “NLO revolution”—in different ways.

Already on the practical side the problems appearing in NLO calculations to multi-particle production are manifold: In $2 \to 4$ particle reactions already some 10^3 complicated Feynman diagrams (full of singularities) occur, leading to an enormous algebraic effort to shape and structure the formulas to a form that is appropriate for numerical evaluation. For more external particles the number of Feynman diagrams explodes factorially. The numerical evaluation is not only challenging in view of speed, but also in view of numerical stability, since typically complicated, severe cancellations take place between many terms. Without extra work, evaluation in double precision arithmetic would not lead to sufficiently precise results in certain regions of phase space.

The group of Prof. Dittmaier refined and further advanced the more traditional Feynman-diagrammatic approach in various directions. The most notable achievements were the first pioneering NLO calculations with $2 \to 4$ complexity for e^+e^- colliders and hadron colliders in 2005 and 2009, respectively. Many NLO multi-leg calculations emerged from this line of research since then, some of them [ditt4, ditt6, ditt8, ditt10] discussed in the subsequent sections. Moreover, automated one-loop matrix-element generators, such as Madgraph5_aMC@NLO, OpenLoops and Recola, make use of or even rely on the methods that were worked out within the collaboration of the groups of S. Dittmaier and A. Denner at the Universities of Freiburg and Würzburg, respectively. Recently the mentioned groups have released of the numerical one-loop library Collier [ditt7], which calculates one-loop scalar and tensor integrals of nearly arbitrary complexity, including several regularization schemes for singularities and supporting complex internal masses, which is important for the description of unstable particles appearing as intermediate resonances. Collier is an integral part of the matrix-element generators mentioned above.

The group of JunProf. Ita contributed to establishing a new numerical approach for providing theory predictions for the LHC. The new approach relies on the unitary of quantum theory and factorisation properties of field theories. The recursive nature of the approach reduces complexity bottlenecks and yields stable numerical algorithms. The initial research to advance the called ‘unitarity method’ to a numerical approach for obtaining particle collider predictions was conducted in collaboration with groups at the University of California, Los Angeles, the SLAC National Accelerator Laboratory, IPhT-CEA Saclay and the IPPP Durham. In recent years the Freiburg group provided a number of cutting edge predictions for multi-particle processes [ita1] including multi-vector-boson final states [ita4] as well as for final states with massive particles most recently [ita10]. Furthermore, the group contributed to the field coordinating standards for program interfaces and setting up a n-tuple event-file format in order to make theory results broadly available to experimenters. The group remains a record holder with theory predictions for $2 \to 6$ particle processes including quantum corrections in QCD, thereby providing important standard-candle predictions for the LHC and future particle colliders [ita5].

In a second, formal line of research the group Ita has developed a new, automatable algorithm for computing multi-loop corrections in QCD [ita3, ita6] based on the established unitarity method. The numerical variant of the method has proven effective and reliable (see Figure 3.20) in a proof-of-principle computation of the four-gluon scattering process including second-order quantum corrections [ita7] and has recently been extended to a first computation of five-gluon amplitudes [ita9]. In an interesting modification of the strategy, analytic results could be constructed from purely numerical evaluations, i.e. while direct analytic computations are very demanding, the intermediate numerical approach lowers the computational load yielding compact analytic results nevertheless. In addition to the flexibility of this approach, the geometric nature of the method serves as an effective organizing principle and points towards interesting ideas in other formal problems such as the classification of Feynman-integral relations [ita3, ita8].

3.6.2 Electroweak Symmetry Breaking and Higgs Physics

Since many years the group of Prof. Dittmaier contributes to precision calculations for the production and decay of the Higgs boson in the SM at hadron colliders. For the LHC experiments, the respective state-of-the-art predictions are collected and coordinated by the *LHC Higgs Cross Section Working Group* (LHCHXSWG), which is formed by the experts of the ATLAS and CMS experiments as well as of the theory community. Various results of our group on the production of Higgs bosons via vector-boson fusion, Higgs-strahlung, and Higgs production in association with top-quark pairs[1] as well as results on the four-body Higgs-boson decays into weak-gauge-boson pairs, $H \to WW/ZZ \to 4$fermions were included in the LHCHXSWG reports, in particular in the most recent one [ditt9].

Some of the precision calculations for Higgs physics performed in the Dittmaier group lead to the development of publicly available Monte Carlo programs, which are actively used in experimental analyses. The program HAWK, for instance, calculates differential Higgs production cross sections for the vector-boson fusion and Higgs-strahlung channels, including NLO electroweak and QCD corrections. Recently, an official release note of HAWK was published in Ref. [ditt3]. Similarly, the program PROPHECY4F provides predictions for the four-body Higgs-boson decays $H \to WW/ZZ \to 4$fermions with full NLO corrections.

Currently PROPHECY4F is generalized to cover various types of extended Higgs sectors, such as the Two-Higgs-Doublet Model (THDM) or extensions of the SM with singlet scalars. Higher-order calculations in extensions of the SM require great care in the renormalization procedure, in order to provide sound parametrizations of observables in terms of appropriate input parameters and not to spoil the self-consistency of the underlying field theory (e.g. by violating gauge invariance). The robustness of predictions should be proven upon investigating the (in)sensitivity with respect to changes in the renormalization scales and the choice of a renormalization scheme. Ref. [ditt10] proposes several renormalization schemes for the THDM and describes their application to the decays $h \to WW/ZZ \to 4$fermions of the light CP-even Higgs boson h, as implemented in a new version of PROPHECY4F. The renormalization group equations for the running parameters are solved numerically, so that the stability of results with respect to scale variations can be investigated. Figure 3.21 shows, for a very common THDM scenario, the LO and NLO predictions for the $h \to 4f$ decay width (summed over all $4f$-decay channels) as a function of the renormalization scale μ_{r} for the renormalization schemes $\overline{\mathrm{MS}}(\alpha)$, $\mathrm{FJ}(\alpha)$, $\overline{\mathrm{MS}}(\lambda_3)$, $\mathrm{FJ}(\lambda_3)$ suggested in Ref. [ditt10]. In contrast to the LO predictions, the NLO results show a nice plateau in the μ_{r} dependence around the central scale μ_0 with mutual agreement between the different renormalization schemes, after a proper conversion of input parameters between the schemes.

3.6.3 Precision Physics with Electroweak Gauge Bosons

Production processes of electroweak gauge bosons W and Z play a double role at the LHC. Firstly, they lead to relatively clean signatures, which are copiously produced in collisions with high statistics.

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[1] See, e.g., Ref. [ditt2] for recent results.

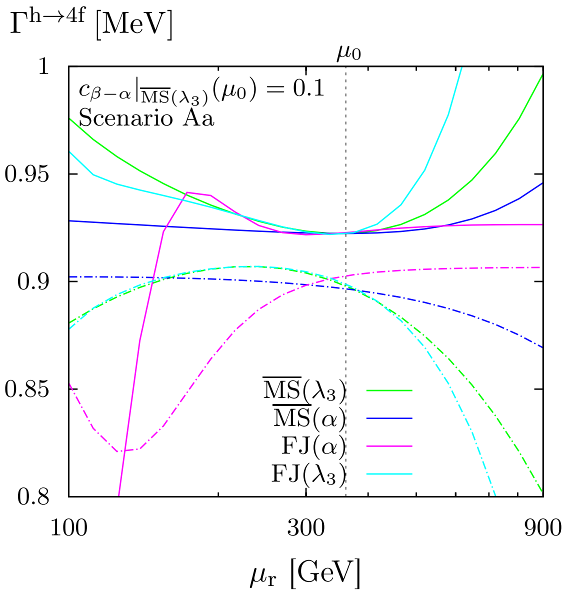

Figure 3.21: The THDM decay width for $h \to 4f$ at LO (dashed) and NLO EW (solid) in dependence of the renormalization scale μ_{r} within the renormalization schemes $\overline{\mathrm{MS}}(\alpha)$, $\mathrm{FJ}(\alpha)$, $\overline{\mathrm{MS}}(\lambda_3)$, $\mathrm{FJ}(\lambda_3)$ (with properly converted input values defined in the $\overline{\mathrm{MS}}(\lambda_3)$ scheme). More details on the model, the renormalization schemes, and the THDM scenario can be found in Ref. [ditt10], from where this plot is taken.

Hence, those processes allow for precision studies of properties of the W and Z bosons, in particular, of their non-Abelian self-interactions in pair-production processes. Secondly, W/Z production processes represent an omnipresent background in the search for new particles. Predictions with the highest possible precision are, thus, mandatory for those processes, either as signal or as background reaction. In a longer termed project, the group of Prof. Dittmaier calculates quantum corrections to various types of production processes of W and Z bosons at the LHC, carefully taking into account the decays of the weak bosons.

In Refs. [ditt1, ditt5] NNLO corrections of mixed QCD–electroweak type were calculated for single-W/Z production, which are important for high-precision measurements of the W-boson mass and the effective weak mixing angle at the LHC. Since the full calculation is technically beyond present capabilities, we worked out the concept of a systematic expansion of the corrections about the resonance poles at the order $O(\alpha_{\mathrm{s}}\alpha)$, which should be sufficient for the mentioned precision analyses. Our results show that *non-factorizable* corrections (induced by photon exchange between production and decay) are negligible [ditt1] and that the dominating *factorizable* corrections can be reproduced by commonly used QED parton showers [ditt5].

Electroweak corrections are particularly important in predictions for the production of electroweak gauge-boson pairs, where those corrections, for instance, reach the order of $30-50\%$ in the domains of high momentum transfer of some TeV. Note that this is also the region where signals of new physics might be expected. In recent years, we have, for instance, calculated NLO electroweak corrections to $W\gamma$ [ditt4], WW [ditt8], and ZZ [ditt6] production processes, taking fully into account leptonic decays of the W and Z bosons as well as all off-shell effects (in contrast to previous calculations). The latter are important both at low and at large scattering energies. Below the WW or ZZ production thresholds, which includes the region where direct WW or ZZ production is a background to Higgs production, at least one of the W/Z bosons is off its mass shell, so that older calculations based on resonant (nearly on-shell) W/Z bosons are non applicable. At high energies, off-shell effects can be enhanced if part of the W/Z production has the characterstics of collinear bremsstrahlung. The latter effect is illustrated in Fig. 3.22 for WW production, where the relative electroweak corrections δ in the transverse-momentum distribution p_{T,e^-} of an electron is compared to the corresponding result of a *double-pole approximation* (DPA) which takes only nearly resonant W bosons into account. As expected, the DPA is good for low p_{T,e^-}, but deviations at the 10% level arise in the TeV range.

3.6.4 QCD-corrections to Multi-Particle Processes

At the LHC, high-multiplicity processes appear as standard candles and typical backgrounds to the expected physics of the Standard Model as well as new physics beyond the Standard Model. Precise theoretical predictions for such processes are, for instance, required to characterize the newly discovered Higgs boson, for exploring the electroweak symmetry breaking mechanism through top-quarks, and to extend the reach of searches for new-physics signals. The complexity of high-multiplicity computations including quantum corrections is very limiting and often requires the development of advanced formal methods in field theory.

In recent years the group of Jun.Prof. Ita has further advanced the implementation of new field theory methods, the so called ‘unitarity methods’ for collider phenomenology. These methods work particularly well when computing often important quantum corrections to high-multiplicity processes. The new computations are implemented in the BLACKHAT software library and are conveniently used together

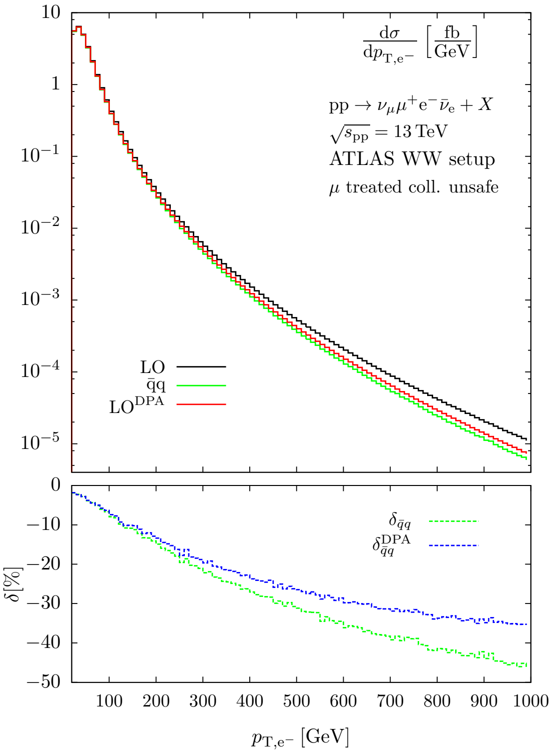

Figure 3.22: Transverse-momentum distribution of the electron produced in $pp \to \nu_\mu \mu^+ e^- \bar{\nu}_e + X$ (upper panel) and corresponding relative electroweak corrections (lower panel), where the full result δ is compared to the DPA result (Plot taken from Ref. [ditt8].).

with SHERPA Monte Carlo program to perform the computations of cross sections. A number of new predictions for high-multiplicity processes including quantum corrections in QCD could be obtained in this way.

An important signature studied by the group is electroweak vector-boson production, accompanied by multiple jets [ita1]. The precise quantitative understanding of this process is helpful in constraining possible anomalous deviations from known physics. Earlier, predictions for the $W + (n \leq 5)$-jet production had been obtained by the group including quantum corrections in QCD. In the recent study the group showed how the cross-section ratios for $W + n$-jet to $W + (n-1)$-jet production can be used to validate and extrapolate differential cross sections to even higher jet multiplicities at next-to-leading order.

Furthermore, the group obtained predictions for di-vector boson production in association with up to three jets, $WW + (n \leq 3)$-jets [ita4]. The predictions include the next-to-leading order corrections in the strong coupling expansion and are an input for measuring the vector-boson couplings in the vector-boson scattering process.

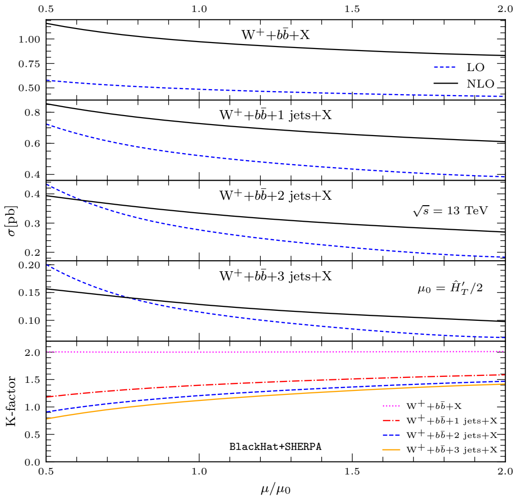

Figure 3.23: The displayed scale dependence of total cross sections for $Wb\bar{b} + 0,1,2,3-$jet+X production is used as an estimator of theoretical uncertainties. The factorization- and renormalization scales are set to $\mu = H'_T/2$ and varied around the central value μ_0. The upper four panels show the dependence of LO (dashed blue line) and NLO (solid black line) predictions. The lower panel shows the ratios (K-factors) of NLO to LO predictions.

Finally, most recently the group could obtain predictions for the diverse final state including a vector boson, light jets and heavy jets [ita10]. These results show the impact of QCD corrections for total cross sections as displayed in Fig. 3.23. In addition the work has made an assessment of theoretical uncertainties of $Wb\bar{b}$+jets viewed as an irreducible background to $H(\to b\bar{b})W$ production. Such predictions with distinct jet multiplicities can be exploited to construct observables with reduced theoretical uncertainties, such as the discussed ‘exclusive sums’ technique. In the future, it will be interesting to use high-multiplicity processes including massive b jets in order to further validate both theory predictions and experimental techniques.

3.6.5 Modified Gravitational Theories and Cosmology

The research of the group of Prof. van der Bij together with Dr. C. Steinwachs also encompasses models of modified gravity and quantum gravity as well as their application to cosmology. General Relativity (GR) has passed all experimental tests with flying colors – impressively confirmed once again by the recent direct detection of gravitational waves. Nevertheless, Einstein’s classical theory is expected to be superseded by a quantum theory of gravity at the fundamental level. While quantum gravitational effects can be safely neglected in terrestrial collider experiments, they are relevant for strong curvature regimes in the early universe and for black hole physics.

Scalar-tensor theories and $f(R)$-gravity provide the phenomenological framework for most cosmologically motivated modifications of GR and even allow for a unified description of inflation and the Standard Model of particle physics – Higgs inflation. The group in Freiburg contributed significantly to the renormalization group improvement of this model, which is crucial for the consistency with observational data. In particular, the quantum parametrization dependence of scalar-tensor theories, relevant for cosmological observables, has been investigated [vdbij4]. At the classical level, $f(R)$-gravity can be equivalently reformulated as a scalar-tensor theory. The one-loop divergences for $f(R)$-gravity, calculated recently for an arbitrary background [vdbij9], generalize previous results and allow for important cosmological applications as well as for the investigation of the aforementioned equivalence at the quantum level [vdbij8].

Lifshitz-theories, which violate Lorentz invariance at the fundamental level, are characterized by an anisotropic scaling of space and time. In the gravitational context such a theory was proposed by P. Hořava. While many results supported the claim that projectable Hořava gravity (a subclass of Hořava gravity) is a unitary and perturbatively renormalizable quantum theory of gravity, a proof was given only recently in [vdbij10, vdbij5]. The most efficient tool for perturbative calculations of ultraviolet divergences in curved spacetime is a combination of the background field method with heat kernel techniques. The heat kernel is an universal tool, used in many different branches in physics and mathematics and has been extended to theories with an anisotropic scaling in [vdbij6]. Based on these new techniques, the explicit calculation of the one-loop counterterms in [vdbij7] revealed that projectable Hořava-gravity in $2+1$ dimensions is asymptotically free. The analogue calculation for the physically most relevant case of $3+1$ dimensions is much more complex and currently in progress.

3.7 GRID Computing

Since the beginning of data taking at the LHC the group of Prof. Schumacher successfully operates an ATLAS-Tier-2-Grid-Centre within the Worldwide LHC Computing Grid (WLCG). As the requirements on CPU power and storage volume increased significantly over the last four years due to the increased collected data at the Large Hadron Collider the computing and storage resources have been extended by a factor of four and two, respectively.

Our group is still responsible for several ATLAS-specific operation tasks in the whole Tier-2 cloud around the Tier-1 GridKa at KIT consisting of 12 sites in 5 countries. On a continual basis the performance of all Tier 2 centres in the cloud (data transfer, job submission, job success rate etc.) is tested and monitored. Freiburg is responsible for summarizing, and analysing the status. Significant contributions are also made to the development and installation of the testing framework “HammerCloud“. All tools have to be adapted regularly to new services and changes in the ATLAS computing model.

Until 2016 the ATLAS-Tier-2 centre and Tier-3 centre for local data analysis were integrated in the interdisciplinary Black Forest Grid (BFG), where 21 groups from 5 faculties, used the common infrastructure and computer cluster located at the university computing centre. The BFG was dominated by the ATLAS Tier2 and other resources from particle physics (90 % of resources) and operated by our group. Since 2016 a new concept by the state of Baden-Württemberg for the future of high performance and high throughput computing has been implemented. Four research cluster ”bwForCluster” have been established at four universities, which each provide the computing power for selected disciplines. In Freiburg the resources for the fields of neuroscience, elementary particles physics and microsystems engineering are hosted in the cluster NEMO.

Cluster	CPU (HEPSPEC06)	Storage (TB)
ATLAS Tier-2	19000	1800
ATLAS Tier-3 / BFG	10000	1000
NEMO	330000	600

Table 3.1: Grid resources hosted in the Freiburg.

Table 3.1 gives an overview of grid computing resources owned by or accessible to the particle physics community in Freiburg, which are operated by our group in cooperation with the HPC-team at the university computer center. The BFG is still used as Tier-3 for local ATLAS data analysis.

In order to use NEMO by ATLAS data analysis the whole ATLAS-specific workflow and services have to be provided via virtualisation. This technology had to be developed, implemented and validated by our group in cooperation with the university computer center. A sketch of the work flow is shown in Fig. 3.24.

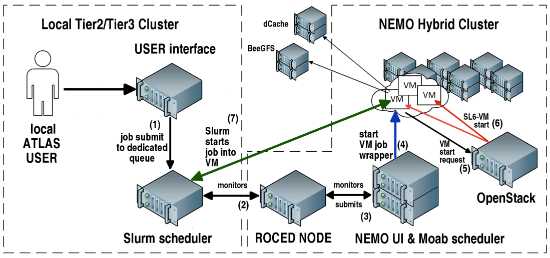

Figure 3.24: Workflow for virtualisation of NEMO

Since autumn 2017 NEMO can be successfully used as a completely virtualised Tier-3 centre for local data analysis. First comparisons of the performance of the virtualised environment with computing on bare metal have been performed e.g. using the HEPSPEC06 benchmark. No hints for a performance loss have been observed as shown in Fig. 3.25. The further increase in data rate and volume expected during Run 3 and Run 4 of the LHC will require to increase the local resources for ATLAS-use by a factor of roughly ten. This already assumes that half of the needed resources can be provided in a different way, e.g. use of opportunistic HPC resources or scientific or commercial computing clouds. The initial virtualisation of NEMO is only a first step. We plan to continue our R&D work on digital technologies for the optimised use of heterogeneous compute resources.

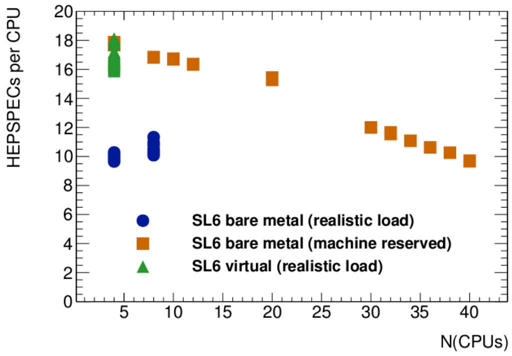

Figure 3.25: Comparison of performance bare metal vs. virtualisation on NEMO

3.8 Important Publications and Conference Talks

Group Dittmaier

Publications

[ditt1] S. Dittmaier, A. Huss and C. Schwinn, "Mixed QCD-electroweak $O(\alpha_s \alpha)$ corrections to Drell-Yan processes in the resonance region: pole approximation and non-factorizable corrections," Nucl. Phys. B **885** (2014) 318 [arXiv:1403.3216 [hep-ph]].

[ditt2] S. Dittmaier, P. Häfliger, M. Krämer, M. Spira and M. Walser, "Neutral MSSM Higgs-boson production with heavy quarks: NLO supersymmetric QCD corrections," Phys. Rev. D **90** (2014) no.3, 035010 [arXiv:1406.5307 [hep-ph]].

[ditt3] A. Denner, S. Dittmaier, S. Kallweit and A. Mück, "HAWK 2.0: A Monte Carlo program for Higgs production in vector-boson fusion and Higgs strahlung at hadron colliders," Comput. Phys. Commun. **195** (2015) 161 [arXiv:1412.5390 [hep-ph]].

[ditt4] A. Denner, S. Dittmaier, M. Hecht and C. Pasold, "NLO QCD and electroweak corrections to $W+\gamma$ production with leptonic W-boson decays," JHEP **1504** (2015) 018 [arXiv:1412.7421 [hep-ph]].

[ditt5] S. Dittmaier, A. Huss and C. Schwinn, "Dominant mixed QCD-electroweak O($\alpha_s \alpha$) corrections to Drell-Yan processes in the resonance region," Nucl. Phys. B **904** (2016) 216 [arXiv:1511.08016 [hep-ph]].

[ditt6] B. Biedermann, A. Denner, S. Dittmaier, L. Hofer and B. Jäger, "Electroweak corrections to $pp \to \mu^+\mu^-e^+e^- + X$ at the LHC: a Higgs background study," Phys. Rev. Lett. **116** (2016) no.16, 161803 [arXiv:1601.07787 [hep-ph]].

[ditt7] A. Denner, S. Dittmaier and L. Hofer, "Collier: a fortran-based Complex One-Loop LIbrary in Extended Regularizations," Comput. Phys. Commun. **212** (2017) 220 [arXiv:1604.06792 [hep-ph]].

[ditt8] B. Biedermann, M. Billoni, A. Denner, S. Dittmaier, L. Hofer, B. Jäger and L. Salfelder, "Next-to-leading-order electroweak corrections to $pp \to W^+W^- \to$ 4 leptons at the LHC," JHEP **1606** (2016) 065 [arXiv:1605.03419 [hep-ph]].

[ditt9] D. de Florian *et al.* [LHC Higgs Cross Section Working Group], "Handbook of LHC Higgs Cross Sections: 4. Deciphering the Nature of the Higgs Sector," arXiv:1610.07922 [hep-ph].

[ditt10] L. Altenkamp, S. Dittmaier and H. Rzehak, "Renormalization schemes for the Two-Higgs-Doublet Model and applications to $h \to WW/ZZ \to$ 4 fermions," JHEP **1709** (2017) 134 [arXiv:1704.02645 [hep-ph]].

Conference Talks

1. H. Rzehak, "Higher-order contributions in Higgs sectors of supersymmetric models", Conference *Loops & Legs in Quantum Field Theory*, Weimar, April/May 2014.
2. S. Dittmaier, "Higgs Theory", plenary talk, *Large Hadron Collider Physics (LHCP) Conference*, New York, June 2014.
3. C. Schwinn, "State-of-the-art theory predictions for Drell-Yan processes", Workshop *Standard Model at LHC 2015*, Florence, April 2015.
4. S. Dittmaier, "Standard Model Theory", plenary talk, *Blois2015: 27th Rencontres de Blois on Particle Physics and Cosmology*, Blois, May/June 2015.
5. S. Dittmaier, "Mixed QCD × EW $\mathscr{O}(\alpha\alpha_s)$ corrections to Drell–Yan processes in the resonance region", plenary talk, *11th International Symposium on Radiative Corrections (RADCOR)*, UCLA, Los Angeles, June 2015.
6. S. Dittmaier, "Electroweak corrections to gauge-boson pair production processes at the LHC including leptonic W/Z decays", Conference *Loops & Legs in Quantum Field Theory*, Leipzig, April/May 2016.

7. P. Maierhöfer, “Multijet merging for vector boson plus jets including electroweak corrections”, Conference *Loops & Legs in Quantum Field Theory*, Leipzig, April/May 2016.
8. T. Schmidt, “(B)SM Higgs Production via Gluon Fusion”, Conference *LoopFest XV*, Buffalo, Aug. 2016.
9. S. Dittmaier, “Standard Model Theory”, plenary talk, *EPS Conference on High-Energy Physics*, Venice, July 2017.
10. C. Schwan, “Vector Boson Scattering at the LHC”, *12th International Symposium on Radiative Corrections (RADCOR)*, St. Gilgen, Sep. 2017.

Group Heinemann

Listed are only publications and conference talks since August 2016.

Publications

[hein1] ATLAS Collaboration, Luminosity determination in pp collisions at $\sqrt{s} = 8$ TeV using the ATLAS detector at the LHC, Eur. Phys. J. C **76** (2016) 653.

[hein2] ATLAS Collaboration, Measurement of $W^{\pm}W^{\pm}$ vector-boson scattering and limits on anomalous quartic gauge couplings with the ATLAS detector, Phys. Rev. D **96** (2017), 012007.

[hein3] ATLAS Collaboration, Search for new phenomena in events containing a same-flavour opposite-sign dilepton pair, jets, and large missing transverse momentum in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector, Eur. Phys. J. C **77** (2017) 144.

Conference Talks

1. B. Heinemann, Searches for New Physics at the LHC, Conference of Brazil Physics Society, Natal/Brazil, September 2016
2. B. Heinemann , LHC Run 2 Results, 10th Annual Meeting of the Terascale Alliance, Hamburg/Germany, November 2016
3. B. Heinemann, Searches for New Physics at the LHC and the role of QCD and PDFs, Workshop on Deep Inelastic Scattering, Birmingham/UK, April 2017

Group Herten

Publications

[hert1] G. Aad *et al.* [ATLAS Collaboration], “Search for supersymmetry at $\sqrt{s}$=8 TeV in final states with jets and two same-sign leptons or three leptons with the ATLAS detector,” JHEP **1406** (2014) 035, arXiv:1404.2500 [hep-ex].

[hert2] G. Aad *et al.* [ATLAS Collaboration], “Measurement of the muon reconstruction performance of the ATLAS detector using 2011 and 2012 LHC proton–proton collision data,” Eur. Phys. J. C **74** (2014) no.11, 3130 doi:10.1140/epjc/s10052-014-3130-x [arXiv:1407.3935 [hep-ex]].

[hert3] G. Aad *et al.* [ATLAS Collaboration], “Measurement of the forward-backward asymmetry of electron and muon pair-production in pp collisions at $\sqrt{s}$ = 7 TeV with the ATLAS detector,” JHEP **1509** (2015) 049, arXiv:1503.03709 [hep-ex].

[hert4] G. Aad *et al.* [ATLAS Collaboration], “Summary of the ATLAS experiment’s sensitivity to supersymmetry after LHC Run 1 - interpreted in the phenomenological MSSM,” JHEP **1510** (2015) 134, arXiv:1508.06608 [hep-ex].

[hert5] G. Aad *et al.* [ATLAS Collaboration], “Search for supersymmetry at $\sqrt{s} = 13$ TeV in final states with jets and two same-sign leptons or three leptons with the ATLAS detector,” Eur. Phys. J. C **76** (2016) no.5, 259, arXiv:1602.09058 [hep-ex]

[hert6] G. Aad *et al.* [ATLAS Collaboration], “Muon reconstruction performance of the ATLAS detector in proton–proton collision data at $\sqrt{s}$ =13 TeV,” Eur. Phys. J. C **76** (2016) no.5, 292 doi:10.1140/epjc/s10052-016-4120-y [arXiv:1603.05598 [hep-ex]].

[hert7] M. Aaboud *et al.* [ATLAS Collaboration], “Search for squarks and gluinos in final states with jets and missing transverse momentum at $\sqrt{s} = 13$ TeV with the ATLAS detector,” Eur. Phys. J. C **76** (2016) no.7, 392, [arXiv:1605.03814 [hep-ex]].

[hert8] M. Aaboud *et al.* [ATLAS Collaboration], “Search for triboson $W^{\pm}W^{\pm}W^{\mp}$ production in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector”, Eur. Phys. J. C **77** (2017) no.3, 141, arXiv:1610.05088 [hep-ex].

[hert9] M. Aaboud *et al.* [ATLAS Collaboration], “Search for supersymmetry in final states with two same-sign or three leptons and jets using 36 fb^{-1} of $\sqrt{s} = 13$ TeV pp collision data with the ATLAS detector”, JHEP **1709** (2017) 084, arXiv:1706.03731 [hep-ex].

[hert10] M. Aaboud *et al.* [ATLAS Collaboration], “Search for squarks and gluinos in final states with jets and missing transverse momentum using 36 fb^{-1} of $\sqrt{s}$=13 TeV pp collision data with the ATLAS detector,” arXiv:1712.02332 [hep-ex], submitted to Phys. Rev. D.

Conference Talks

1. Zuzana Rurikova, Inclusive SUSY Particle Searches with Jets and MET in ATLAS, The 22nd International Conference on Supersymmetry and Unification of Fundamental Interactions, SUSY 2014, Manchester, UK, July 2014.
2. Andrea Di Simone, Sensitivity of future mono-jet searches for WIMPS at the 14 TeV LHC, Dark Matter at the Large Hadron Collider, DM@LHC 2014, Oxford, UK, September 2014.
3. Andrea Di Simone, Weak mixing angle measurements at hadron colliders, Twelfth Conference on the Intersections of Particle and Nuclear Physics, CIPANP2015, Vail, CO, USA, May 2015.
4. Stephanie Zimmermann, LHC(ATLAS, CMS, LHCb) Run 2 commissioning status, Flavor Physics & CP Violation 2015, FPCP2015, Nagoya, Japan, May 2015.
5. Gregor Herten, Event-by-event flow in ATLAS and CMS, Large Hadron Collider Physics Conference 2015, LHCP-2015, St. Petersburg, Russia, August 2015.
6. Gregor Herten, SUSY Searches, Planck-2016, Valencia, May 2016.
7. Martina Javurkova, Squark/gluino in leptonic channels with ATLAS, Large Hadron Collider Physics, LHCP 2016, Lund, Schweden, June 2016.
8. Andrea Di Simone, SUSY searches with the ATLAS detector, Hadron Structure and QCD, HSQCD2016, Gatchina, Russia, 27.06.-01.07.2016.
9. Manfredi Ronzani, Inclusive searches for squarks and gluinos in fully hadronic final states with the ATLAS detector, SUSY 2016 Conference, Melbourne, Australien, July 2016.
10. Fabio Cardillo, Searches for electroweak production of supersymmetric gauginos and sleptons with the ATLAS detector, PASCOS, June 2017, Madrid

Group Ita

Publications

[ita1] Z. Bern, L. J. Dixon, F. Febres Cordero, S. Höche, H. Ita, D. A. Kosower and D. Maître, “Extrapolating W-Associated Jet-Production Ratios at the LHC,” Phys. Rev. D **92** (2015) no.1, 014008 [arXiv:1412.4775 [hep-ph]].

[ita2] F. Coradeschi, D. de Florian, L. J. Dixon, N. Fidanza, S. Höche, H. Ita, Y. Li and J. Mazzitelli, “Interference effects in the $H(\to \gamma\gamma)+2$ jets channel at the LHC,” Phys. Rev. D **92** (2015) no.1, 013004 [arXiv:1504.05215 [hep-ph]].

[ita3] H. Ita, “Two-loop Integrand Decomposition into Master Integrals and Surface Terms,” Phys. Rev. D **94** (2016) no.11, 116015 [arXiv:1510.05626 [hep-th]].

[ita4] F. Febres Cordero, P. Hofmann and H. Ita, “W^+W^- + 3-jet production at the Large Hadron Collider in next-to-leading-order QCD,” Phys. Rev. D **95** (2017) no.3, 034006 [arXiv:1512.07591 [hep-ph]].

[ita5] M. L. Mangano *et al.*, “Physics at a 100 TeV pp collider: Standard Model processes,” CERN Yellow Report (2017) no.3, 1 [arXiv:1607.01831 [hep-ph]].

[ita6] S. Abreu, F. Febres Cordero, H. Ita, M. Jaquier and B. Page, “Subleading Poles in the Numerical Unitarity Method at Two Loops,” Phys. Rev. D **95** (2017) no.9, 096011 [arXiv:1703.05255 [hep-ph]].

[ita7] S. Abreu, F. Febres Cordero, H. Ita, M. Jaquier, B. Page and M. Zeng, “Two-Loop Four-Gluon Amplitudes from Numerical Unitarity,” Phys. Rev. Lett. **119** (2017) no.14, 142001 [arXiv:1703.05273 [hep-ph]].

[ita8] Z. Bern, M. Enciso, H. Ita and M. Zeng, “Dual Conformal Symmetry, Integration-by-Parts Reduction, Differential Equations and the Nonplanar Sector,” Phys. Rev. D **96** (2017) no.9, 096017 [arXiv:1709.06055 [hep-th]].

[ita9] S. Abreu, F. Febres Cordero, H. Ita, B. Page and M. Zeng, “Planar Two-Loop Five-Gluon Amplitudes from Numerical Unitarity,” arXiv:1712.03946 [hep-ph].

[ita10] F. R. Anger, F. Febres Cordero, H. Ita and V. Sotnikov, “NLO QCD Predictions for $Wb\bar{b}$ Production in Association with up to Three Light Jets at the LHC,” arXiv:1712.05721 [hep-ph].

Conference Talks

1. H. Ita, “Di-vector Boson Production in Association with Multiple Jets at the LHC”, The European Physical Society Conference on High Energy Physics, Vienna, Juli 2015.
2. F. Febres Cordero, “Divector Boson Production with Jets at the LHC”, Loops & Legs in Quantum Field Theory, Leipzig, April/Mai 2016.
3. H. Ita, “Towards a Numerical Unitarity Approach for Two-loop Amplitudes in QCD”, Loops & Legs in Quantum Field Theory, Leipzig, April/Mai 2016.
4. H. Ita, “Numerical Unitarity Method for Two-Loop Amplitudes in QCD”, Nordita program, Aspects of Amplitudes, Stockholm, Juni/Juli 2016.
5. M. Jaquier, “Towards a Numerical Unitarity Approach at Two Loops in QCD”, Loopfest XV, Buffalo, Aug. 2016.
6. F. Febres Cordero, “Divector Boson Production with Jets at the LHC”, “International Conference for High Energy Physics, in Chicago, August 2016.
7. H. Ita, “Numerical Two-loop Amplitudes in QCD from Unitarity”, Loopfest XVI, Argonne National Laboratory, Mai 2017.
8. B. Page, “First Two-Loop Amplitudes with the Numerical Unitarity Method”, Amplitudes Conference, at Higgs Centre, The University of Edinburgh, UK, Juli 2017.

9. H. Ita, “Methods for Numerical Unitarity @ Two Loops”, Scientific Programme, “Automated, Resummed and Effective: Precise Computations for the LHC and Beyond”, Munich Institute for Astro- and Particle Physics (MIAPP) of the DFG cluster of excellence “Origin and Structure of the Universe”, Garching, Aug. 2017.
10. B. Page, “First Two-Loop Amplitudes with the Numerical Unitarity Method”, 12th International Symposium on Radiative Corrections (RADCOR), St. Gilgen, Sept. 2017.

Group Jakobs

Publications

[jak1] ATLAS Collaboration, “Evidence for the Higgs-boson Yukawa coupling to tau leptons with the ATLAS detector”, JHEP 04 (2015) 117.

[jak2] ATLAS Collaboration, “Observation and measurement of Higgs boson decays to WW^* with the ATLAS detector”, Phys. Rev. D. 92 (2015) 012006.

[jak3] ATLAS Collaboration, “Summary of the ATLAS experiment’s sensitivity to supersymmetry after LHC Run 1 - interpreted in the phenomenological MSSM”, JHEP 1510 (2015) 134.

[jak4] ATLAS and CMS Collaboration, “Measurements of the Higgs boson production and decay rates and constraints on its couplings from a combined ATLAS and CMS analysis of the LHC pp collision data at $\sqrt{s}$ = 7 and 8 TeV”, JHEP 08 (2016) 45.

[jak5] ATLAS Collaboration, “Search for a scalar partner of the top quark in the jets plus missing transverse momentum final state at $\sqrt{s}$ = 13 TeV with the ATLAS detector”, arXiv:1709.04183 [hep-ex], accepted by JHEP.

[jak6] ATLAS Collaboration, “Measurement of total and differential W^+W^- production cross sections in proton-proton collisions at $\sqrt{s}$ = 8 TeV with the ATLAS detector and limits on anomalous triple-gauge-boson couplings”, JHEP 09 (2016) 29.

[jak7] ATLAS Collaboration, “Precision measurement and interpretation of inclusive $W^+, W^-$and Z/γ^* production cross sections with the ATLAS detector”, Eur. Phys. J. C 77 (2017) no.6, 367.

[jak8] ATLAS Collaboration, “Evidence for the $H \to b\bar{b}$ decay with the ATLAS detector”, JHEP 12 (2017) 24.

[jak9] M. Wiehe et al., “Measurements of the reverse current of highly irradiated silicon sensors to determine the effective energy and current related damage rate”, Nucl. Instrum. Meth. A (2018) 877: 51.

[jak10] ATLAS Collaboration, “Technical Design Report for the ATLAS Inner Tracker Strip Detector”, CERN-LHCC-2017-005.

Conference Talks

1. Köneke, K., *ATLAS Results* (invited plenary talk), 20th International Symposium on Particles, Strings and Cosmology (PASCOS 2014), Warschau, Polen, Juni 2014.
2. Jakobs, K., *Conference Summary talk, Higgs Couplings 2014*, Conference on Higgs Couplings (HC 2014), Turin, Italien, Oktober 2014.
3. Karl Jakobs: Physics at the Large Hadron Collider - from the discovery of the Higgs particle to searches for new physics - Stern-Gerlach Laureate plenary talk, Annual DPG spring conference, Wuppertal, March 2015
4. Daniel Büscher, *Search for the bb decay of the SM Higgs boson in associated $(W/Z)H$ production with the ATLAS detector*, Higgs Couplings 2015, Durham (England), Oktober 2015.

5. Christian Weiser, *Deciphering the Higgs boson: New results from the LHC* (invited plenary talk), Annual DPG spring conference, Hamburg, Februar 2016.
6. Frederik Rühr, *Searches for new physics at the LHC* (invited plenary talk), Annual DPG spring conference, Hamburg, February 2016.
7. Christian Weiser, *Higgs and more: Results from the LHC*, (invited plenary talk), Loops and Legs in Quantum Field Theory, Leipzig, April 2016.
8. Philip Sommer, *High precision measurement of the differential W and Z boson production cross sections with the ATLAS experiment*, 25th International Workshop on Deep Inelastic Scattering, Birmingham, United Kingdom, April 2017.
9. Susanne Kuehn, (for the ATLAS Collaboration), *First testbeam results of prototype modules for the upgrade of the ATLAS strip tracking detector*, ICHEP, Chicago (USA), August 2016.
10. Carlos Garcia-Argos, *Modules and Front-End Electronics Developments for the ATLAS ITk Strips Upgrade*, International Conference on Technology and Instrumentation in Particle Physics (TIPP2017), Beijing (China), Mai 2017.

Group Schumacher

Publications

[schumach1] ATLAS Collaboration], “Search for neutral Higgs bosons of the minimal supersymmetric standard model in pp collisions at $\sqrt{s}$ = 8 TeV with the ATLAS detector”m JHEP **1411** (2014) 056, [arXiv:1409.6064 [hep-ex]].

[schumach2] ATLAS Collaboration, ”Search for charged Higgs bosons decaying via $H^{\pm} \to \tau \pm \nu$ in fully hadronic final states using pp collision data at $\sqrt{s}$ = 8 TeV with the ATLAS detector”, JHEP03 (2015) 088, arXiv:1412.6663.

[schumach3] ATLAS Collaboration, ”Identification and energy calibration of hadronically decaying tau leptons with the ATLAS experiment in pp collisions at $\sqrt{s}$ = 8 TeV”, Eur. Phys. J. C75 (2015) 303, arXiv:1412.7086.

[schumach4] ATLAS Collaboration, ”Evidence for the Higgs-boson Yukawa coupling to tau leptons with the ATLAS detector”, JHEP 04 (2015) 117, arXiv:1501.04943.

[schumach5] ATLAS Collaboration, ”Modelling $Z \to \tau\tau$ processes in ATLAS with tau-embedded $Z \to \mu\mu$ data”, 2015 JINST 10 P09018, arXiv:1506.05623 [hep-ex]].

[schumach6] ATLAS Collaboration, ”Measurements of the Higgs boson production and decay rates and coupling strengths using pp collision data at $\sqrt{s} = 7$ and 8 TeV in the ATLAS experiment”, Eur. Phys. J. C **76** (2016) no.1, 6, [arXiv:1507.04548 [hep-ex]].

[schumach7] ATLAS and CMS Collaborations, ”Measurements of the Higgs boson production and decay rates and constraints on its couplings from an combined ATLAS and CMS analysis of the LHC pp collision data at s = 7 and 8 TeV”, JHEP 08 (2016) 45, [arXiv:1606.02266 [hep-ex]].

[schumach8] ATLAS Collaboration, ”Test of CP Invariance in vector-boson fusion production of the Higgs boson using the Optimal Observable method in the ditau decay channel with the ATLAS detector”, Eur. Phys. J. C 76 (2016) 658, [arXiv:1602.04516 [hep-ex]].

[schumach9] ATLAS Collaboration,”Search for lepton-flavour-violating decays of the Higgs and Z bosons with the ATLAS detector”, Eur. Phys. J. C **77** (2017) no.2, 70, [arXiv:1604.07730 [hep-ex]].

[schumach10] D. de Florian et al. [LHC Higgs Cross Section Working Group], ”Handbook of LHC Higgs Cross Sections: 4. Deciphering the Nature of the Higgs Sector”, arXiv:1610.07922 [hep-ph].

Conference Talks

1. E. Coniavitis, Higgs Boson decays to Leptons with the ATLAS detector, 37th Int. Conference on High Energy Physic (ICHEP), Valencia, July 2014.
2. A. Kopp, Search for charged Higgs bosons in ATLAS using the tau+jets final state, Prospects for Charged Higgs Discovery at Colliders (CHARGED 2014), Uppsala, September 2014.
3. M. Schumacher, Experimental Summary, Flavour of the Higgs Workshop , Weizmann Institute of Science, Rehovot, Israel, June 2014.
4. M. Boehler, Improved ATLAS HammerCloud Monitoring for local Site Administration, 21st International Conference on Computing in High Energy and Nuclear Physics, Okinawa, Japan, Apr 2015.
5. M. Boehler, Evolution of ATLAS conditions data and its management for LHC run 2, 21st International Conference on Computing in High Energy and Nuclear Physics, Okinawa, Japan, Apr 2015.
6. Markus Schumacher, Das Higgs-Boson – Charakterisierung seiner Natur, Eingeladener Plenarvortrag, Frühjahrtagung der Deutschen Physikalischen Gesellschaft, Münster, March 2017.
7. Duc Bao Ta, Cross section and coupling measurements with the ATLAS detector for the 125 GeV Higgs Boson in the fermion decay channels, 25th In. Workshop on Deep Inelastic Scattering and Related Topics 2017, Birmingham, United Kingdom, April 2017.
8. Ulrike Schnoor, Higgs Decays to Bottom and Tau Pairs With the ATLAS and CMS Experiments, Standard Model at the LHC 2017, Amsterdam, The Netherlands, May 2017.
9. Elias Coniavitis, ATLAS H(125) Lepton Decays Results, 8th Higgs Hunting 2017, Orsay-Paris, France, July 2017.
10. Anton Gamel, Virtualization of the ATLAS software environment on a shared HPC system (Poster), 18th International Workshop on Advanced Computing and Analysis Techniques in Physics Research, Seattle, WA, USA, August 2017.

Group Schumann

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Conference Talks

1. H. Fischer, ”Experimental Overview on DVCS Measurements”, invited talk SPIN 2014, Beijing, October 2014.
2. M. Schumann, ”Direct Searches for WIMP Dark Matter”, plenary talk COSMO-15, Warsaw, September 2015.
3. M. Schumann, ”DARWIN: Dark Matter (and more) with a multi ton-scale Xenon Detector”, TAUP 2015, Torino, September 2015.
4. M. Schumann, ”The Direct Search for Dark Matter - Status and Perspectives”, plenary talk DPG Spring Meeting, Hamburg, March 2016.
5. M. Schumann, ”Dark Matter Direct Detection - the next 5 years (and beyond...)”, LHCSki, Obergurgl, April 2016.
6. D. Coderre, ”The XENON1T Dark Matter Search”, PPC 2016, Sao Paulo, July 2016.
7. M. Schumann, ”Direct Dark Matter Searches - Status and Perspectives”, plenary talk TeVPA, CERN, September 2016.
8. D. Coderre, ”XENON1T: First Results from the First Ton-Scale Xe Detector”, TIPP 2017, Beijing, May 2017.
9. M. Schumann, ”DARWIN”, LAUNCH 17, Heidelberg, September 2017.
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1. M. Bicer *et al.* [TLEP Design Study Working Group], "First Look at the Physics Case of TLEP," JHEP **1401** (2014) 164.
2. C. F. Steinwachs, 28.10.2015 - 30.10.2015, Madrid, Windows of quantum gravity, Season 2, "Question of quantum equivalence between Jordan frame and Einstein frame".
3. C. F. Steinwachs, 18.05.2016 - 20.05.2016, Isfahan, First Isfahan-Freiburg meeting on quantum science, "Higgs Inflation: connecting cosmology with particle physics".
4. C. F. Steinwachs, 29.05.2017 - 03.06.2017, Moscow, Lebedev Institute, Ginzburg centennial conference on physics, "Quantum properties of Lifshitz theories".
5. J. J. van der Bij, HiggsTools Final Network Meeting, IPPP Durham 11-19 September 2017, "Physics after the discovery of the Higgs boson," arXiv:1711.03898 [hep-ph].

3.9 PhD, Diploma and Master Theses

Group Dittmaier

Habilitations

1. Christian Schwinn, “Heavy particles at the LHC and future colliders: theoretical methods and precise predictions”, 2014.

2. Heidi Rzehak, “Theoretical input for the search of deviations from the Standard Model”, 2016.

PhD Theses

1. Alexander Huss, “Mixed QCD-electroweak $O(\alpha_s\alpha)$ corrections to Drell-Yan processes in the resonance region”, Sep. 2014.

2. Luisa Oggero, “Radiative corrections to the decay of the top quark”, Dez. 2014.

3. Markus Hecht, “NLO QCD and electroweak corrections to $W\gamma$ and $Z\gamma$ production”, Oct. 2015.

4. Lukas Altenkamp, “Precise Predictions within the Two-Higgs-Doublet Model”, Dec. 2016.

Diploma/Master Theses

1. Martin Rotzinger, “Higgs-Boson Decay Processes in an Effective Field-Theory Approach – First Steps towards Automation”, June 2014.

2. Michael Kordovan, “Electroweak Next-to-Leading-Order Corrections to $t\bar{t}H$ Production at the Large Hadron Collider”, July 2014.

3. Lynn Meissner, “Higgs-Boson Decays into Four Fermions in an Effective Field Theory Approach”, Oct. 2015.

4. Gernot Knippen, “Next-to-leading order electroweak corrections to triple-W-boson production at proton-proton colliders”, Nov. 2015.

5. Wladimir Tschernow, “Evaluation of scalar Feynman integrals via differential equations”, Dec. 2016.

6. Ramon Winterhalder, “Approximations for Vector-Boson Scattering at the LHC”, Sep. 2017.

Group Herten

PhD Theses

1. Martina Javurkova, Measurement of WWW production and search for supersymmetric particles in multi-lepton final states in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector at the LHC, 2017.
   `http://www.freidok.uni-freiburg.de/data/12802/`

2. Tomas Javurek, Search for squarks and gluinos in final state with jets, missing transverse momentum and boosted W bosons with the ATLAS Experiment, 2016.
   `https://freidok.uni-freiburg.de/data/11176/`

3. Simone Amoroso, Tuning of event generators to measurements of $t\bar{t}$ production and a general search for new physics with the ATLAS Experiment, 2015.
   `http://www.academia.edu/23763406`

4. Valerio Consorti, Search for squarks and gluinos in final states with jets and missing transverse momentum with the ATLAS detector at the LHC, 2014.
   `https://freidok.uni-freiburg.de/data/10906/`

5. Kim Temming, Construction and Calibration of a Setup for Micro-Pattern Gaseous Detectors Using UV Laser Photoelectrons, 2014.
   `https://freidok.uni-freiburg.de/data/9390/`

6. Riccardo Maria Bianchi, A model-independent General Search for new physics with the ATLAS detector at LHC, 2014.
   `https://freidok.uni-freiburg.de/data/9492/`

Diploma/Master Theses

1. Patrick Scholer, Simulation and Measurement of Position Inaccuracies in Large Micromegas Chambers, 2017.

2. Franziska Nöthling, Real rate estimation for three charged gauge boson processes in the Standard Model, 2015.

Group Ita

Diploma/Master Theses

1. Jonas Wenzler, "Towards an unitarity based implementation of Higgs production in association with jets including quantum corrections",2016.

2. Evgenij Pascual, "Recursive methods of the numerical unitarity approach for two-loop amplitudes", 2015.

3. Philipp Hofmann, 'Di-Vector Boson Production in Association with Jets in NLO QCD', 2014.

4. Andreas Ikkert, 'Unitarity Methods for One- and Two-Loop Integral Reduction', 2015.

Group Jakobs

Habilitations (submitted)

1. Karsten Köneke, "Electroweak Interactions, the Higgs Boson, and the Search for new heavy Bosons", submitted November 2017.

2. Susanne Kühn, "Semiconductor Detectors for High Energy Physics Experiments", submitted January 2018.

PhD Theses

1. Manuela Venturi, "Search for the Standard Model Higgs boson in the $WW \to \ell\nu\ell\nu$ final state with the ATLAS experiment and study of its spin and parity quantum numbers", February 2014.

2. Andreas Zwerger, "Entwicklung und Charakterisierung von spektroskopischen und ortsauflösenden Cadmiumtellurid-Halbleiterdetektorsystemen", October 2014.

3. Nils Ruthmann, "Search for the Standard Model $H \to \tau\tau$ decays in the lepton-hadron final state in proton-proton collisions with the ATLAS detector at the LHC", December 2014.

4. Claudia Giuliani, "The quest for the top squark in semi-leptonic and hadronic final states with the ATLAS Experiment", 2015

5. Matthias Werner, "Improvement of FastCaloSim and Measurement of k_T Splitting Scales in $W \to e\nu$ Events with the ATLAS Experiment", 2015

6. Francesca Consiglia Ungaro, "Search for the Supersymmetric Partner of the Top Quark with the ATLAS Detector via $\tilde{t}_1 \to t\tilde{\chi}_1^0$ and $\tilde{t}_1 \to b\tilde{\chi}_1^\pm$ Decays", 2015

7. Christopher Betancourt, “Measurement of the W+c production cross-section in pp collisions at $\sqrt{s}$=8 TeV with the ATLAS detector and charge multiplication detectors for use in the HL-LHC”, April 2016.
8. Vakhtang Tsiskaridze, “Search for the top squark in semileptonic final states in compressed scenarios with the ATLAS detector”, August 2016.
9. Daniel Büscher, “Search for Higgs bosons with b-jets in the final state in proton-proton collisions with the ATLAS experiment”, October 2016.
10. Philip Sommer, “A Measurement of W boson pair production in pp collisions at $\sqrt{s}$=8 TeV with the ATLAS experiment”, November 2016.
11. Phuong Nguyen Dang, “Search for the neutral Higgs boson in $H \rightarrow WW^{*} \rightarrow \ell\nu\ell\nu$ decays with the ATLAS experiment”, December 2016.
12. Liv Wiik-Fuchs, “Search for heavy lepton resonances decaying to a Z boson and a lepton in proton-proton collisions at $\sqrt{s}$ = 8 TeV with the ATLAS detector and investigations of radiation tolerant silicon strip detectors for the high-luminosity LHC upgrade of the ATLAS inner detector”, March 2017 (Bonn and Freiburg).
13. Carsten Burgard, “Measurement of H $\rightarrow WW^{*} \rightarrow \ell\nu\ell\nu$ decays at $\sqrt{s}$ = 13 TeV with the ATLAS experiment and analysis of effective Higgs boson couplings”, July 2017.

Diploma/Master Theses

1. Maira Thomas, “Vergleichende Studien zur Signalentwicklung in strahlenharten Siliziumstreifendetektoren”, May 2014.
2. Ralf Gugel, “Background rejection studies using multivariate techniques in the $H \rightarrow W^{\mp}W^{\pm *} \rightarrow \ell^{-}\bar{\nu}\ell'^{+}\nu$ channel with the ATLAS detector”, September 2015.
3. Fabian Schnell, “Aufbau und Inbetriebnahme eines Edge-TCT-Teststands zur Untersuchung von Siliziumdetektoren”, October 2015.
4. Thorben Swirski , “Estimation of the $t\bar{t}+Z$ background for SUSY searches of pair production of top squarks with the ATLAS detector”, September 2015.
5. Frank Sauerburger, “Search for H $\rightarrow \tau\tau$ decays in the lepton-hadron final state using multivariate techniques in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS Detector at the LHC”, March 2017.
6. Aliya Ismailova, “Search for WH production in the final state with two same-charge muons and two jets in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS experiment at the LHC”, 2017
7. Brian Moser, “Investigations of the Top-Quark Pair-Production Process as a Background in the Search for $H \rightarrow b\bar{b}$ with the ATLAS Experiment at the Large Hadron Collider”, November 2017
8. Benjamin Jäger, “Investigation of the Higgs Boson Production via Gluon Fusion in the $H \rightarrow WW^{*} \rightarrow l\nu l\nu$ Decay Mode with the ATLAS Experiment at the Large Hadron Collider”, November 2017
9. Christopher Böhm, “Improvements to a search for a supersymmetric partner of the top quark in a di-tau final state with multivariate techniques using data recorded with the ATLAS detector”, November 2017
10. Moritz Wiehe, “Testbeam Studies of Silicon Strip Detectors for the ATLAS ITk-Upgrade”, November 2017

Group Schumacher

PhD Theses

1. Holger von Radziewski, “Search for Neutral Higgs Bosons of the Minimal Supersymmetric Standard Model in the $\tau_e\tau_\mu$ Decay Mode at $\sqrt{(s)}$ = 7 TeV with the ATLAS Detector”, March 2014.

2. Anna Kopp, “Search for charged Higgs bosons decaying via $H \to \tau\nu$ fully hadronic final states with the ATLAS detector at the LHC”, September 2015.

3. Christian Schillo, “Search for the Standard Model Higgs Boson and Test of CP Invariance in Vector-Boson Fusion Production of the Higgs Boson in the Fully Leptonic $H \to \tau\tau \to ll4\nu$ Final State in Proton-Proton Collisions with the ATLAS Detector at the LHC”, May 2016.

Diploma/Master Theses

1. Michaela Oettle, ”Studien zur CP-Natur des Higgs-Bosons mithilfe von Optimalen Observablen in der Vektorbosonfusion im Zerfallskanal $H \to \gamma\gamma$ mit dem ATLAS-Detektor”, July 2014.

2. Marco Zimmermann, ”Investigation of the Higgs-gluon Coupling Tensor Structure in the Decay Channel $H \to \gamma\gamma$ with the ATLAS Experiment”, December 2014.

3. Ulrich Baumann, ”Search for the lepton-flavor-violating Higgs boson decays $H \to \tau\mu$ and $\tau\ell$ in di-lepton final states with the ATLAS experiment”, October 2015.

4. Alena L”osle, ”Study of CP properties of the Higgs boson produced in gluon fusion with two jets in proton-proton collisions at $\sqrt{s}$ = 8 TeV with the ATLAS Experiment”, November 2015.

5. Fabian Becherer, ”Estimation of background processes with a jet misidentified as a hadronically decaying τ-lepton and measurements of Simplified Template Cross Sections in the $H \to \tau_{lep}\tau_{had}$ decay channel with the ATLAS experiment at $\sqrt{s}$ = 13 TeV”, September 2017.

6. Benjamin Rottler, ”Optimizing the measurement of the signal strength for Higgs-boson production in the $H \to \tau\tau$ decay using multivariate techniques at $\sqrt{s}$ = 13 TeV with the ATLAS detector”, October 2017.

Group Schumann

PhD Theses

1. Katharina Schmidt, Transverse target spin asymmetries in exclusive vector meson muoproduction, 2014.
`https://freidok.uni-freiburg.de/data/9893`

2. Johannes ter Wolbeek, Azimuthal asymmetries in hard exclusive meson muoproduction off transversely polarized protons, 2015.
`https://freidok.uni-freiburg.de/data/10172`

3. Stefan Sirtl, Azimuthal asymmetries in semi-inclusive deep-inelastic hadron muoproduction on longitudinally polarized protons, 2015.
`https://freidok.uni-freiburg.de/data/11139`

4. Christopher Regali, Exclusive event generation for the COMPASS-II experiment at CERN and improvements for the Monte-Carlo chain, 2016.
`https://freidok.uni-freiburg.de/data/11449`

5. Lukas Bütikofer, From XENON100 to XENON1T: direct dark matter searches with dual phase liquid xenon time projection chambers, 2017.

6. Tobias Szameitat, New Geant4-based Monte Carlo software for the COMPASS-II experiment at CERN, 2017.
`https://freidok.uni-freiburg.de/data/11686`

7. Philipp Jörg, Deeply virtual compton scattering at CERN - what is the size of the proton?, 2017.
`https://freidok.uni-freiburg.de/data/12397`

8. Basho Kaminsky, Optimizing Liquid Xenon TPCs, 2017.

9. Maximilian Büchele, Development of Time-to-Digital Converter based on Field-Programmable Gate Arrays, 2017.

Diploma/Master Theses

1. Paul Kremser, Optimierung und Charakterisierung eines Transientenrekorders für Teilchenphysikexperimente, 2014.
2. Arne Gross, Extraction of cross sections for Rho and Phi muoproduction at the COMPASS experiment, 2014.
3. Steffen Landgraf, Luminosity Calculation for the COMPASS Experiment using the F2 Structure Function, 2015.
4. Carl Schaffer, Development of a FPGA based trigger module for the COMPASS-II experiment, 2017.

Group van der Bij

Diploma/Master Theses

1. Michael Ruf, ”Quantum Effective Action and Heat Kernel Methods in Curved Spacetime”, 2017.

Part III

Teaching

Chapter caption: Top left: Experimental Physics lecture in the renovated large lecture hall. Top right: Experiment in the *Advanced Physics Laboratory*. Bottom: BSc students attending the lecture *Introduction to Experimental Physics* held by B. von Issendorff with the assistance of H. Wentsch.

1.1 Overview

The Institute of Physics offers its students a broad variety of courses ranging from mathematical preparatory classes, over bachelor- and master-level courses to specialized physics lectures and seminars. The taught subjects cover topics from fundamental basic principles to practical applications with early exposure to contemporary modern research. Since basic knowledge in physics is also required in many other natural science disciplines our institute contributes to external study programmes by offering dedicated lectures and laboratory classes to various other faculties.

Various course formats are offered in order to train the students in basic and advanced physics as well as to teach the necessary skills. Fundamental and specialized physical content is taught in different **lectures**, with the number of participants ranging from 100–400 in the large experimental and theoretical physics lectures to 10–15 in advanced elective courses. In all degree programmes the lectures are accompanied by **tutorials**/**exercises** with typically less than 15 participants each. In our bachelor and master programmes **seminars** are implemented as central modules, where students give talks on a topic of current research. These formats train the participants in handling scientific literature and provide skills in presenting and discussing scientific topics. Each term, the research groups offer various seminars for bachelor students and term paper seminars for master students covering all three main research fields at the institute. In several practical **laboratory courses** for bachelor and master students the participants perform basic and advanced physics experiments in teams of two and obtain hands-on experience in running an experiment, as well as analyzing and presenting their results. For their **final thesis work**, the students join a research group at the Institute of Physics or one of the associated and participating research institutes.

At the Institute of Physics students can currently enrol in the following modular degree programmes:

- **Bachelor of Science (BSc) Physics**
  The BSc programme started in winter term 2008/09. It encompasses six terms with a total workload of 180 credit points (CP). The degree programme has been successfully accredited in 2015.

- **Master of Science (MSc) Physics**
  This English-taught MSc programme started in winter term 2011/12. It encompasses four terms with a total workload of 120 CP. The degree programme has been successfully accredited in 2015.

- **Master of Science (MSc) Applied Physics**
  This English-taught MSc programme started in winter term 2016/17. It encompasses four terms with a total workload of 120 CP. This degree programme explicitly includes contributions from associated institutes of the university, the university medical center and the local Fraunhofer Institutes.

- **Polyvalent two-subject Bachelor Physics (with teacher training option)**
  The Bachelor programme started in winter term 2015/16. In this programme students study physics in combination with a second subject. It encompasses six terms with a total workload of 180 credit points (75 CP each subject and 30 CP didactics and Bachelor thesis). The Polyvalent Bachelor in combination with the Master of Education has substituted the previous teacher-training for secondary schools (*Erstes Staatsexamen* / first state examination) in winter term 2015/16.

- **Master of Education (MEd)**
  The programme will start in winter term 2018/19. It encompasses four terms with a total workload of 120 CP. In combination with a second subject the programme qualifies for teaching physics at secondary schools.

The evolution of the number of new enrolments in each course programme since the introduction of the BSc programme in 2008/09 is summarised in Fig. 1.2. The number of enrolments in the BSc programme has steadily increased over the initial years reaching a level of approximately 100 beginners per

Figure 1.1: Students working in the beginners physics lab.

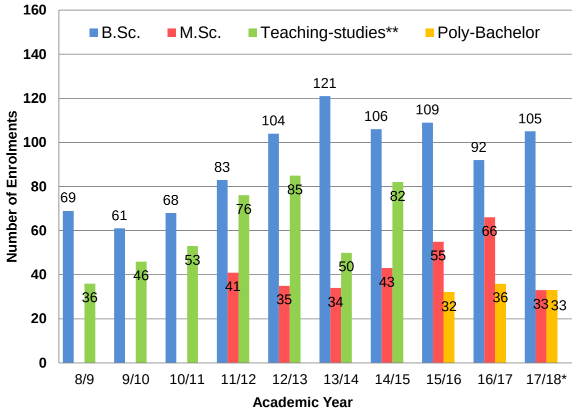


Figure 1.2: New enrolments in our degree programmes per academic year. Enrolment to the BSc and Poly programmes is possible only for the winter terms, to the MSc programmes for winter and summer terms. (*For the academic year 17/18 only MSc-enrolments for the winter term contribute to the graph. **In winter term 2015/16 the Teaching-studies programme has been replaced by new polyvalent Bachelor in combination with a Master of Education, which will start in winter term 2018/19.)

academic year over the last few years. Enrolments in the MSc programme follow the same trend as the bachelor enrolments with a delay of 3 years (i.e. the duration of the bachelor). The number of beginners in the teaching-studies programme showed originally a similar trend as for the bachelor programme until the introduction of the new Polyvalent Bachelor, replacing the Teaching-study programme in winter term 2015/16. Due to organizational uncertainties and ambiguities in the regulations the number of enrolments in this new programme initially dropped to a significantly lower level as before for the Teaching-study programme, but is expected to hopefully rise again with the introduction of the Master-of-Education in winter term 2018/19.

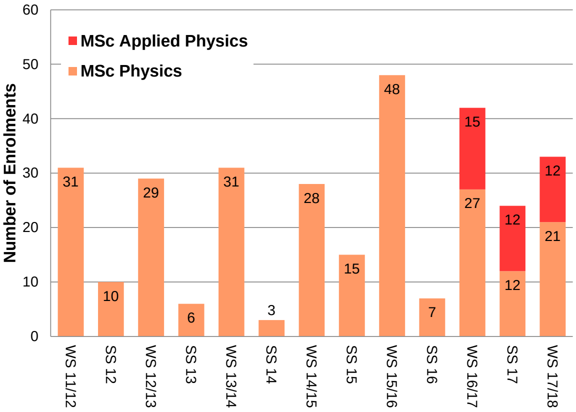


Figure 1.3: New enrolments in our MSc programmes per semester.

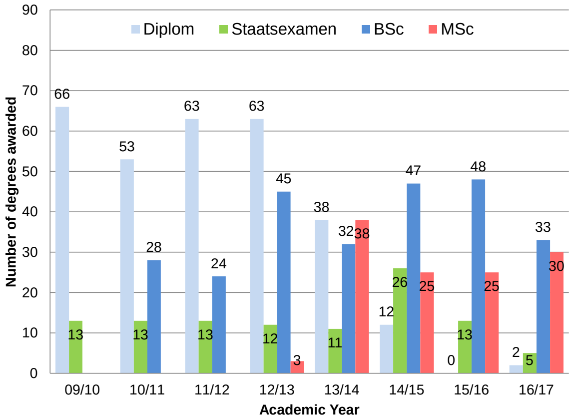


Figure 1.4: Number of degrees awarded since winter semester 2009.

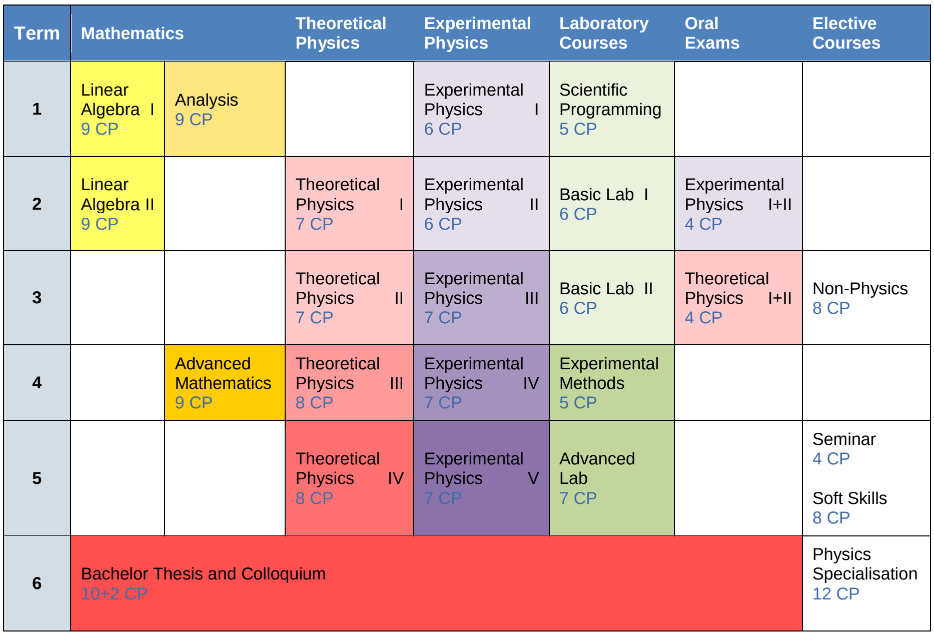
The number of degrees awarded (see Fig. 1.4) shows some fluctuations over the years with the BSc and MSc degrees having replaced the Diplom. Notably, the number of MSc degrees has not yet reached the level of the number of the Diplom degrees in previous years. However, it is expected that the general increase in master enrolments since 2015/16 will also result in an increased number of master degrees awarded within the next years.

1.2 Degree Programmes

1.2.1 BSc Physics

For the enrolment in the BSc programme no specific requirements have to be fulfilled by the candidates apart from the general qualification for university entrance. However, they have to take part in an online self-assessment (http://www.osa.uni-freiburg.de/physik) in order to check whether their interests and expectations about the study programme are sufficient and realistic.

The compulsory part of the course programme provides basic knowledge and key competences in the areas of mathematics, theoretical physics, experimental physics, and laboratory work. These classes also include an introduction course in scientific programming and basic knowledge in statistics, electronics and detection techniques. The remaining one fifth of the course programme can be chosen according to the preferences of the students. This allows the students to specialise already during the BSc programme and to get a first insight into mod-



Term	Mathematics		Theoretical Physics	Experimental Physics	Laboratory Courses	Oral Exams	Elective Courses
1	Linear Algebra I 9 CP	Analysis 9 CP		Experimental Physics I 6 CP	Scientific Programming 5 CP		
2	Linear Algebra II 9 CP		Theoretical Physics I 7 CP	Experimental Physics II 6 CP	Basic Lab I 6 CP	Experimental Physics I+II 4 CP	
3			Theoretical Physics II 7 CP	Experimental Physics III 7 CP	Basic Lab II 6 CP	Theoretical Physics I+II 4 CP	Non-Physics 8 CP
4		Advanced Mathematics 9 CP	Theoretical Physics III 8 CP	Experimental Physics IV 7 CP	Experimental Methods 5 CP		
5			Theoretical Physics IV 8 CP	Experimental Physics V 7 CP	Advanced Lab 7 CP		Seminar 4 CP Soft Skills 8 CP
6	Bachelor Thesis and Colloquium 10+2 CP						Physics Specialisation 12 CP

Figure 1.5: Overview of the six semester BSc course programme together with the allocated ECTS-credit points (CP).

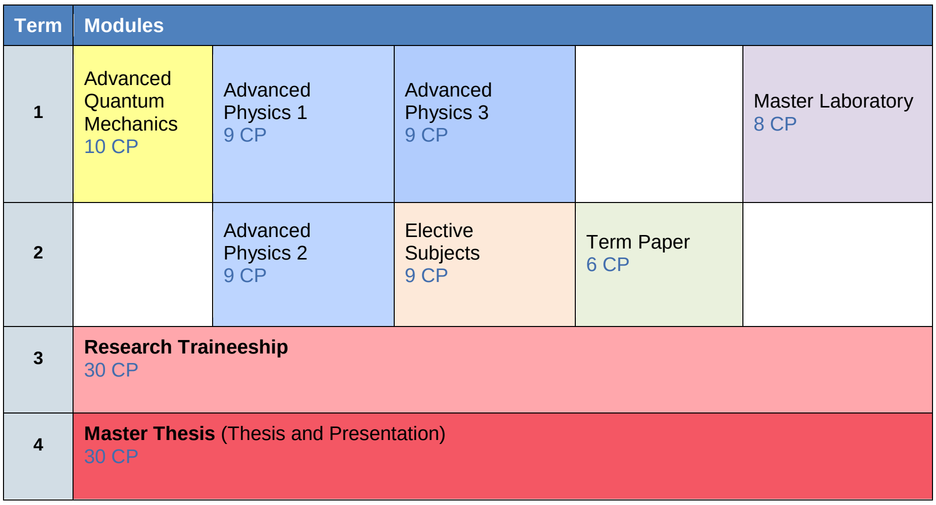
ern research topics by choosing up to two lectures and a seminar. Elective subject classes are offered not only by lecturers from the Institute of Physics, but also from the associated institutes. Soft skills are obtained in specific classes at the *Zentrum für Schlüsselqualifikationen ZFS* (Centre for Key Competences), e.g. in the fields of foreign languages, scientific writing, and communication and presentation techniques. In addition, one or two classes are required to be in a non-physics discipline. An overview of the BSc course programme is given in Fig. 1.5. The BSc studies are completed by the bachelor thesis work. Students perform for the first time a small and independent research project during a period of three months in one of the research groups at the Institute of Physics or at the associated institutes. The project closes with documenting their work and their scientific results in a written thesis and give a faculty-public presentation on their thesis work.

As there are no specific admission requirements, the drop-out rate is at the level of 40% to 50% with most of these students leaving the challenging course programme already during the first year. This rate is comparable to other BSc physics programmes in Germany. However, most of the students, who drop out of the BSc programme in physics, do not leave university, but enrol in a different discipline, e.g. in engineering sciences. In this case the accomplished academic achievements in the BSc physics programme are usually accredited in the new programme so that the students can enter the new discipline in an advanced term.

1.2.2 MSc Physics

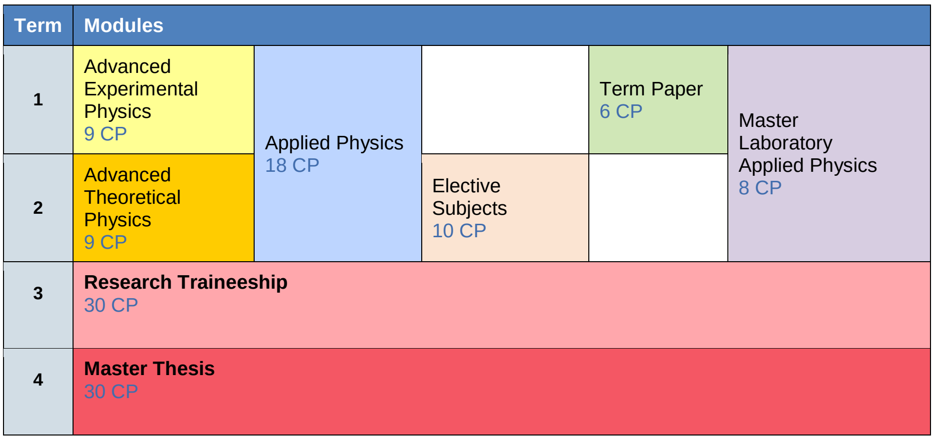
The MSc programme in Physics is taught in English in order to provide additional skills in the dominating academic language English to the native German students and to attract also students from non-German-speaking countries. Application to the MSc programme is possible in both winter and summer terms. The selection and admission process is undertaken by a MSc Admission Committee.

The MSc Physics programme (see overview in Fig. 1.6) provides a comprehensive scientific education in advanced physics, together with a specialisation in a particular field during a final, one-year long research phase, during which students participate in a current project of one of the research groups at the Institute of Physics or at the associated institutes. In the first MSc year, participants consolidate their knowledge in advanced theoretical and experimental physics. Advanced quantum mechanics and the advanced laboratory are mandatory classes. Students can choose each term among various ”Term Papers”, where they learn to give oral presentations in English on a topic of modern research, accompanied by a written ”paper-style” summary in English. Three courses have to be choosen from state-of-the-art topics in the main research areas of the depart-



Term	**Modules**				
1	Advanced Quantum Mechanics 10 CP	Advanced Physics 1 9 CP	Advanced Physics 3 9 CP		Master Laboratory 8 CP
2		Advanced Physics 2 9 CP	Elective Subjects 9 CP	Term Paper 6 CP	
3	**Research Traineeship** 30 CP				
4	**Master Thesis** (Thesis and Presentation) 30 CP				

Figure 1.6: Overview of the four semester MSc Physics programme together with the allocated credit points (CP).



Term	**Modules**				
1	Advanced Experimental Physics 9 CP	Applied Physics 18 CP		Term Paper 6 CP	Master Laboratory Applied Physics 8 CP
2	Advanced Theoretical Physics 9 CP		Elective Subjects 10 CP		
3	**Research Traineeship** 30 CP				
4	**Master Thesis** 30 CP				

Figure 1.7: Overview of the four semester MSc Applied Physics programme together with the allocated credit points (CP).

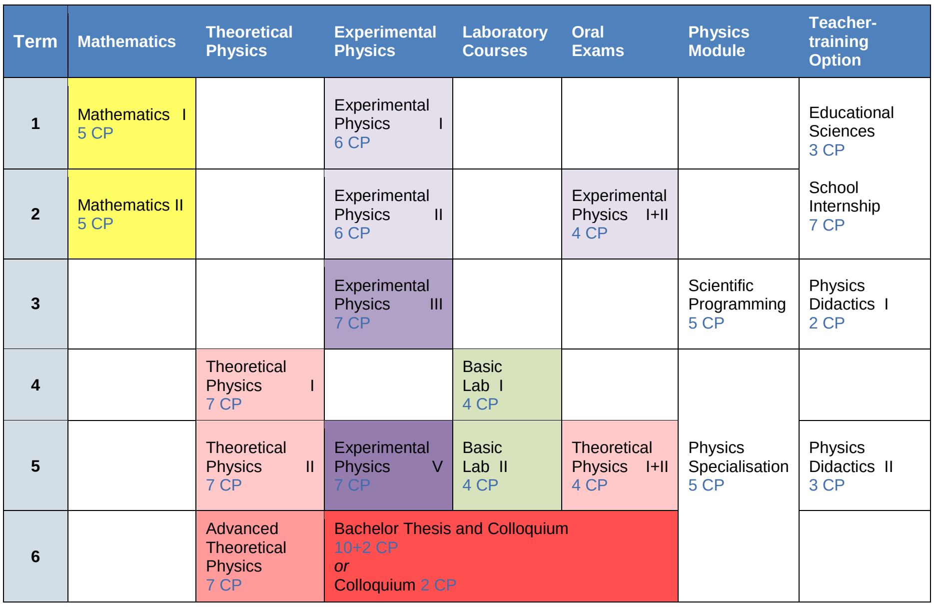
ment. In addition, students can select from a variety of elective courses in physics, from the MSc or Master of Arts (MA) programmes of other faculties. During the second year, the students carry out their Research Traineeship and their Master Thesis project. The study programme concludes with the submission of the MSc thesis and a faculty-public presentation of the results.

By advertising the programme e.g. on the web pages of the *Deutscher Akademischer Austauschdienst DAAD* (German Academic Exchange Service), we were able to increase the ratio of international students in the programme since its introduction from a few % to currently 18%. The drop-out rate in the master programme is continuously at a low level of only a few percent.

1.2.3 MSc Applied Physics

Following the advice of the Scientific Advisory Board after its first visit in 2014, the Institute of Physics implemented a Master of Applied Physics programme. In this frame, funding could be attracted for a new professorship for ”Applied Theoretical Physics - Computational Physics” financed through the ”Master 2016” programme of the Baden-Württemberg Ministry of Science, Research and the Arts. Prospective candidates have been interviewed in March 2017 and an offer to the first-placed candidate of the list is currently under negotiation.

The module plan of the MSc Applied Physics programme is shown in Fig. 1.7. In the first year, participants consolidate their knowledge in advanced experimental and theoretical physics. They can choose among various Term Paper seminars and may se-



Term	Mathematics	Theoretical Physics	Experimental Physics	Laboratory Courses	Oral Exams	Physics Module	Teacher-training Option
1	Mathematics I 5 CP		Experimental Physics I 6 CP				Educational Sciences 3 CP
2	Mathematics II 5 CP		Experimental Physics II 6 CP		Experimental Physics I+II 4 CP		School Internship 7 CP
3			Experimental Physics III 7 CP			Scientific Programming 5 CP	Physics Didactics I 2 CP
4		Theoretical Physics I 7 CP		Basic Lab I 4 CP		Physics Specialisation 5 CP	
5		Theoretical Physics II 7 CP	Experimental Physics V 7 CP	Basic Lab II 4 CP	Theoretical Physics I+II 4 CP		Physics Didactics II 3 CP
6		Advanced Theoretical Physics 7 CP	Bachelor Thesis and Colloquium 10+2 CP *or* Colloquium 2 CP				

Figure 1.8: Overview of the course programme in Physics of the Polyvalent two-subject Bachelor (CP - ECTS credit points).

lect from a variety of elective courses in physics, or from the master programmes of other faculties. In the large *Applied Physics* module and in the *Master Laboratory Applied Physics* many courses and experiments are contributed, to a substantial extend, by other faculties and external institutes (e.g. University Hospital, Fraunhofer Institutes, KIS), offering the possibility for specialization in a particular area of applied physics, such as optical technologies, physics in the life science, or interactive and adaptive materials. In their final year the students pursue their Research Traineeship and their Master Thesis project.

The new Master program started with the winter term 2016/2017, and 40 students are currently enrolled after a period of now three terms. With 33% international students and only 50% of the participants coming from our own bachelor in Freiburg compared to 18% international students and 76% participants from Freiburg in the regular MSc Physics, the new master programme is not competing with the established Master of Physics but attracts additional students and to a great extend international participants to Freiburg. As envisioned by the Scientific Advisory Board, 50% of the lectures were offered by colleagues from outside the Institute of Physics, including the Fraunhofer Institutes and the Faculties for Biology, Medicine and Environment & Natural Resources. For the programme, a dedicated new *Master Laboratory Applied Physics* has been established. Again, 50% of the experiments in this new master lab are contributed by external colleagues.

In order to serve for sustainable teaching activities of our external colleagues, the Institute of Physics co-opted Professor Stefan Rotter, whose field of research and teaching is neurobiology, from the Faculty for Biology and Professor Michael Bock, whose field of research and teaching is magnetic resonance imaging, from the Faculty of Medicine. For Dr. Frank Kühnemann from the Fraunhofer Institute for Physical Measurement Techniques (IPM), the institute transferred his Habilitation from the Faculty for Physics at the University of Bonn to our faculty. The now retired director of the Fraunhofer Institute for Solar Energy Systems (ISE), Prof. Eicke Weber, was a professor at the Institute of Physics. Recently, two new directors of the ISE were appointed.

1.2.4 Polyvalent Bachelor & Master of Education (MEd)

Starting with the winter term 2015/2016 the former Teaching-studies programme (*Staatsexamen*) in the federal state of Baden-Würtemberg was replaced by a consecutive bachelor-master study. In the frame of the new bachelor programme *Polyvalent two-subject Bachelor* prospective teachers are able to study two major subjects in a single bachelor degree. An overview of the study programme in physics comprising 80 ECTS credit points is shown in Fig. 1.8. By selecting the teacher-training option the programme incorporates in addition to the classes in the scientific disciplines (lectures, tutorials and lab courses) also didactics courses in each of the two major subjects, classes in general educational sciences, and a school internship. The final bachelor thesis can be written in either one of the main subjects.

If physics is one main subject it is generally recommended to select mathematics as second subject, since in this case the required mathematical knowledge is covered and no additional mathematics lectures have to be selected. In this case the students can freely choose two elective courses in physics instead, allowing to gain some specialized physics knowledge.

Starting in winter term 2018/2019 the new Master-of-Education (MEd) will be implemented as consecutive master programme for graduates of the Polyvalent Bachelor (with teaching-training option). The programme comprises courses in the scientific discipline, subject didactics in each of the two major subjects, classes in general educational sciences, and an internship at a secondary school of 12 weeks duration. The final master thesis can be written in either main subject, or alternatively in educational sciences.

Recently, the university has entered a cooperation with the *Pädagogische Hochschule* (PH, University for Education) in Freiburg, so that students of the Polyvalent Bachelor and the MEd programmes attend their basic and advanced courses in subject didactics at the PH.

As discussed in the previous section the number of enrolments in the Polyvalent Bachelor programme is significantly lower than for the former Teaching-training studies (see Fig. 1.2). This trend has been also observed in other disciplines and also at other universities in Baden-Württemberg and has been attributed to the initially rapid introduction of the study programme for prospective teachers without providing a detailed outline of the changes. With the consolidation of the Polyvalent Bachelor and the introduction of the Master of Education (MEd) programme it is expected that the number of enrolments will increase again in the near future.

The current drop-out rate in the Polyvalent Bachelor programme is currently at the same level as in the BSc programme. Also in this case, most of the students dropping out do not leave the university, but enrol in a different discipline, where the accomplished academic achievements can usually be accredited.

1.3 Postgraduate Studies / PhD Programme

A significant fraction of master graduates continues with postgraduate studies aiming for the PhD degree ”Dr. rer. nat.” awarded by the joint Faculty for Mathematics and Physics. Since 2016 at the University of Freiburg new PhD regulations are in effect, which require that the candidate and his or her supervisor sign a supervision agreement prior to the PhD project. In this agreement the candidate and supervisor comply to regular official meetings where they assess their progress and discuss and plan the further time-line for the thesis. The supervisor reports the progress to the doctoral examination board.

For obtaining a PhD degree no structured course programme is mandatory. However, at the Institute of Physics three Research Training Groups, funded by the *Deutsche Forschungsgemeinschaft DFG* (German Science Foundation), are currently hosted, which offer an educational programme for the participating PhD students including specialised lectures, seminars, topical workshops and annual conventions. The established Research Training Groups promoting young researchers cover all three main research areas at our institute and comprise the Research Training Group (RTG 2044) ”Mass and Symmetries after the Discovery of the Higgs Particle at the LHC”, the International Research Training Group (IRTG 2079) ”Cold Controlled Ensembles in Physics and Chemistry”, and the International Research Training Group (IRTG 1642) ”Soft Matter Science: Concepts for the Design of Functional Materials”.

In total 155 PhD students are currently performing the research for their dissertation in physics, about two thirds directly at the Institute of Physics and one third at one of the associated research institutes or in the group of a co-opted member.

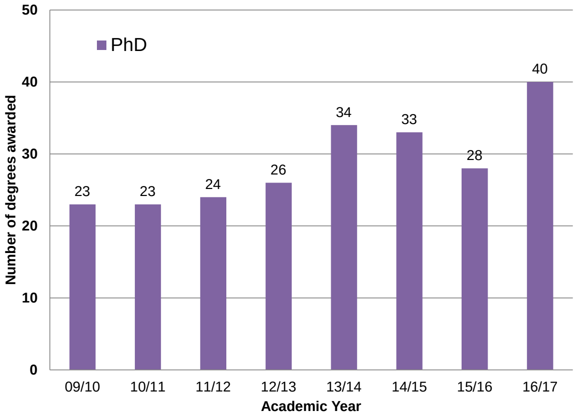


Figure 1.9: Number of PhD degrees in Physics awarded during the last eight academic years.

1.4 Teaching Export

The Institute of Physics supplies the largest teaching supports to other departments and faculties at the University of Freiburg. Basic physics knowledge is mandatory in many course programmes or recommended as an elective subject in nine BSc, five MSc and three *Staatsexamen* programmes, i.e. in BSc Biology, BSc and MSc Chemistry, MSc Chrystalline Materials, BSc Embedded Systems, BSc Environmental Sciences, BSc Geography, BSc and MSc Geology, BSc and MSc Computer Science, Bsc and MSc Mathematics, BSc Microsystems Engineering, and state examinations in Medicine, in Dentistry, and in Pharmacy. In some of the programmes, the external students participate in the basic experimental physics lectures of the regular BSc physics programme, e.g. students from engineering sciences, computer science and mathematics. However, for students from other natural sciences, and from medicine and pharmacy dedicated lectures, tutorials and laboratory classes are offered. Nearly thousand students from all over the university participate in these dedicated lectures and laboratory courses each year.

1.5 Office for Studies

The Office for Studies is the central contact point for the students at the Institute of Physics. The examination office constitutes a central part of this office, offering advice and information on examination details and procedures during the regular consultation-hours. Two study councellors are another important corner stone, who offer individual advice and guidance with respect to the study plan and general aspects of the study programmes, one for the BSc/MSc programmes and one for the Polyvalent Bachelor/MEd (Teacher) programmes. Both also coordinate the course programmes. The official head of the Office for Studies is the Dean of Studies, who signs responsible for all affairs related to teaching and examinations. In addition three professors, one from each main research area, offer consultations on specific questions related to the particular research field.

1.6 Quality Management

All basic courses including tutorial classes and all specialised courses are evaluated with a questionnaire each term. The survey is organised by the student representatives and programme coordinator in cooperation with the central evaluation service (ZES) of the university. The evaluation consists of a statistical analysis and a collection of individual comments by the students. Direct feedback is given to the lecturers and to the tutors. This enables continual improvement in the quality of teaching.

New developments and structural changes in the course programme and all issues related to teaching are discussed in regular meetings of the Committee for Study Affairs in Physics. The committee consists of four students, two members from the academic staff and four professors.

1.7 Teaching Infrastructure

The Institute of Physics offers a competitive infrastructure for its students. It provides a large reference library with many copies of standard textbooks and a large variety of specialised literature for advanced studies. A central piece of the library is a large reading room, which offers fifty places to students for individual literature studies. Two computer pools, each equipped with sixteen modern desktops, allow students to exercise their skills in programming, using scientific software and perform studies online. The computer pools are also used regularly in the tutorial classes accompanying several lectures. Additionally, a large number of open office space and work rooms for private research or group discussion is provided: the ”Common Room” on the top floor of the physics high-rise building, the “Garden of Physics”, and nine equipped discussion rooms encompassing approximately 50 temporary work places in the basement of the West Building. The department holds three lecture halls with 340, 150, 60 seats, respectively, and six seminar rooms with up to 30 seats each. The two large export lectures ”Physics for Medical and Pharmacy Sciences” and ”Physics for Natural Sciences” are nominally attended by more than 380 and 600 students, respectively, so that the capacity of the large lecture hall (340 seats) is insufficient. Therefore, a modern video recording and transmission system has been installed, which enables live streaming of the lectures via the streaming channel of the Institute of Physics.

1.8 Support for Students

1.8.1 New Students

The body of student representatives (Fachschaft Physik) offers various forms of assistance to students, particularly to new students at the start of their studies and during their first semesters. They pro-

Figure 1.10: Physics lecture in the large lecture hall.

vide practical help in organising the students' life and in planning their studies and their individual time tables. Before the beginning of the winter term, a one-week long ”Welcome and Kick-Off event” is organised, which helps students in a viable transition from school to university. The welcome week of the Fachschaft incorporates guided tours of the natural science campus, the libraries and the physics institute, as well as an overnight stay at a local hut, where the new students get to know each other and connect to students in higher semesters.

Welcome and introduction seminars are organised by the Dean of Studies and the study counsellors during the first week of each teaching period. The presentations give an overview of the study programme, the examination procedures and regulations and the various options to obtain advice and support. General help is also provided by the central Service Centre for Studies (SCS).

Starting with the winter term 2017/2018 the Institute of Physics implemented a new mentoring programme for first year students where allocated professors and lecturers meet with up to five students six times during the first year of their studies. In these meetings students and mentors especially discuss their expectations, in particular also the requirements in terms of the personal responsibility and motivation of the students. Furthermore, these meetings enable the students to personally get to know one of the professors or lecturers which is typically difficult in the large first year's lectures. We hope that this programme will help especially students who have the talent to study physics but do not succeed to deal with the challenges of the transition from school to university.

1.8.2 Gender and Diversity

The fraction of female students in the course programmes is currently at the level of 18%, 14% and 27% in the BSc, MSc and teacher-training (including Polyvalent Bachelor) programmes, respectively. By the appointments of Beate Heinemann and Tanja Schilling in 2017 as new professors, the fraction of female professors at the Institute of Physics could be increased to 14% (3 of 21), which is above the average of 10% at German universities. Hopefully this will have positive impact also on female students at the institute who plan to pursue a scientific career in physics.

In order to increase the number of female students in physics and to help women in organising their studies and career planning, specific programmes have been implemented:

Each year a special open day originally for pupils at secondary schools is organised, where they are informed about the study programmes and the research activities at the institute and also have the possibility to participate in small practical workshops organised by the research groups. Originally, the event was only available for female pupils but has been opened recently also for male pupils. Nevertheless, the institute aims to especially deploy female PhD students as supervisors of the workshops, which may act as role models for the students.

A specific mentoring programme MeMPhys (mentoring in mathematics and physics) has established at the Faculty for Mathematics and Physics. Each interested student is mentored by an experienced student in a tandem approach. In addition, specific seminars and social events are organised by coordinators of the MeMPhys programme in cooperation with the faculty member responsible for equal opportunities. Although this programme was initially designed only for female students, the event has now been opened for all genders.

1.8.3 International Students

Dedicated support is provided to students from foreign countries, who enrol in the MSc programme or spend several months to two terms in Freiburg with an international exchange programme. The International Office of the university provides general help, particularly related to questions concerning housing and visa issues. The EU Office provides additional support for students participating in the European exchange programme ERASMUS. The Institute of Physics also has its own ERASMUS counsellor who is organising the stays of about 15–20 students each year who participate in the student exchange programme and go for one or two terms to one of the partner universities abroad, and of the 5–10 students from foreign countries are visiting the Institute of Physics. The *Studierendenwerk Freiburg Schwarzwald* (Student Services Freiburg) offers advice to students looking for an apartment or a possibility to finance their stay in Freiburg. Language courses in German are offered regularly at various levels by the *Sprachlehrinstitut SLI* (Language Teaching Centre). Help with the regulations for applications and enrolments is provided by the International Admissions and Services (IAS) in the Service Centre for Studies (SCS).

Currently 6% international students are participating in the BSc programme, which requires them to have an advanced proficiency in German (C1-level). The English-taught MSc programmes are attracting much more students from abroad, with a fraction of currently 21% internationals. Beginning in winter term 2017/18, the state of Baden-Württemberg implemented tuition fees of 1500 € per term for international students from non-EU countries. Some students will be exempted from the tuition fees if they fulfill specific criteria. These tuition fees led to a reduction of enrolments from non-EU countries in the winter term 2017/18 by 30% counteracting the ambition of the Universtiy of Freiburg to promote internationalisation.

1.9 Outreach - Promoting the Physics Programmes

A large number of well-trained physicists and physics teachers is a benefit for the future of our society. In order to attract more students to the field of physics, several measures are followed to promote the quality and variety of the course programmes at our institute and to inform about the research activities.

Each year an ”Open Day” for interested pupils from secondary schools is organised by the Office for Studies. The pupils are informed about the content of the various course programmes in physics and the research activities at the Institute of Physics and the associated institutes. They get the opportunity to discuss with the Dean of Studies and the study counsellors about their plans to study physics. Specific lectures covering aspects of experimental and theoretical physics adapted to the level of secondary school students are held by professors. About 100 to 200 pupils attend this event each year.

In the module *Berufs- und Studienorientierung am Gymnasium BOGY* (Orientation for Profession and Studies at Secondary Schools) pupils at the age of sixteen to seventeen have to visit a service provider, company, research institute or research group at a university to perform an internship for one week. Each year on average ten pupils choose to join a research group at the Institute of Physics for this project.

The Institute of Physics participates every year in a science fair called ”Science Days”, held at the theme park in Rust close to Freiburg. During this three-day event pupils from secondary schools can interactively perform experiments, and are informed about the opportunities to study physics in Freiburg.

The particle physics groups participate in the international Master Classes ”Hands on Particles Physics”, organised simultaneously at 210 institutes in 52 countries worldwide every year in March. Secondary school pupils have the opportunity to attend lectures on particles physics and to perform analysis of data from collider experiments themselves during the course of one day. At the end of each day, the participants join an international video conference for the discussion of their results. In addition, teachers can also invite scientists from the Institute of Physics to visit their school for a day and perform the Master Classes on site. On average five such visits take place every year.

Other activities for the general public include the participation in the biannual two-day long Science Market centrally organised by the University of Freiburg in the centre of the city and the well attended public Christmas Lectures in physics every year.

A comprehensive list of the outreach activities of the Institute of Physics is given in Chapter V.

Part IV

Infrastructure

Chapter caption: Physics lecture in the newly renovated main lecture hall (Großer Hörsaal Physik).

1.1 Buildings of the Institute

With few exceptions all facilities used by and available to the researchers, students, and administration of the Institute of Physics are located at the Physics Campus (see overview map in Fig. 1.1). This campus is part of the University's Natural Sciences Campus (Institutsviertel), just about 1000 m away from the Freiburg city center. The institute and its facilities are distributed over several buildings.

With its eleven floors, the *Physics High-Rise* (Physik Hochhaus) provides office spaces for theoretical and experimental research groups, some smaller, basic experimental laboratories, the offices of the IT support group, as well as two large lecture halls and several seminar rooms for tutorial classes in the first floor. The eleventh, top floor hosts the institute's Common Room.

The *Gustav-Mie Building* (Gustav-Mie Gebäude) offers high-quality experimental lab spaces and further offices. Several chemical labs and clean rooms are also located here. In addition, the Gustav-Mie building hosts the advanced laboratory courses with the corresponding experiments on the second floor, as well as computer pools for students, a seminar room and the students' "social room".

The *Low-Rise Building*, which connects the Physics high-rise and the Gustav-Mie building, provides space for the mechanical and electrical workshops, and the electronic design and development lab. In addition, the experimental labs of four research groups are located here on an iterim basis. The tower for the old Van de Graaf accelerator, that has been dismantled already in the last century, remained essentially unused in the last years. It was fully refurbished from August 2017 to February 2018 to host the laboratory of the new astroparticle physics group.

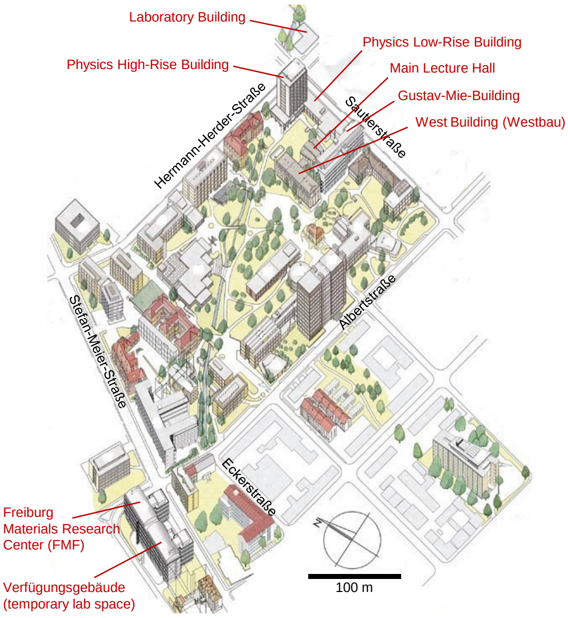


Figure 1.1: Map of the Natural Sciences Campus of the University (Institutsviertel) with the physics buildings being labeled.

Figure 1.2: The main lecture hall (*Großer Hörsaal*) after its renovation in December 2017.

The *West Building* (West Gebäude) houses additional seminar rooms, the offices of the institute and the student administration, the library of the Institute of Physics, and the offices for some theoretical research groups. Furthermore, there are two meeting rooms furnished with modern multimedia equipment and work space for students. The *Fachschaft Physik* (body of student representatives) has its own rooms in the basement.

The *Main Lecture Hall* (Großer Hörsaal Physik) is located in a dedicated building in the center of the physics campus. It also provides additional rooms for the preparation and storage of demonstration experiments. The building with a capacity of $\sim$350 seats has been renovated from February to December 2017 and is now equipped with state-of-the-art building automation and modern multimedia equipment.

The *Laboratory Building* (Praktikumsgebäude) just across the road hosts the experimental setups and lab spaces of the introductory physics lab courses for physics students and students of other natural sciences (teaching export).

Given the size of the institute, the available space for offices and laboratories is not sufficient. After the transformation of the old accelerator tower into a laboratory, there is currently no further space available at the physics campus. For this reason, the laboratories and offices of two experimental research groups (Sansone, von Issendorf) are located in the Verfügungsgebäude adjacent to the Freiburg Materials Research Center (Freiburger Materialforschungszentrum, FMF) since many years. This leads to the very unfortunate situation that these groups are located rented space, separated by a distance of 500 m from the work shops and support groups while hampering the direct contact with the physics students and their colleagues.

1.2 General Organization

The Institute of Physics is organized as a 'Department System', which provides central management of the human, financial and other resources. The procurement of research equipment is in the hands of the individual groups.

An essential element of the Department System is that in addition to their individual resources, all full professors participate equally in a common "pool of resources". It provides central infrastructure such as administration, mechanical and electronics workshops, electronic design and development lab, IT support, technical staff, liquid nitrogen supply and further resources. A similar pool also exists for scientific personnel from which positions can be allocated based on demand (largely reflecting the institute's obligations from hiring negotiations), as well as for financing the joint infrastructure and short term needs of individual groups.

The institute's administration comprises the senior manager who also acts as head of administration, the deputy senior manager/head of technical services and four administrators. It manages the human and financial resources, including the various third-party funding from the DFG, BMBF, and EU. Dedicated team assistants, most of whom are working part-time, support the research groups and the administration.

1.3 Workshops and Technical Support Groups

The Institute of Physics operates five central support units, see Fig. 1.3. The Mechanical Workshop (MW), the Electronic Workshop (EW), and the Electronic Design and Development Laboratory offer highly specialized technical services and are essential resources for the experimental physics groups. They constitute a central cornerstone of physics research in Freiburg and their work is internationally recognized thanks their contribution to large-scale multi-national projects such at ATLAS at CERN. The mechanical and electronic workshops regularly train young apprentices as *Feinwerkmechanikern/innen* (precision mechanics) or electricians. Typical numbers are eight and four apprentices for the two units, respectively.

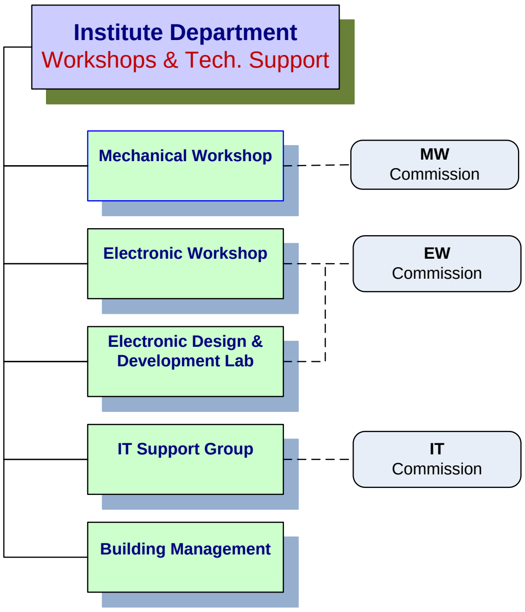


Figure 1.3: Organisation chart of the workshops and technical support groups.

The recently founded IT group provides computing support and advice to the theory groups and some of the experimental research groups. Each unit is lead by a dedicated head with additional support by commissions, which consist of representatives of the workshops and of the professors. The fifth unit takes care of managing the institute's buildings and infrastructure.

1.3.1 Mechanical Workshop

The mechanical workshop has 19 members (plus apprentices). It serves the experimental groups in all their requirements to build and operate their experiments. The workshop supports the researchers starting from the design phase of a project (even though the institute cannot offer dedicated support by a mechanical engineer), to production, assembly/installation and maintenance. The full integration of the workshop into the institute allows for the efficient realization of prototypes, time-critical components, special shapes and new developments, and facilitates solving complicated experimental problems via continuous feedback between workshop and scientists. It considerably reduces experimen-

Figure 1.4: Mechanical workshop at the Institute of Physics.

tal down-times and allows the Freiburg groups to take leading roles in the construction of international large-scale projects. If required, the number of workshop members also allows for mass production. The workshop is conveniently located on the first two floors of the Low-Rise Building, which allows young researchers at the PhD level, but also already during the BSc or MSc thesis, to directly interact with machining experts to realize their own projects.

The workshop team also operates the forklift truck and the various cranes of the institute, and provides general support in larger logistic operations.

The workshop is equipped to manufacture all sorts of high-precision parts, up to sizes of $1.5 \times 0.7\,\mathrm{mm}^2$ (see Fig.1.4). The available manufacturing tools allows achieving essentially any specification currently attainable by state-of-the-art mechanical manufacturing technology. Besides the usual lathe and milling tools the mechanical workshop currently operates

- seven CNC milling machines;
- three of the seven milling centers with four- and five-axis control;
- one CNC turning center;
- two CNC turning centers with driven tools;
- 3-D printer for rapid prototyping;
- welding equipment for stainless steel, aluminum and copper;
- sheet metal working machines for complex designs.

Simultaneous five-axis manufacturing is possible thanks to a CAD/CAM cross linking. Sophisticated parts can be treated by clamping, which enhances the manufacturing efficiency and quality.

1.3.2 Electronic Workshop

The electronics workshop consists of six technicians, who offer a wide range of services, starting from counseling in all electronics related questions, management and provision of electronic parts, assembly of cables and connectors, and repair and maintenance of custom-made and commercial equipment. If required, equipment in the research laboratories is also being checked in terms of safety. The core expertise of the workshop is the development and production of instruments and measurement systems with a special emphasis on CAD aided printed circuit board (PCB) layout routing and in-house production of two-layer print boards and well as the procurement of multi-layer PCBs and SMD parts.

To this end the workshop is equipped with all required standard tools and machines. PCBs with a small number of electronic components are produced by hand using stereo microscopes. For projects involving many components, protoypes or small batch series, an automatic pick & place machine (Fritsch PlaceALL 510) is employed. It features a broad range of components and allows for a flexible realization of complex projects. For such projects, the workshop also operates a large high-end reflow soldering oven (Rehm) while smaller ones are handled using a compact table-top oven.

1.3.3 Electronic Design and Development Lab

This group of four electronics engineers supports the experimental research groups of the Institute of Physics. It provides consulting and proof-of-concepts for new designs in first instance. The expertise in high-speed or ultra-sensitive electronic sensor devices for research is its prime specialty. The group offers the full range portfolio from analog, e.g., low voltage sensors or power electronics, to digital, e.g., high speed FPGA or micro-controller based. During developments the group makes vast use of state-of-the-art ECAD tools for the design and simulation of new circuits. Moreover, the group operates a clean room for the assembling of semiconductor sensors. Highlights of designed and/or developed electronic circuits through the last three years include:

- 200 MHz multi-channel pulse generator with burst mode option
- programmable multi-channel delay and gate generator
- 200 MHz event counter with count to voltage output
- μC based and USB or Ethernet interfaced controller and readout systems for power supplies and interlock systems

In many cases, the projects realized in past years have led to designs that could later be adapted to meet new and/or common requirements of the Freiburg researchers. This is a big advantage of in-house designed, custom-built and tested equipment.

1.3.4 IT Support Group

The institute's IT support group of four computer specialists represents a central service unit of the institute. It was founded in 2016 by combining IT experts from individual research groups into a dedicated team, in order to exploit synergies and to optimize expertise and the availability of support. It serves the needs of a large fraction of the institute, including the theoretical and many experimental groups and the administration. However, due to limited manpower, not all experimental groups can benefit from the IT support group.

The tasks of the group include:

- maintenance, configuration and trouble-shooting of computers and other IT infrastructure;
- operation of complex IT infrastructures;
- administration of UNIX/Linux, OSX and Windows based clients and servers;
- hardware and software installations for personnel computers;
- procurement of IT components;
- assistance in IT and network questions and coordination with other faculties and the computer center (”Rechenzentrum”);
  item coordination, administration and deployment of Wolfram Mathematica and OriginLab campus licenses;
- maintenance, configuration and trouble-shooting of multimedia facilities;
- administration of institute copiers

1.3.5 Building Management

The building management team is responsible for the maintenance and servicing of building installations and infrastructure such as heating, ventilation, air-conditioning, postal delivery services and further tasks. It is handled by a janitor and a desk officer, who is based in the entry area of the Physics High-Rise. Further advice, planning and implementation of building technology installation is offered by the *Technisches Gebäude Management* (technical building management), a central service unit of the university.

1.4 Facilities for Teaching and Students

The central administration unit for students is the ”Office for Studies” is staffed with two officials, supporting the dean of studies. The unit is located in the West Building and comprises the examination office, the programme coordination (for details see Part III, Section **1.3**) and the student advisers (one for BSc/MSc physics students, one for students who want to become physics teachers). Detailed additional academic counseling is provided by three professors, representing the three main research areas of the institute.

Three large lecture halls are available to the Institute of Physics on its own premises: the main lecture hall (340 persons), and lecture halls I (150 persons) and II (60 persons) on the first floor of the Physics High-Rise Building. A total of six seminar rooms with capacities ranging from 15 to 40 persons are located in the Physics High-Rise, the Gustav-Mie and the West Buildings. In order to compensate for space shortcomings, especially in highly-demanded time slots in the morning or the early afternoon, student seminars or tutorials are occasionally held in the seminar/common rooms of individual research groups for a full semester.

The basic laboratory courses for physicists and the lab courses for medical students, students of phar-

Figure 1.5: The ”Common Room” on the top floor of the physics highrise building.

macy and other natural sciences are all given in the Laboratory Building (Fig. 1.1), where the experimental setups are distributed over four floors. All experiments are maintained by a laboratory course technician. The 25 experiments for the advanced laboratory classes are located in the Gustav-Mie Building, and maintained by another technician. Two Computer Pools (34 workplaces) for students are available in the Gustav-Mie Building.

The Institute of Physics provides ample space for both learning and recreation. A large Common Room (Fig. 1.5) at the top floor of the Physics High-Rise offers a relaxed atmosphere for students to meet with other students or teaching staff and scientific personnel. It features a stunning view over Freiburg with several tables and a public coffee vending machine and is regularly used by students for discussions, preparation for lectures and tutorials, or relaxing.

The student representatives of the *Fachschaft Physik* occupy separate rooms in the basement of the West Building. A social room in the Gustav-Mie Building is equipped with a black board and desks, as well as kitchen equipment (cooker, dishwasher, etc.). It is regularly used for student gatherings or meetings of the Fachschaft, but can also be booked for tutorial classes.

1.5 Other Infrastructure

1.5.1 Clean Room Facilities

After significant extensions in 2014, the Gustav-Mie building houses now an industrial-style class 10000 clean room of approximately 100 m^2, with about 15 m^2 under laminar flow boxes qualified as class 100. The clean room shown in Fig. 1.6 is primarily designed for testing and manipulating semiconductor wafers and detectors made from, e.g., Silicon, GaAs, or CdTe. It is also well adapted to handling delicate electronic boards. The clean room is equipped with a Delvotec ultrasonic wire bonder, a wire pull tester, an automatic probe station, a semi-automatic metrology microscope and a dispensing robot.

1.5.2 Library

The Physics Library occupies the entire first floor of the West building. It is organized as a reference library (*Präsenzbibliothek*), and is open to researchers 24 hours a day, seven days a week and to students during the week. Apart from providing scientific literature it also offers silent work space.

1.5.3 Computational Infrastructure

Major computational hardware of the Institute of Physics is located in two server rooms in the basement of the High-Rise and the Gustav-Mie building. Almost all of the installed systems are operated by the IT support group, the rest by the research groups themselves. Additional computing infrastructure, e.g. web and mail servers, wiki-services, home-directory storage space with automated backup functionality, etc. is provided by the University IT Services (computer center/”Rechenzentrum”). The two computer rooms for students offer 34 PC workstations and two printers. The IT support group is in charge of the student computer pools and organize software installation and updates.

Major compute resources are provided in big clusters financed by the state of Baden-Württemberg and the German Research Foundation (DFG) for the use by all scientists at universities in Baden-Württemberg: cluster bwUniCluster for all users and four research clusters bwForCLuster supporting each a few scientific communities. The Freiburg University Computer Center hosts NEMO for the communities of particle physics, neuro-science and microsystem engineering. The groups of S. Dittmaier and M. Schumacher are stakeholders of NEMO via additional investments. For a more detailed discussion of Grid

Figure 1.6: Left: View of the clean room in the Gustav-Mie building. Right: The Delvotec 6400 series ultrasonic wire bonder housed in the clean room.

computing in the area of particle physics and the resources operated for ATLAS data analysis we refer to section II 3.7.

Part V

Activities of the Institute

Chapter caption: The Institute of Physics at the annual Science-Days for elementary and high school students.

During the reporting period, members of the Institute of Physics have organized various International Conferences, workshops, and symposia. The institute offers several weekly or bi-weekly colloquia and seminar series in the different research areas. The *Freiburger Physikalisches Kolloquium* is the main colloquium that spans across research areas and offers a forum for scientific exchange between scientists and students. It takes place every Monday afternoon during the semester and also provides an ideal forum for presentations and discussions of topics not directly addressed in the Freiburg research areas.

As part of our outreach activities scientists from our institute are actively promoting physics in general and the institute's research areas in particular at local schools, in public lectures, or at science fairs. The goal is to attract interested students and encourage them to enrol in physics or other natural sciences as well as to familiarize high school teachers with the topics of current research. Another important aspect of the outreach activities is to increase the awareness of the general public that physics is an important science for the society.

The various activities are listed in the following sections.

1.1 Conferences

- **Standard Model at LHC (SM@LHC)**, CIEMAT, Madrid, April 2014, Organizing Committee: S. Dittmaier (`http://wwwae.ciemat.es/smlhc`).
- **Standard Model at LHC (SM@LHC)**, GGI, Florence, April 2015, Organizing Committee: S. Dittmaier (`http://smlhc2015.fi.infn.it`).
- **Radcor 2015 and Loopfest XIV**, UCLA, Los Angeles, June 2015, Organizing Committee: H. Ita (`https://hepconf.physics.ucla.edu/radcor-loopfest/`).
- **International Conference on Quantum Fluid Clusters**, Toulouse, Jun 6 – Jun 11, 2015, Secretary of the conference series and Advisory Committee: F. Stienkemeier (`http://www.quantum-fluid-clusters.info/`)
- **Spring Meeting of the German Physical Society, Section AMOP**; Hannover Feb 29 – Mar 4, 2016; Mainz Mar 6 – Mar 10, 2017, Chair of Scientific Organisation: A. Buchleitner (`http://hannover16.dpg-tagungen.de/`; `http://mainz17.dpg-tagungen.de/`).
- **Casimir and van der Waals Physics: Progress and Prospects**, International Organizing Committee: S. Y. Buhmann, Hongkong, China, April 2016 (`http://iasprogram.ust.hk/201604casimir/index.html`).
- **Standard Model at LHC (SM@LHC)**, University of Pittsburgh, May 2016, Organizing Committee: S. Dittmaier (`https://indico.cern.ch/event/470105`).
- **Axion-WIMP 2017 (PATRAS)**, Thessaloniki, May 2017, Organizing Committee: M. Schumann (`https://axion-wimp2017.desy.de/`).
- **International Conference on Quantum Fluid Clusters**, Obergurgl, Jun 7 – Jun 9, 2017, IRTG CoCo co-organization, Secretary of the conference series and Advisory Committee: F. Stienkemeier (`https://www.uibk.ac.at/congress/qfc2017/`)
- **International Symposium on Molecular Beams 2017**, Nijmegen, Jun 25 – Jun 30, 2017, Advisory Committee: F. Stienkemeier (`http://www.ru.nl/ismb2017/`)
- **4 Conferences in the Series "Higgs Hunting"**, Orsay / Paris, 5th 21-23 July, 6th 30 July – 2 August, 7th 31 August – 2 September, 8th 24 - 26 July 2017. International Advisory Committee: M. Schumacher
- **Axion-WIMP 2018 (PATRAS)**, DESY/Hamburg, June 2018, Organizing Committee: M. Schumann (`https://axion-wimp2018.desy.de/`).
- **High Precision for Hard Processes (HP2)**, University of Freiburg, 1.-3.10.2018; Organizers: S. Dittmaier, F. Febres Cordero, H. Ita, P. Maierhöfer (`http://hp2-2018.physik.uni-freiburg.de`)

1.2 Workshops, Symposia and Schools

- **IRTG "Soft Matter Science" Workshops**, University of Freiburg, 24.-25.05.2016 and 29.11.2016, Organizer: G. Reiter (`http://www.softmattergraduate.uni-freiburg.de/allevents/worksh`).
- **Workshop "Quantum Mechanics Tests in Particle, Atomic, Nuclear and Complex Systems: 50 years after Bell's renowned theorem"**, European Center for Theoretical Studies in Nuclear Physics and Related Areas, Trento, 24.-28.02.2014 Organizing Committee: A. Buchleitner (`http://www.ectstar.eu/node/769`)
- **8th General Assembly Meetings of the LHC Higgs Cross Section Working Group**, CERN, June 2014, Int. Organizing Committee; M. Schumacher
- **HIGGS COUPLINGS 2014**, University of Torino, Oct 2014, International Advisory Commettee: S. Dittmaier (`http://higgscoupling2014.to.infn.it`).
- **2nd International Workshop on Dendrimers and Hyperbranched Polymers**, Strasbourg, France, 23.-24.11.2015, Organizing Committee: M. Dolgushev and J. Wittmer (`http://www.softmattergraduate.uni-freiburg.de/hyperbranched2015`)
- **Winterschool on "Applications of Quantum Mechanics 2015"**, Instituto de Física, UNAM, México D.F., Mexico, 12.-23.01.2015, Organizers: A. Buchleitner, T. Gorin, C. Pineda (`http://gioc.fisica.unam.mx/ws2015/`)
- **9th General Assembly Meetings of the LHC Higgs Cross Section Working Group**, CERN, January 2015, Int. Organizing Committee; M. Schumacher
- **First Annual Meeting of EU-ITN HiggsTools**, University of Freiburg, 11.-15.4.2015; Organizer: S. Dittmaier, K. Jakobs and M. Schumacher (chair) (`http://higgstools2015.uni-freiburg.de`)
- **10th General Assembly Meetings of the LHC Higgs Cross Section Working Group**, CERN, Junly 2015, Int. Organizing Committee; M. Schumacher
- **HIGGS COUPLINGS 2015**, IPPP Durham, Oct 2015, Internation Advisory Commettee: S. Dittmaier (`https://www.ippp.dur.ac.uk/higgs-couplings-2015`).
- **11th General Assembly Meetings of the LHC Higgs Cross Section Working Group**, CERN, January 2016, Int. Organizing Committee; M. Schumacher
- **First Isfahan-Freiburg Joint School on "Quantum Science"**, Isfahan, May 17 – May 20, 2016, Organizers: A. Buchleitner, R. Roknizadeh
- **HIGGS COUPLINGS 2016**, SLAC, Stanford, Nov 2016, Internation Advisory Commettee: S. Dittmaier (`http://www-conf.slac.stanford.edu/hc16`).
- **SoMaS School**, Mittelwihr, France, Annual Summer School 2014-2017, Organizer: G. Reiter, (`http://www.softmattergraduate.uni-freiburg.de/allevents/summerschools`).
- **DARWIN Meeting**, Freiburg, Sep 12–Sep 13, 2017, Organizer: M. Schumann, (`www.darwin-observatory.org`)
- **1st CoCo Summer School: "Ultracold few- and many-body systems: Quantum mechanics made crystal clear"** , Mittelwihr, France, Jul 24 – Jul 29, 2016 Organizer: F. Stienkemeier, M. Walter, S. Y. Buhmann
- **12th General Assembly Meetings of the LHC Higgs Cross Section Working Group**, CERN, July 2016, Int. Organizing Committee; M. Schumacher
- **625. WE-Heraeus-Seminar "The High-Energy LHC - Interplay between Precision Measurements and Searches for New Physics"**, Physikzentrum Bad Honnef, October 2016, Organizers: M. Schumacher together with M. M. Mühlleitner and T. Müller (both KIT).

- **Quantum-classical transition in many-body systems: Indistinguishability, Interference and Interactions**, Max Planck Institute for the Physics of Complex Systems, Dresden, Feb-7 – Feb-17, 2017, Organizers: A. Buchleitner, J.-D. Urbina
- **2nd CoCo Summer School: "Ultracold few- and many-body systems: Cold on quantum's trail"**, Squamish, Canada, Aug 6 – Aug 11, 2017, Organizer: F. Stienkemeier, M. Walter, T. Momose
- **Clustertreffen 2015**, Lindow, Sep 20 – Sep 25, 2017, IRTG CoCo co-organization, Programm Committee: F. Stienkemeier, B. von Issendorff (`http://web.physik.uni-rostock.de/cluster/clustertreffen`)
- **First Interdisciplinary and International Summer School of the Universities Strasbourg, Nagoya and Freiburg on "Light, Frontiers, Time"**, Nagoya, Aug 30 – Sept 5, 2017, Organizers: V. Robert, H. Kunieda, G. Neuhaus, A. Buchleitner
- **Quantum Cup 2017**, Max-Planck-Institute for Quantum Optics, Garching, Germany, Oct 01 – Oct 04, 2017, Organizer: S. Y. Buhmann

1.3 Workshops co-organized by FRIAS[1]

- **FRIAS Research Focus *Designed Quantum Transport in Complex Materials***, Sept. 2014 — Oct 2015; Organizers: A. Buchleitner, T. Schaetz, E. Weber, S. Weber
- **Physics School: New trends in many-particle quantum transport**, Freiburg, 23.02.-06.03.2015, Organizers: A. Buchleitner, A. Rodriguez
- **Journée quantique**, FRIAS Focus Designed Quantum Transport in Complex Materials & Académie Nationale de Médecine, Freiburg, Sep 11, 2015, Organizer: A. Buchleitner
- **Spin-Boson physics - from trapped ions to metamaterials**, FRIAS Focus Designed Quantum Transport in Complex Materials, Freiburg, Sep 18, 2015, Organizer: A. Buchleitner
- **FRIAS Junior Researcher Conference - Nonlinear spectroscopy meets quantum optics**, Freiburg, Oct 8 – Oct 10, 2015, Scientific Coordinators: Frank Schlawin, Manuel Gessner, `https://www.frias.uni-freiburg.de/en/events/frias-junior-researcher-conferences/junior-researcher-conference-nonlinear-spectroscopy-meets-quantum-optics`
- **Workshop "Symmetry, proportion and seriality, the semantics of mirroring and repetition in science and the art"**, International Conference of the Academia Europea, Freiburg, May 2016, Organizers: Andreas Buchleitner, Monika Fludernik, Martin Midekke
- **FRIAS Junior Researcher Conference - Beyond molecular movies: Bringing time-domain spectroscopy to diffraction imaging**, Freiburg, Sep 13 – Sep 19, 2017, Scientific Coordinators: Lukas Bruder, Simon Doldt, Aaron LaForge, `http://www.frias.uni-freiburg.de/en/events/frias-junior-researcher-conferences/junior-research-conferences-2017-2018`

1.4 Colloquia and Seminars

- **Colloquium of the Physics Institute**: During the semester, weekly (every Monday), University of Freiburg, 2014-2017; Organizers: Professors of the Institute of Physics, `http://www.physik.uni-freiburg.de/aktuelles/vortraegekolloquien/physikkolloq`
- **Astrophysical Colloquium of the KIS**: weekly around the year, Kiepenheuer-Institut für Sonnenphysik (KIS), 2014-2017; Organizers: O. von der Lühe, S. Berdyugina, M. Roth, `http://www.leibniz-kis.de/en/institute/events/kolloquium/`

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[1] Freiburg Institute for Advanced Studies (FRIAS), https://www.frias.uni-freiburg.de

- **Seminar "Fundamentale Wechselwirkungen" (Fundamental Interactions)**, Every semester, University of Freiburg, 2014-2017; Organizers: S. Dittmaier, H. Ita, J. van der Bij,
`http://portal.uni-freiburg.de/ag-dittmaier/seminars/fundi`
- **RTG-Seminar "Mass and Symmetries after the Discovery of the Higgs Particle at the LHC"** organized within the Research Training Group (Graduiertenkolleg), every semester, University of Freiburg, 2015-2017; Organizers: S. Dittmaier, H. Fischer, G. Herten, H. Ita, K. Jakobs / C. Weiser, M. Schumacher, M. Schumann, J. van der Bij,
`http://www.grk2044.uni-freiburg.de/seminars`
- **IRTG-Seminar "Cold Controlled Ensembles in Physics and Chemistry"** organized within the International Research Training Group (IRTG 2079), every semester, weekly, University of Freiburg, biweekly as a joint seminar together with the University of British Columbia (UBC), Canada, 2014-2017; Organizer: F. Stienkemeier, A. Buchleitner, S. Y. Buhmann, B. von Issendorff, T. Schätz, M. Walter,
`http://www.irtg-coco.uni-freiburg.de/`
- **IRTG-Seminar "Soft Matter Science"** organized within the International Research Training Group (IRTG 1642), every semester, weekly, University of Freiburg, 2014-2017; Organizer: G. Reiter,
`http://www.softmattergraduate.uni-freiburg.de/events`

1.5 Public Lectures

- **"Weihnachtsvorlesung" (public Christmas lecture)**, every year, December 2014, 2015, 2016, 2017; Lecturer: H. Fischer; Experiments: H. Wentsch
- **"Chaos, Quanta, Uncertainty"**, Physics House, Isfahan, Mar 18, 2016, Lecturer: A. Buchleitner

1.6 Lectures at Physics and Interdisciplinary Schools

- **"Hypothesis Testing, Confidence Intervals and Limits"**, Heidelberg B-Physics School, Neckarzimmern, 6 March, 2014, Lecturer: M. Schumacher.
- **"Quantum correlations in finite dimensional systems"**, ICTP-School on "Advances in Quantum Information: Theory and Application", Rabat, Morrocco, Sept 15 – Sept 19, 2014, Lecturer: A. Buchleitner.
- **"Quantum chaos and control"**, Applications of Quantum Mechanics 2015, Instituto de Física, UNAM, México D.F., Mexico, 12.-23.01.2015, Lecturer: A. Buchleitner.
- **"Non-Markovian dynamics in open quantum systems"**, Applications of Quantum Mechanics 2015, Instituto de Física, UNAM, México D.F., Mexico, Jan 12 – Jan 23, 2015, Lecturer: H.-P. Breuer.
- **"Markovian and non-Markovian quantum dynamics of open systems"**, 51 Winter School of Theoretical Physics on Irreversible Dynamics: Nonlinear, Nonlocal and Non-Markovian Manifestations, Ladek Zdroj, Poland, Feb 9 – Feb 14, 2015, Lecturer: H.-P. Breuer.
- **"Electroweak Physics at the LHC"**, HiggsTools Summer School on Higgs Physics, Aosta, June 28 – July 4, 2015, Lecturer: S. Dittmaier.
- **"Higgs Physics at the LHC"**, Herbstschule für Hochenergiephysik, Maria Laach, Sep. 8 – 18, 2015, Lecturer: S. Dittmaier.
- **"Quantum information (more theory than computation)"**, ICTP-School on "Cooperative phenomena in Condensed Matter: From Bose-Einstein Condensates to Quantum Optics", Nov 2 – Nov 13, 2015, Buea, Cameroon, Lecturer: A. Buchleitner.
- **"Non-Markovian Quantum Dynamics"**, Arctic School on Open Quantum Systems, Kilpisjärvi Biological Station, Finland, Dec 14 – Dec 18, 2015, Lecturer: H.-P. Breuer.

- **“Mesoscopic Physics with Cold Atoms”**, International Summer School “Spatio-Temporal Control of Waves: From Imaging to Sensing”, Cargese, France, Apr ? – Apr ?, 2017, Lecturer: T. Wellens.
- **”Dark Matter: Experimental searches”**, XVIII FRASCATI SPRING SCHOOL ”BRUNO TOUSCHEK” in Nuclear Subnuclear and Astroparticle Physics, Frascati, May 9 – May 13, 2016, Lecturer: M. Schumann
- **“Quantum Control: Determinism, Chaos, Disorder”**, XVIII Giambiagi Winter School “Quantum Chaos and Control”, Buenos Aires, Jul 25 – Jul 29, 2016, Lecturer: A. Buchleitner.
- **“Electroweak Standard Model”**, Summer School and Workshop on the Standard Model and Beyond, Corfu Summer Institute, Aug. 31 – Sep. 12, 2016, Lecturer: S. Dittmaier.
- **”Dark Matter”**, CHIPP Winter School of Particle Physics 2017, Sörenberg, Feb. 12 – Feb. 17, 2017, Lecturer: M. Schumann
- **“Transport in complex quantum systems: from photons to atoms to photosynthesis”**, Fourth CUI (Hamburg Centre for Ultrafast Imaging) Winter School, Rügen, Feb 20 – Feb 24, 2017, Lecturer: A. Buchleitner.
- **”Dark Matter”**, GRK1504/2: Spring Block Course 2017, Rathen, Mar. 13 – Mar. 16, 2017, Lecturer: M. Schumann
- **“Theoretical Quantum Optics”** Review course at the African Institute for Mathematical Sciences (AIMS) at Limbe, Cameroon, Mar 19 – Apr 4, 2017, Lecturer: A. Buchleitner.
- **”Direct Dark Matter Searches - Status and Perspectives”**, LHCb Week 2017, Neckarzimmern, Mar. 24, 2017, Lecturer: M. Schumann

1.7 Presentations of the Institute of Physics to the Public

- **Presentation at the “Science Days”** at the Europa-Park Rust near Freiburg, October 2014, 2015, 2016, 2017; Organizers: M. Walther, H. Dummin, `http://www.science-days.de/science-days/`
- **Exhibition ”Von Einstein to Higgs”** at Buergerhaus Seepark, 15 to 21 June 2015, Organizer: M. Schumacher for the RTG-2044, Silke Mikelskis-Seifert for the Paedagogische Hochschule
- **Presentation at the “Freiburger Wissenschaftsmarkt”** in the city centre of Freiburg:
  “Ein Quantum Kälte – Cool. Kühler. Physik!” & “Die faszinierende Welt der Elementarteilchen”, 14./15.07.2017; Organizers: T. Schätz, M. Schumann
  `http://www.uni-freiburg.de/innovation/wissenschaftsmarkt`

1.8 Lectures, Presentations & Events for High-school Teachers and Students

- **Open house presentations (“Tag der offenen Tür”)**, every year, November 2014-2017; Organizers / Lecturers: M. Schumacher, G. Reiter, J. Timmer, H. Fischer, T. Filk, M. Walther
- **Freiburg Study Information Day (”Freiburger Hochschultag”)**, every year, November;
  About 540 students from 17 high schools in the Freiburg area attend lectures on study programmes at the University; Information event of the Physics Institute by M. Walther
- **Breakfast for school students (”Schülerfrühstück”)**, once a year, organised by the Young German Physical Society (jDPG)
  About 20 students meet with three Professors of the Institute of Physics at the institute’s Common Room. They can discuss physics and ask questions and can join a lecture and lab tour.

- **Junior Studies for high school students ("Schülerstudium")**, University of Freiburg;
  Every year about one to two extremely talented high schools students participate in the junior study programme, where they visit lectures and turorials parallel to their school classes. Passed exams will be accredited if they later enrol at the university.
- **Master Classes for High-school students at the Particle Physics Department of the Institute of Physics**, University of Freiburg, March 2014-2017; Organizer: M. Schumacher
- **Schnupperstudium** (one-day internship in groups and various workshops at the Institute of Physics) for high-school students, University of Freiburg, April 2014-2017; Organizers: M. Kaschek, T. Filk, `http://www.studium.uni-freiburg.de/service_und_beratungsstellen/zsb/schnupperstudium`
- **BOGY internship for high-school students at the Institute of Physics**, every year, Students apply for a one-week internship at the institute, where they visit and work with various research groups; participating groups and researchers: H. Fischer, T. Schätz, B. von Issendorff, K. Dulitz, F. Stienkemeier, G. Reiter, K. Jakobs, C. Weiser, U. Parzefall, M. Schumann
- **Several lectures at high-schools in the Freiburg area** (about two to five per year), Lecturers: T. Filk, H. Fischer
- **One-day visits by high-school classes**, introduction lecture and lab tours organized by differnet groups at the Institute of Physics
- **Excursions to CERN for Schools Classes from Freiburg** (1-2 per year), Organizer: H. Fischer
- **DPG-Fortbildungskurs für Physiklehrerinnen und Physiklehrer "Das frühre Universum"**, Bad Honnef; contributed by group v. d. Bij through lecturer C. Steinwachs, July 2014

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