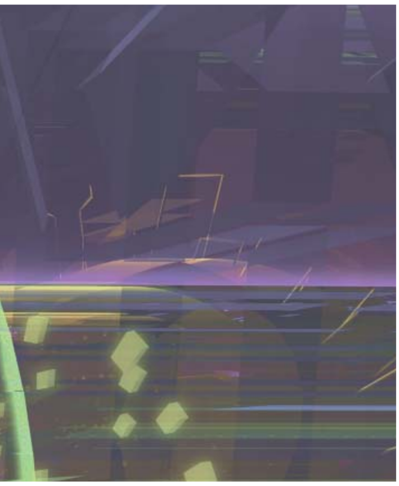
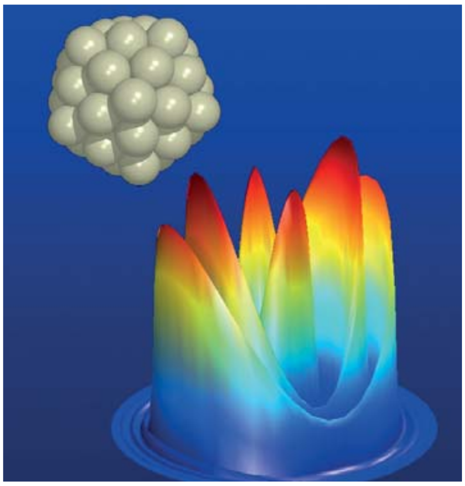
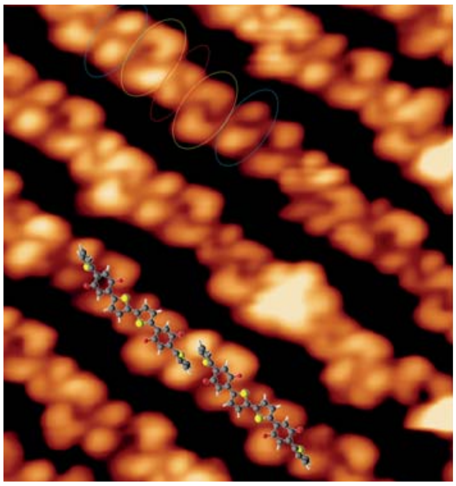
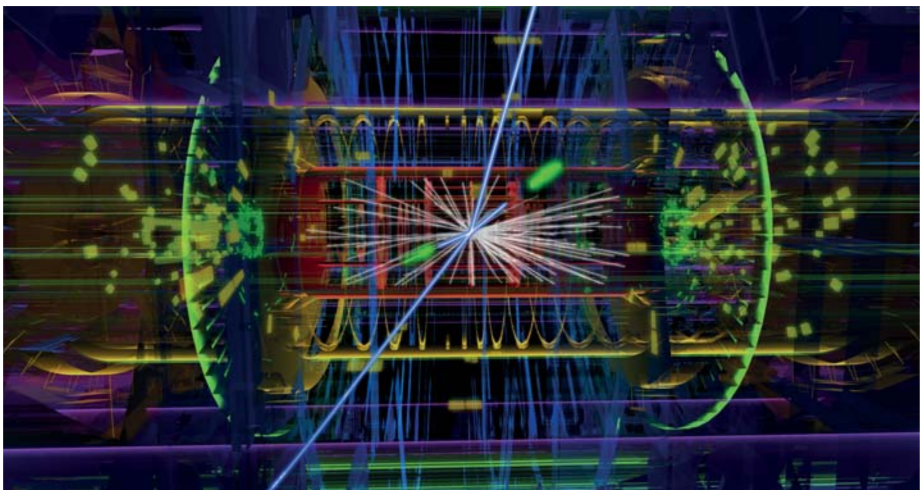
Freiburg Institute of Physics

Activity Report 2011-2013









Albert-Ludwigs-Universität Freiburg

UNI FREIBURG

INSTITUTE OF PHYSICS
UNIVERSITY OF FREIBURG

ACTIVITY REPORT
2011 - 2013

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

Front cover
Measured angular distribution of photoelectrons emitted from a Na_{55}^{-} cluster, scanning tunneling microscope image showing chains of oligomeric molecules, 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 2011 to 2013, 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.

The inaugural meeting of the Scientific Advisory Board is scheduled for 17 and 18 February 2014, and will be embedded into a public workshop programme, where cutting edge research on a broad selection of topics will be presented by members of the institute.

Contents

Part I

The Institute of Physics

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

1.1 Structure, Research & Education

The Institute of Physics, part of the Faculty of Mathematics and Physics of the University, is actively involved in an unusual range of research areas, from particle physics and field theory to organic electronics and photovoltaic applications. Given the moderate size of the department, as compared to others in Germany, with 22 professors and three co-opted members, students enjoy a broad diversity of topics covered by lecture courses and seminars. The diversity and quality of the research and teaching programme of the institute, embedded in the rich and interdisciplinary research landscape defined through the University of Freiburg and other institutions committed to research and development in the larger Freiburg area, are key ingredients for the attractiveness of the institute nation-wide, but also on the international level. At present, 336 students are enrolled for Bachelor of Science (BSc) and Master of Science (MSc) studies, 162 students work on their PhD, and 52 young researchers are at the PostDoc stage of their career. Together with faculty and the administrative staff of the institute, our team comprises approx. 750 individuals who are committed to foster and deliver first class academic training and research.

The Institute of Physics is composed of eleven experimental and eleven theoretical research groups which are almost all located (see site map, Fig. 1.1) at the central site of the Institute at Hermann-Herder-Str. 3 and 6. At present, three groups (Gross, Helm, von Issendorff) are located at other sites nearby, due to a shortage of laboratory and office space at the central location. Also all teaching, including the library of the institute, is located at the central site, so that contact between research and teaching staff, and students is intense and regular.

Support for our experimental research is provided by a mechanics and an electronics workshop which together represent a crucial and highly renowned element of our research infrastructure. The central administration takes care of general management issues, ranging from infrastructure maintenance to budget management. Its second key responsibility concerns the teaching programme of the institute, which includes compatibility issues with respect to teaching programmes of different faculties. General management is led by the Acting Director of the institute, assisted by the Director of Administration, while teaching administration is overseen by the Dean of Studies (see organisation chart, Fig. 1.2). The offices of Acting Director and Dean of Studies are executed by professors of the institute for a period of two years (presently by Andreas Buchleitner and Markus Schumacher).

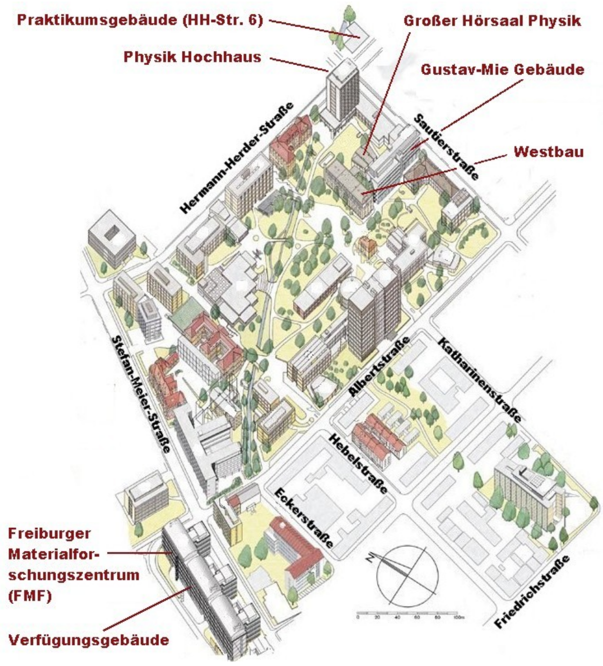


Figure 1.1: Site map of the Institute of Physics

On the institutional level within the University, the Institute of Physics is integrated into the Faculty for Mathematics and Physics, and the Acting Director and the Dean of Studies are members of the Faculty Board, the executive body of the faculty. The Offices of Dean (at present, Michael Růžička, Institute of Mathematics) and Vice-Dean (at present, Andreas Buchleitner) of the faculty alternate between Mathematics and Physics, in general in intervals of two years.

Research at the Institute of Physics can be grouped into three main areas (see Fig. 1.3): *Atomic, Molecular and Optical Sciences*[1], *Condensed Matter and Applied Physics*, and *Particles, Fields, Cosmos*.

A strong 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, together with the sun physics group (see Part I, Sec. 1.2), strongly relies on light-matter-interaction for the detailed analysis of complex structures and transport processes on very diverse scales. Classical and quantum theory of complex systems, with a strong computational component, join with experimental polymer science, nano-

[1] The terms 'Atomic, Molecular and Optical Sciences (AMO)' and 'Light-Matter-Interaction (LMI)' for this research area are used synonymously throughout the report.

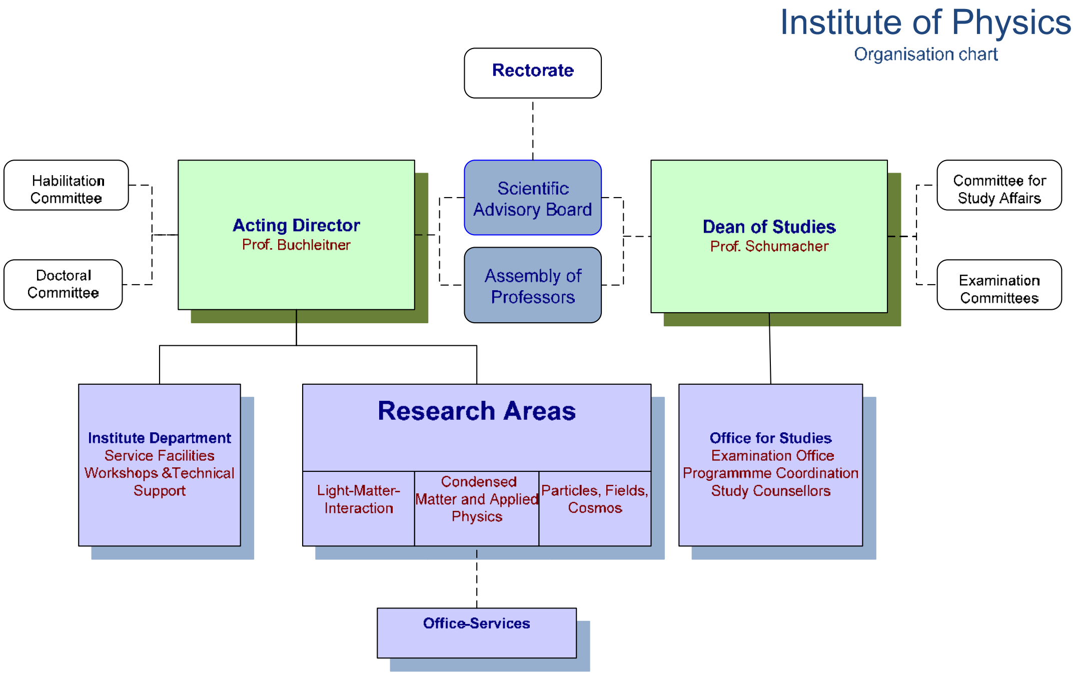


Figure 1.2: Organisation chart of the Institute of Physics. Together with the Institute of Mathematics, the Institute of Physics constitutes the Faculty of Mathematics and Physics.

magnetism and photovoltaic research in the broad context of condensed matter and applied physics. The institute has strong and internationally very visible experimental and theoretical particle physics groups. The experimental programme is focussed 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 activities in particle theory range from precision studies of the strong and electroweak interactions over quantum-field-theoretical aspects to the exploration of model extensions with new theoretical structures.

During the past years, the institute has seen several important developments, and new challenges are waiting ahead: In total, researchers at the Institute of Physics have published more than 700 papers in international, peer-reviewed journals during the reporting period (excluding publications by researchers from the associated institutes, see Section 1.2). We have attracted competitive funds which amount to about 6 times the funding provided directly by the university, from national and international sources (BMBF, DFG, EU, etc).

The Institute of Physics succeeded to establish the Research Training Groups (RTG) *Physics at Hadron Accelerators* (funding period 2005-2014) and *Soft Matter Science* (together with the Faculty of Chemistry and Pharmaceutics of the University of Freiburg, and partner groups at Strasbourg and Mulhouse, funding period 2010 - 2015) and the International Training Network *HiggsTools* (together with nine partners from eight European countries; funding period 2014-2017).

The institute attracted funding, through different sources (ERC, German Excellence Initiative, State of Baden-Württemberg, DFG) for the establishment of four junior research groups (Mintert, Gross, Ita, Buhmann).

Five junior researchers of the institute (Caron, Dingfelder, Mintert, Schelter and Vivarelli) received permanent academic positions at Nijmegen, Bonn, London, Aberdeen and Sussex. Since mid 2011 E. von Hauff was a very active researcher at our institute holding an associate professorship. She accepted an offer from the University of Amsterdam and left the institute end of 2013.

The University of Freiburg awarded a Honorary Professorship to Peter Jenni, who took a pioneering and leading role in the design and construction of the ATLAS experiment at the Large Hadron Collider. International long-term visitors are Greg Scholes, one of the leading experimentalists characterising quantum effects in biological matter, who was awarded a one year guest professorship by the *Ministry of Science and the Arts of Baden-Württemberg* and the *Wissenschaftliche Gesellschaft in Freiburg im Breis-*

Research and Teaching

Institute of Physics

Atomic, Molecular and Optical Science		Condensed Matter and Applied Physics		Particles, Fields, Cosmos	
Berdyugina	(Theo KIS)	Blumen	(Theo)	Dittmaier	(Theo)
Buchleitner	(Theo)	Grabert	(Theo)	Herten	(Exp)
Gross	(Theo)	Moseler	(Theo IWM)	Ita	(Theo)
Helm	(Exp)	Reiter	(Exp)	Jakobs	(Exp)
von Issendorff	(Exp)	Timmer	(Theo)	Königsmann	(Exp)
Schaetz	(Exp)	von Hauff	(Exp ISE, until 2013)	Schumacher	(Exp)
Stienkemeier	(Exp)	Waldmann	(Exp)	van der Bij	(Theo)
Stock	(Theo)	Weber	(Exp ISE)		
von der Lühe	(Exp KIS)				
		Aertsen	(Biology, co-opted)		
		Hennig	(Medicine, co-opted)		
		Rohrbach	(Engineering, co-opted)		

Figure 1.3: Professors and co-opted members of the Institute of Physics, with their main research areas.

gau, and Rienk van Grondelle (Amsterdam), one of the pioneers of the spectroscopic elucidation of the primary physical processes of photosynthesis, who received a Research Award of the Alexander von Humboldt foundation hosted by the Institute.

Within our teaching programme, we launched the Master of Science programme, fully taught in English, to enhance its international visibility. We implemented a reform of the legal framework for the education of high school teachers. We are now preparing the formal accreditation of our BSc and MSc programmes in 2014, as stipulated by the Bologna process and its legal ramifications.

Four colleagues will retire within the next three years (Blumen 2016, Grabert 2016, Helm 2015, Königsmann 2015). The opening of these four full professor positions is an enormous chance and challenge for the strategic long-term development of the institute. We will compete for the best candidates on the international academic market.

Much as in the past, a successful recruiting and research strategy will be an important prerequisite for further cooperative research initiatives presently under preparation: The International Research Training Group (IRTG) *Soft Matter Science* will submit a proposal for a second funding period. The particle physics groups are preparing a new proposal for a graduate programme focussing on *Mass and symmetry after the discovery of the Higgs particle*. Furthermore, physics-led proposals for an IRTG on *Cold Ensembles in Atomic, Molecular and Optical (AMO) Physics and Chemistry* (with partners at the University of British Columbia at Vancouver), and for Cooperative Research Centres on *Quantum mechanics of efficient light-energy conversion* and on *Polymers* are in an advanced stage of preparation.

1.2 Associated Institutes and Co-opted Members

In various subject areas, the institute has long-term institutional partnerships with other faculties within the university, as well as with external research institutions (see Fig. 1.3).

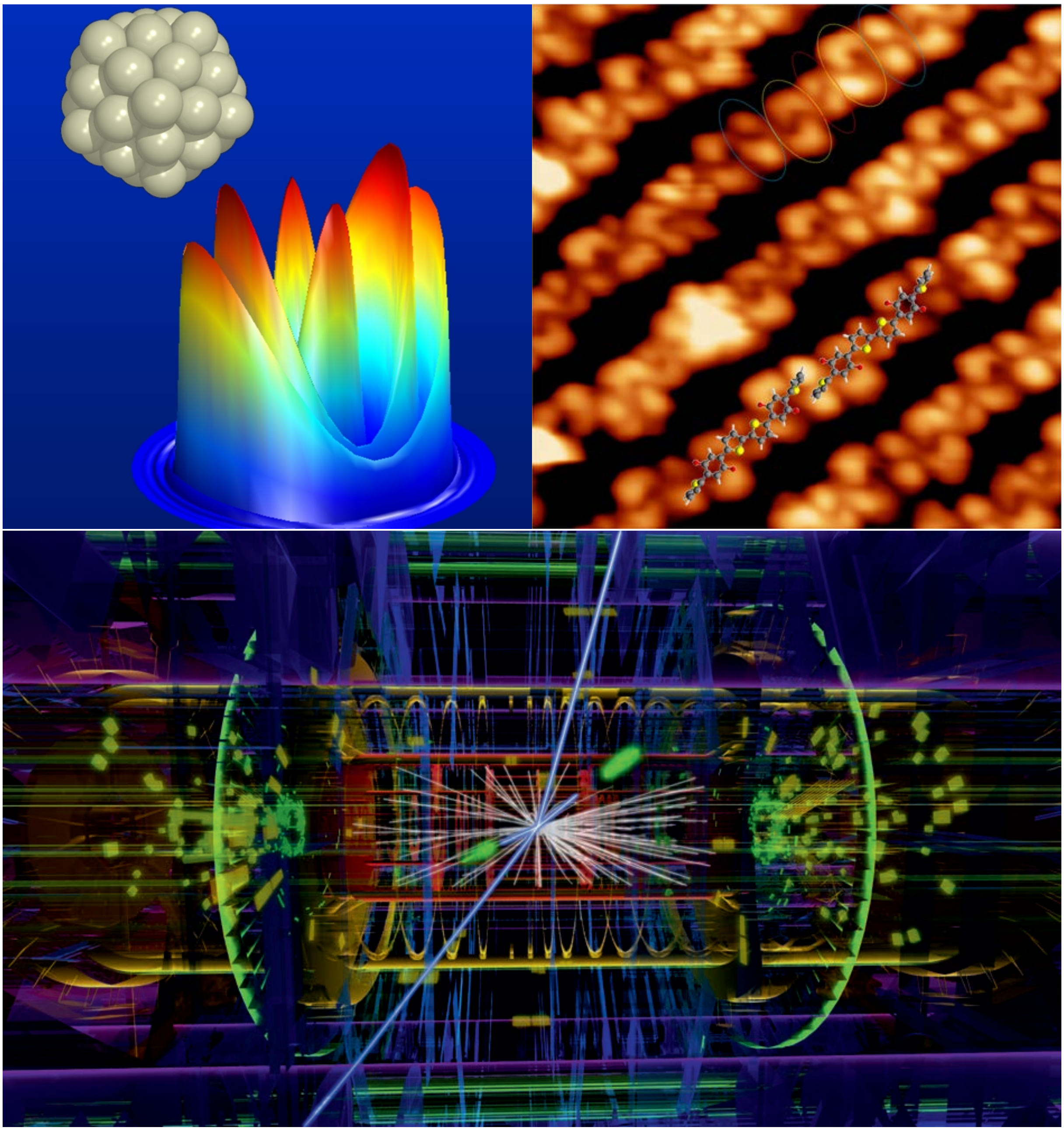
Three colleagues from the Faculty of Biology, the Faculty of Medicine, and the Department of Microsystems Engineering (IMTEK) are co-opted members of the institute.

Four professors of the Institute of Physics hold joint appointments with the *Kiepenheuer-Institut für Sonnenphysik (KIS)* of the Leibniz-Gemeinschaft, the *Fraunhofer Institute for Material Mechanics (IWM)*, and the *Fraunhofer Institute for Solar Energy Systems (ISE)* in Freiburg. Several members of the institute run 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)*. Four senior and one junior member of the institute were awarded fellowships at the *Freiburg Institute for Advanced Studies (FRIAS)*, the international research college of the University of Freiburg. Some of our faculty members (Hermann Grabert and Jens Timmer) serve(d) on the Board of Directors of FRIAS, and the institute competed successfully for the establishment of a physics-led research focus in the academic year 2014/15.

Under the perspective of an enhanced cooperation with the local Fraunhofer Institutes (Freiburg being the largest site of Fraunhofer research in Germany), we aim at the establishment of permanent Fraunhofer professorships at the institute.

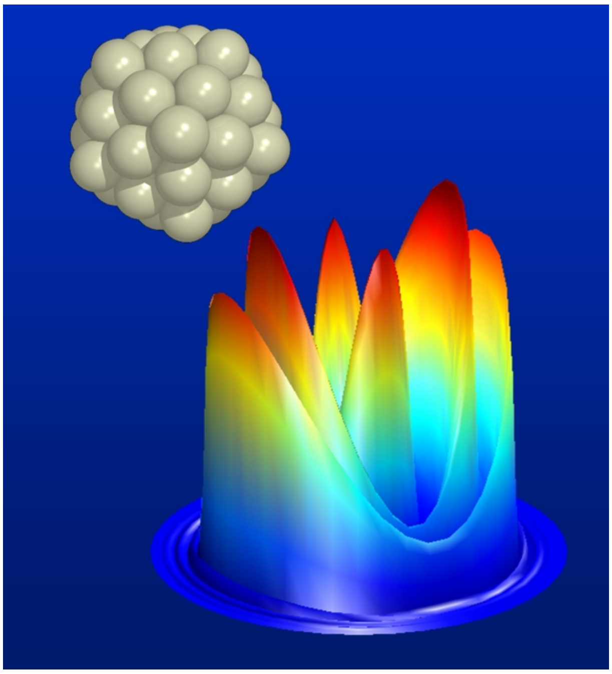
Part II

Scientific Activities 2011 - 2013



Chapter 1

Atomic, Molecular and Optical Sciences



Experimental Physics

- Prof. H. Helm
- Apl. Prof. B. v. Issendorff
- Prof. T. Schaetz
- Prof. F. Stienkemeier
- Prof. O. v. d. Lühe (KIS)

Theoretical Physics

- Prof. S. Berdyugina (KIS)
- Prof. A. Buchleitner
- JProf. D. Gross
- Prof. G. Stock

Chapter caption: Measured angular distribution of photoelectrons emitted from a size selected Na_{55}^{-} cluster, revealing its electron shell structure.

1.1 Overview

Gaining insight on scales ranging from the single photon regime to intense laser fields and from individual atoms to large molecular entities is at the heart of Atomic, Molecular and Optical Sciences (AMO). At the level of single particles of light or matter the seemingly bizarre phenomena predicted by quantum mechanics can be directly observed and exploited via the manipulation of photons and atoms. For this purpose AMO physics has developed a realm of novel technologies, both in pursuit of new questions and to lay the foundation to modern technologies, ranging from the currently most precise atomic clocks to methods of storing antimatter in traps of light.

Erwin Schrödinger's remark of 1952 that *'... it is fair to state that we are not experimenting with single particles, any more than we can raise ichtosauria in the zoo'* has long been disproven in the laboratory where particles are guided by electromagnetic fields or matter waves are diffracted by standing waves of light. Thought experiments, long the cornerstone of the development of quantum mechanics, are now realized in the lab, allowing to directly study truly fundamental questions. In parallel the quest to understand how quantum properties enter macroscopic domains and how quantum coherence dephases under the action of the environment are currently pillars of study in theory and experiment.

Simultaneously, the development of new laser technology has led to table-top equipment providing light intensities exceeding 10^{15} W/cm^2 and pulse durations in the range of femtoseconds and below. This has opened the avenue to study matter distorted by strong electromagnetic fields (beyond perturbation theory) and enabled the time-resolved study of atomic and molecular quantum mechanics. The advent of free-electron lasers allows to perform such studies in completely different photon energy ranges, and opens the possibility to use novel measurement techniques like time-resolved diffraction. In a seemingly different context, ultra-short pulses of visible light serve in optoelectronic devices, which now operate in and explore the Terahertz frequency range, capable of resolving the electromagnetic field vector rather than monitoring intensity. Modern optical technologies are aided by intelligent hard- and software, enabling near diffraction free imaging with active suppression of atmospheric distortion in novel telescopes for observation of stellar objects as well as imaging of atomic-scale many body wavefunctions through novel microscopic techniques.

Front-line research in all these areas has grown in the Freiburg Institute of Physics over decades and common research initiatives were established. 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 **A. Buchleitner** and **D. Gross**, as well as the experimental groups of **T. Schaetz** and **H. Helm** study the fundamental interaction between light and isolated atoms, ions and molecules. By extending the capabilities to observe and control nature on the atomic scale and at the quantum level we gain deeper insight into complex quantum behaviour. The experimental tools employed allow a strong link to idealized model systems. However, due to an exponential growth of the number of resources required to describe a quantum system of increasing size and its dynamics, only tens of quantum particles remain tractable by numerical (classical) means. Still, the basic concepts are predicted to be of substantial relevance in nature. In a bottom-up approach, we are assembling larger quantum entities - to gain deeper insight into complex quantum dynamics and to elucidate the frontiers of quantum mechanics. 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 for narrowing state definition 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. 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. Stock** is concerned with the theory and computation of structural dynamics and spectroscopy of biomolecules. Employing all-atom molecular dynamics simulations and mixed quantum-classical calculations of the relaxation dynamics and multidimensional spectra, they provide approximate results for "real systems" as benchmark for idealized models.

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, in particular the magneto-acoustic wave propagation in the solar atmosphere under the influence of complex magnetic field structures, and polarimetric signatures of exoplanets in starlight. KIS designed, built and operates one of the most powerful solar telescopes and works on image stabilization of ground- and satellite-based observatories.

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 underlaying 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.

Cold controlled ensembles in physics and chemistry

This initiative focuses on ensembles in the ultracold regime, where wavelike quantum behavior might dominate the properties of the system and its related dynamics. In order to study the physics and chemistry involved, we aim at producing and characterizing cooled and trapped atomic and molecular systems and using state selectivity and quantum control to study their properties and dynamics. Experimentally, the programme combines groups in the fields of ultra-cold atoms, ion traps, cold molecules and clusters, and quantum control with femtosecond lasers. The complementary expertise of the theorists (DFT calculations, quantum chemistry, molecular dynamics, reactive scattering, quantum many-body simulations and spectral theory, molecules in strong fields) adds substantial theoretical support for the research programme.

The international initiative is based on the ongoing joint activities between groups in theory and experiment from the Physics Institute, one Fraunhofer Institute and the University of British Columbia (UBC) in Vancouver, Canada. They already led to joint projects, joint Master students and many fruitful interactions. We intend to deepen the collaborations between the two locations, for example, by realizing a DFG/NSERC-funded International Research Training Group (IRTG). The designated spokespersons are: F. Stienkemeier (Freiburg Institute of Phyiscs) and T. Momose (UBC); The consortium further consists of: A. Buchleitner, 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, M. Shapiro (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).

Quantum contribution for efficient light-energy conversion

The initiative is dedicated to gain a systematic and quantitative understanding of microscopic quantum transport processes in complex materials, with a special focus on their potential relevance for light-energy conversion.

Due to the high structural complexity of biological or technological functional units which mediate energy or charge transfer (e.g. in photosynthesis or photovoltaics), the relevant mechanisms are far from active and deterministic control. The consortium aims to respond to the following guiding questions:
1) Are there relevant and nontrivial quantum phenomena in light-energy conversion? That is, under which conditions can quantum coherence exist in large, disordered and open quantum systems?
2) To which level can we control them, together with the potentially related coherent transport?
3) Can we exploit them? That is, can we identify ways to adopt such quantum effects, in the presence of imperfections and noise, for an improvement of light energy conversion technology, as used e.g., in solar cells or light emitting diodes?

For this endeavor several groups in Freiburg are joining forces, which will cover subjects from the experimental and theoretical study of quantum transport in idealized model systems, via experimental quantum simulators, over the study of quantum coherence in larger systems, like molecular clusters or biological molecules, to the characterization of engineered devices like solar cells. The initiative was started in 2011 (speaker A. Buchleitner), with 19 contributing principal investigators: All members of the AMO research area, actively involved partner groups at Chemistry, IMTEK, Fraunhofer ISE, IWM in Freiburg and Bayreuth (J. Köhler) as well as various research centres abroad (Berkeley, Mulhouse, Ohio, Strasbourg, Toronto).
In order to focus the common effort, a seminar series was installed to which many of the leading experts in fields related to that of the initiative contributed (among others: H. Briegel, I. Burghardt, R. Cogdell, E. Collini, R. van Grondelle, R. Hildner, A.S. Mukamel, G. Scholes, ...).

To establish the basis for a solid bridge between the envisioned scientific poles - abstract theory, on the one hand, and device engineering, on the other - we unfold our work programme on different levels of detail and integration. To enhance the coherence of the consortium, four PIs (A. Buchleitner and T. Schaetz of the Institute of Physics, E.Weber of the Fraunhofer institute ISE and S.Weber of the Chemistry Department) initiated a Research Focus at the Freiburg Institute of Advanced Studies (mentioned above). Furthermore, active cooperation with R. van Grondelle (Amsterdam) and G. Scholes (Toronto) were secured through the Alexander von Humboldt Research Award and a Guest Professorship, co-funded by the *Ministry of Science and Arts of Baden-Württemberg* and the *Wissenschaftliche Gesellschaft* in Freiburg.

Common programme for education

The collaborative research will enhance the educational programme of the Institute of Physics, from the Bachelor to the PhD level, by dedicated seminars, summer schools, meetings and guest lectures. The research is of interdisciplinary character and will connect to diverse fields of mathematical physics, atomic and molecular physics, quantum optics, condensed-matter physics, and physical chemistry. The involved groups are expected to efficiently foster synergy effects in scientific achievements as well as for creating a unique training environment for young scientists. The doctoral projects of the IRTG will be embedded into binational collaborations and include long-term stays at both locations.

1.2 Research Groups

1.2.1 Quantum Optics and Statistics

The **Quantum Optics and Statistics Group (coached by Andreas Buchleitner, together with Deputy Coach Thomas Wellens)** conceives Modern Quantum Optics as a diverse and challenging sub-field of advanced Quantum Statistics, with high potential for modern AMO experiments in diverse physical settings. The overarching theme of our research is the quantitative theoretical analysis of few to many-body quantum dynamical and transport phenomena, in possibly disordered, nonlinear, and/or open quantum systems, with tools from spectral, diagrammatic and control theory combined with advanced (quantum) statistical and computational methods.

Quantum transport

One of our main activities concerns the propagation of quantum particles (or classical waves) in *disordered* environments. In particular, we studied *excitation transport in disordered molecular networks*, designed to model certain essential features of photosynthetic light harvesting complexes [abu2]. We established a general mechanism for highly efficient coherent transport [abu10] demonstrating the possibility of exploiting quantum coherence in order to increase the efficiency of transport processes required for photosynthesis. Furthermore, we studied incoherent upconversion by triplet-triplet annihilation – a promising candidate for improving solar cells – and showed that its efficiency can be optimized by varying the ratio between two molecular species [abu8].

Whereas these works are concerned with a statistical analysis of transport *fluctuations* for various disorder realizations, our group also applied and developed diagrammatic methods for calculating the *average* over many such realizations. In this case, transport is typically suppressed by destructive interference. For classical waves in weak random potentials, this manifests itself in the phenomena of weak localisation and coherent backscattering. Furthermore, we studied how these effects can be controlled by properly chosen non-linearities [abu3]. Our interest also lies in understanding the interplay between disorder and interactions in bosonic many-particle quantum systems. For this purpose, we derived a microscopic stationary scattering theory of *interacting bosons in a three-dimensional, weakly disordered potential*, describing thermalization of the single-particle energies due to atom-atom collisions and the impact of these on the coherent backscattering signal [abu4]. We further derived equations for the time-dependent propagation of a Bose-Einstein condensate in mean-field approximation. In a different context, we developed a novel pump-probe approach for treating *multiple scattering of intense laser light in clouds of cold atoms* [abu6], where diagrammatic scattering theory is combined with quantum optical Bloch equations. These theoretical advances will allow us to shed new light on experimental results on Bose-Einstein condensates in random potentials or on coherent backscattering of light from cold atoms.

Quantum chaos

We consider helium as a prototype of a strongly correlated few-body system. Using parallel computation and semiclassical tools, we investigate the role of electronic correlations in ionization processes, the existence of long-lived excited states and electronic transport along the energy axis. In driven atomic systems dynamical localization prevents fast fragmentation by hampering the excitation process. Understanding how dynamical localization is affected by particle-particle interactions is essential to unravel the correlations observed in laser-driven atomic ionization. Using numerical simulations within a collinear model of microwave-driven helium Rydberg atoms we proved that *dynamical localization survives the impact of electron-electron interaction*, even for doubly excited states in the presence of fast autoionization. For a better understanding of the decay of driven and field-free helium, we developed a *formalism to calculate partial decay rates* of doubly excited states. Thus we can analyse independently all the available auto- and photo-ionization channels. We also studied the phase-space structure of classical two-dimensional helium with vanishing angular momentum, the so-called Wannier ridge. We found that in the presence of a weak external driving field, new islands of stability are induced in phase-space, while stronger fields always give rise to non-sequential correlated double ionization.

Cold atoms

We studied how the properties of a *BEC loaded in an optical lattice* can be deduced from those quantities accessible in a scattering experiment (transmission or inelastic cross section), and thereby analysed the fingerprint of the bosonic interaction in the scattering quantities. We have as well investigated the dynamical behaviour of condensates in tilted optical lattices. Recently, we focused on the *scattering of matter-waves from interacting bosonic gases* in one-dimensional lattices. Using Bogoliubov's formalism we derive an analytical expression for the inelastic scattering cross-section, and find a universal decay of the latter as a function of the interaction in the lattice, independent of system size and number of particles. We have also succeeded in identifying the decay phenomena for interacting bosons loaded into asymmetric double-well potentials. For *fermionic optical lattices*, we deduced an expression for the critical polarization below which the Fulde-Ferrell-Larkin-Ovchinnikov state emerges in one-dimensional lattices with spin-imbalanced populations, and investigated the impact of the excited state entanglement content on fermionic transport.

Quantum information

The focus of our group's quantum information section lies on the exploration and exploitation of many-particle interference and entanglement, the generation and control of entanglement, its protection against decoherence, and open system dynamics.

Many-particle interference and entanglement. The well-known Hong-Ou-Mandel effect, where two bosons or fermions bunch or anti-bunch in the output ports of a beam splitter, impressively demonstrates that quantum statistics and the entailed many-particle interference can have characteristic effects on the dynamics of identical particles. Starting out from an innovative definition of the entanglement of identical particles, we could show that the collective interference of three or more particles leads to much more diverse behavior than expected from the boson-fermion dichotomy. This is prominently reflected by non-monotonic relations between the occurrence of many-particle interference and the indistinguishability of the particles [abu1]. Currently, we are also including the impact of disorder on many-particle interference and correlations [abu5].

Towards larger numbers of particles, the full treatment of the many-particle dynamics becomes rapidly intractable, as it is convincingly demonstrated by the computational effort to describe boson sampling. Taming the complexity of many-particle interference thus becomes crucial to reliably predict the behavior of large systems. To this end, we could establish a simple law for the strict suppression of counting events in a Bell multiport beam splitter (Fig. 1.1), which serves to prooftest the underlying dynamics up to all orders of many-particle interference. Along different lines of research, we are currently developing a semiclassical approximation for systems of identical particles and an open system theory to efficiently describe subsystems of identical particles. In addition, we have developed several approaches to produce,

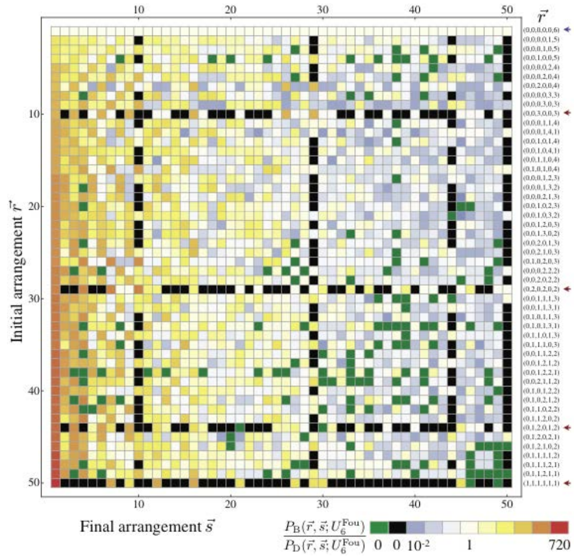


Figure 1.1: Many-boson interference in a setup with $N = 6$ bosons and $n = 6$ modes. The colour coding indicates the quotient of the probability for bosons, P_B, to the classical probability P_D, as a function of the input state $\vec{r}$ and of the output state $\vec{s}$. Black fields denote transitions that are suppressed due to the suppression law, while green fields represent suppressed events that are not predicted by the law.

detect and quantify many-particle entanglement.

Entanglement and decoherence in open systems. The generation and protection of entangled states becomes increasingly important with the upcoming of more and more applications of quantum technology. To this end, we have developed a time-local optimal control scheme to drive multipartite systems rapidly into highly entangled, robust quantum states. We complemented this by a general coherent control approach to uphold entanglement in the presence of dissipation in the long-time limit [abu9]. Currently, we are extending our method to also include monitoring and feedback. In different lines of research, we investigate the evolution of quantum correlations [abu7], their detection by local monitoring of open systems, and the effective description of complex, disordered systems, e.g. networks, by an open system dynamical approach.

1.2.2 Quantum Correlations

The research group **Quantum Correlations in Physics, Math, and Computer Science of D. Gross** was established in November 2011. The stated purpose was to provide a mathematical perspective on quantum mechanics, as well as to strengthen the links between the Institute of Physics on the one hand, and mathematicians and computer scientists on the other hand.

The group is led by a tenure-tracked assistant professor (Gross) and includes in late 2013 two postdoctoral researchers, three PhD students (two local and one visiting), and three students writing master theses. It is very international, with all postdocs and PhD students being foreign nationals.

Research

The group works on the interface between quantum mechanics and applied mathematics. Our main emphasis lies on the application of rigorous mathematical methods to problems in quantum information and many-body theory. Conversely, we aim to use methods originating in quantum physics to classical problems, e.g. in machine learning theory.

Selected recent activities: One focus lies on **compressed sensing** and **low-rank matrix recovery**, two highly active research fields in machine learning. Ref. [gro1], on estimating low-rank matrices, may be the most significant contribution of the group over all subjects. Derived from it are, e.g., our theoretical and experimental [gro2] papers on **characterisation of large-scale quantum systems**, and our work on **classical data recovery** from quadratic measurements. Close to 200 citing papers (Scholar) give further applications, from image enhancements, over face recognition, to robust statistics. Turning to theoretical physics, the **quantum marginal problem** concerns the relation between global and reduced states. Building e.g. on asymptotic representation theory, we have pointed out its applications to many-body physics [gro3] and quantum information [gro4]. In the context of traditional **mathematical physics**, we work e.g. on dynamics of infinite spin systems [gro5]. Two experienced postdocs drive research on **quantum contextuality** and **quantum thermodynamics** respectively.

In 2013, publications in "high impact" journals included one in Science, two in Nature Communications, and three in PRL. In the same year, the group contributed e.g. to pure and applied mathematics journals, including on Algebraic Combinatorics, Linear Algebra, and Information Theory.

Focus on Mathematical Physics

We aim to promote research and teaching on mathematical physics in Freiburg. The group organizes the intrafaculty colloquium on mathematical physics (with K. Wendland, Institute of Mathematics, and A. Buchleitner, Institute of Physics), and maintains a website listing activities in the field. In the summer terms 2013 – 2015, Gross will teach one newly developed course each on mathematical physics ('13: Hamiltonian Dynamics, '14: Structure of QM, '15: rigorous results in Statistical Physics).

Outlook

From 2014, two five-year grants (with O'Brien, experimental quantum optics, Bristol; and Flammia, theory, Sydney) will fund a PhD student and a postdoc working on experimental characterisation of large quantum systems. In the context of the proposed CRC on Quantum Efficiency, a similar project has been coordinated closely with the group of Schaetz in Freiburg, which will be pursued further.

Gross is involved in ongoing efforts to establish a DFG-funded Priority Programme on compressed sensing (as the only physics group). In preparation, a DFG proposal on low-rank methods for coding theory has been submitted late 2013 (with Prof. Bossert, telecomm. engineering, Ulm). Relatedly, with colleagues from Göttingen, Barcelona, and Texas, the group has received funding for a workshop "Mathematical Physics meets Sparse Recovery" at the Oberwolfach Math Research Institute (April 2014).

We collaborate with D. Janzing of the MPI for Intelligent Systems, Tübingen on a project linking ideas from quantum contextuality to the young field of causal inference (which aims to discover causal connections underlying empirical data). To further this, Dr. Chaves of our group has applied in late 2013 for startup funding from Freiburg's Innovation Fund.

In January 2014, the group will present itself to the Freiburg Center for Data Analysis and Modeling. The goal is to become an associate member – in order to strengthen connections to the math institute (and gain access to office space needed for the growing group).

1.2.3 Molecular and Optical Physics

The current research activities of the **Molecular and Optical Physics group of H. Helm** fall into four main topics. All experiments are done in our laboratories in Freiburg at the VF and FMF (see Part I, Fig.1.1). The group is embedded in German, European and international networks.

Superposition states of atoms in tailored laser fields

The non-classical nature of superposition of two states is at the heart of modern methods of high resolution measurement. A specific class of superposition states are dark states when atoms are immune to illumination but are strongly absorbing when they are not dark. The phase of the amplitudes of the superposition is the critical parameter for darkness and we have explored its significance in the preparation of atoms and the survival of the state in presence or absence of phase-controlled light fields. We have studied the atomic dynamics of evolving into the dark state condition as well as the free induction decay which is observed when the coherent superposition is illuminated by nonresonant fields. This led to the development of a phase-switching method capable of measuring the quantum phase difference of the states involved in the superposition [hel1]. This phase can be determined in a nearly nondestructive manner. This method permitted a concise investigation of Berry's geometric phase which we can imprint in an atomic superposition state by rotating a laboratory magnetic field [hel2]. We have also explored a

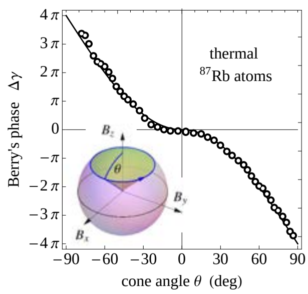


Figure 1.2: Observation of Berry's geometric phase imprinted in quantum superposition states of Rb-atoms by rotating the laboratory magnetic field [hel2].

classical analogue of the dark state in a metamaterial containing split-ring resonators.

Among the many applications of dark states in metrology is their entanglement with translational degrees of freedom of the atoms. The controlled darkness of vibrational transitions of an atom in a trapping potential promises a method for reaching Bose-Einstein condensation without evaporative cooling. We have pursued this topic in experiments with laser cooled trapped atoms in a far detuned optical dipole trap and prepared our understanding of this tool by numerical simulation of realistic environments [hel3].

Nonadiabatic coupling in triatomic hydrogen

Triatomic hydrogen is a ubiquitous and frequently the predominant molecular species in hydrogen plasmas and in interstellar clouds. In its most stable form it is ionized, H_3^+. This ion controls the local electron density as it recombines with slow electrons to form H_2+H or $H+H+H$. The rate of recombination has been studied in many laboratories with greatly diverging results and has been a controversial topic in experiment and theory for the past 30 years. Recombination involves the temporary formation of neutral H_3 which subsequently decays. We have developed means to prepare by laser excitation these intermediate forms of neutral H_3 and have studied their autoionization and predissociation as these represent the intimate paths involved in recombination.

Our latest work deals with the breakup of state-selected H_3 molecules into three slow hydrogen atoms. The experiment uses time and position sensitive wire-detectors for neutral hydrogen atoms with 30 ps time- and 50 μm spatial resolution. We succeed in the coincident detection of the three H(1s)-atoms released by a single molecule and determine the correlated momentum vectors of the three atoms. Nuclear symmetry plays a decisive role in the se-

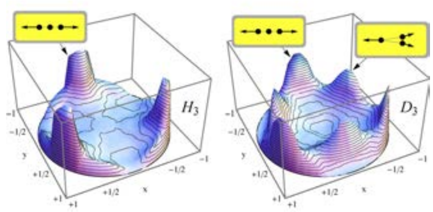


Figure 1.3: A profound isotope effect in predissociation of Rydberg states in the vicinity of the ionization thresholds of H_3 and D_3 [hel4].

lection of mechanical degrees of freedom as shown by isotope effects between D_3 and H_3 [hel4]. When viewed in the laboratory frame, the correlated momentum vector image is an analogue of the optical far-field of a diffracting object, in our case the intermediate H_3 molecule at the time of breakup. As the lifetime of the molecule is typically larger than the rotational and vibrational period, the image of momentum correlation represents a view of the available phase space in which nonadiabatic coupling opens a door for the molecule to enter the continuum of three separating hydrogen atoms. This is the first time that direct views of the modulus of a many particle wavefunction are obtained in an experiment. The results attest to the complex forms of nonadiabatic coupling in polyatomic molecules and provide stringent tests for many-body quantum dynamics theory [hel5].

Strong field physics

At light intensities above 1 TW/cm^2 the wavefunction and energy spectrum of atoms and molecules can be greatly distorted from the nascent form. Our pioneering development of photoelectron imaging has led to tools (now in use in over 40 laboratories world wide) capable of imaging the distorted electronic wavefunction, as it is projected by a final photon into the continuum of free electrons. Theory has kept apace with simulating the light-field induced distortion of the atomic wavefunction using analytical models or numerical simulation of the time-dependent Schrödinger equation, even for nearly exact atomic structure, when exposed to strong light fields. By comparison the understanding of molecular structure and the structure of negative ions in strong fields is far less developed.

Recent Freiburg experiments deal with molecular hydrogen and fluorine [hel6]. They show that the commonly accepted ponderomotive shifting of electronic states can be greatly modified due to electronic coupling in bound-bound transitions. In collaboration with the Univ. Goeteborg high resolution studies of threshold photodetachment were undertaken. A latest highlight is the time-resolved study of strong-field ionization of a superposition of fine structure states

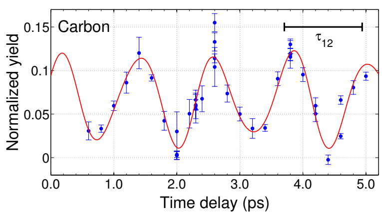


Figure 1.4: The time-resolved spatial oscillation of electron density in the carbon atom ground state is detected along a laboratory coordinate [hel7].

of the carbon atom ground state. The neutral atom is formed in the gas phase by fs-pulse photodetachment of C$^-$ producing C(^{3}P) in a coherent superposition. The isolated atom evolves with time as manifested by the oscillation of the spatial distribution of the electron density along an axis chosen by the detachment laser [hel7].

In a seemingly unrelated subject the Deutsche Wetterdienst and a local company requested measurements of the sinking velocity of airborne pollen for calibration of commercial pollen counters and simulation of pollen flight over Europe. We responded by constructing Paul traps for holding and studying single pollen over long periods of time in controlled temperature-humidity environments. We discovered that the sinking velocity controls the stability boundary in the Paul trap via the drag coefficient. The dependence of sinking velocity on the number of conglomerated pollen was determined.

THz radiation and applications

Our group has pioneered electro-optic detection of electromagnetic radiation fields in the THz range and has over the years concentrated on microscopic structure related vibration and relaxation of biological molecules and ionic liquids. Recently our focus has moved to plasmonics and metamaterials. Metamaterial structures are build from micro resonators and feature unusual optical properties. A latest highlight is the development of a near-field microscope capable of detecting the electromagnetic field vectors of an ac-field with sub-picosecond time and 5 or 25 μm spatial resolution [hel8]. This microscope has proven to be a worldwide unique tool for characterizing the near-field properties of micro resonators or surface-plasmon polaritons and for sub-wavelength resolution imaging. Using radially polarized light we visualized surface-plasmon polaritons, focused to sub-wavelength spotsize. We demonstrated sub-diffraction imaging and focussing using metamaterial fibers fabricated at the Univ. Sidney [hel9]. Coupling between micro resonators has been studied in the near- and far-field. In cooperation with the univer-

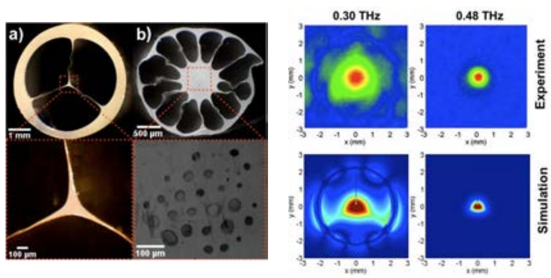


Figure 1.5: Sub-wavelength sized, solid-core fibers used for transport of electromagnetic radiation and THz near-field images at the fiber exit. [hel10]

sities Adelaide and Southampton coaxial micro cavities for localized plasmons and a switchable liquid crystal based metamaterial device were developed and characterized.

1.2.4 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, thermodynamical or chemical properties significantly. In order to characterize and understand such effects in detail the **Cluster Physics group of B. von Issendorff** studies size-selected and temperature controlled clusters in the gas phase, employing a range of spectroscopic methods. In the following his main research projects are briefly described:

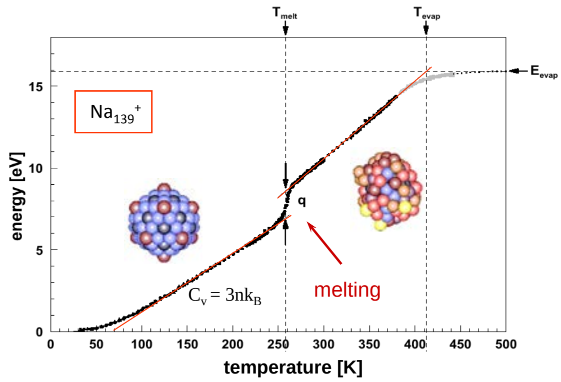


Figure 1.6: Caloric curve of a free sodium cluster.

Electronic and geometric cluster structures

Using photoelectron spectroscopy, the electronic density of states of the clusters is monitored. This allows to directly study quantum size effects, but also, in combination with high level theory (mainly DFT calculations, performed e.g. in the group of Michael Moseler), the determination of the geometric structure of the clusters. Systems examined are, e.g., alkaline and noble metal clusters, divalent metal clusters, or negatively charged water clusters, where the additional electron is localized in a hydration shell. The application of angle resolved photoelectron spectroscopy allows to obtain direct information about the form of the electron wavefunctions [iss1]. Recent achievements were the determination of the electron binding energy in very large water clusters, the discovery of an unusual doping behavior of silicon atoms in gold clusters [iss3], or the observation of the mixing of angular momentum eigenstates in deformed sodium clusters [iss1].

Ultrafast dynamics

Using time-resolved femtosecond pump-probe photoelectron spectroscopy, the electron dynamics is studied. Systems examined are metal, semiconductor and carbon clusters (fullerenes). In C_{60}^{-} for example recently 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.

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. Recently the focus was put on water clusters, which were shown not to undergo melting, but to exhibit rather a glass transition.

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 (Helmholtz Zentrum Berlin), a new setup has been constructed which allows to measure XMCD spectra on size selected clusters stored in a liquid helium cooled ion trap within a 5T magnetic field. The recent measurements of high quality XMCD spectra of free clusters can be considered a breakthrough in nanoparticle magnetism research [iss2].

FEL experiments

The advent of XUV and X-ray free electron lasers offers exciting possibilities for cluster research. The group is part of a consortium which performs photoelectron spectroscopy experiments on free size-selected clusters at the FEL FLASH in Hamburg. Full use of the time structure and intensity of FEL pulses can be made by measuring time-resolved diffraction patterns of particles, which will yield movies of the motion of these particles and thereby yield unprecedented insight into nanoparticle dynamics. Experiments of this type are currently prepared in a cooperation with the group of Thomas Möller (TU Berlin).

1.2.5 Atomic and Molecular Physics

The endeavor to control increasingly large systems of particles at the quantum level will be one of the driving forces for physical sciences in the coming decades. The **Atomic and Molecular Physics group of T. Schaetz** aims to gain (i) 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 experimental work builds on different trapping technologies. On the one hand, on conventional rf-traps (see Figs. 1.7 and 1.10). We further extended this approach in size and dimension towards two-dimensional arrays of individual traps spanned by micro-fabricated surface electrodes (see Fig. 1.9, work contributing to the initiative at FRIAS, see Part II, Section 1.1). On the other hand, we aim to explore and exploit trapping of ions and atoms by optical means (This project is embedded in the IRTG initiative). The group moved into its novel laboratories in February 2012.

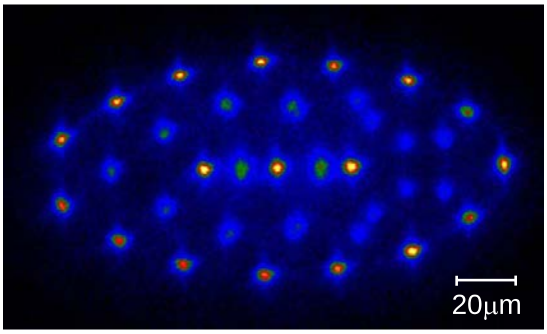


Figure 1.7: Scaling Coulomb crystals in size and dimension while maintaining the unique controllability of the individual ion might allow addressing intriguing quantum effects in many different fields of physics. Here: Fluorescence image of ≈ 40 ions within one single trapping potential of our conventional 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 get precisely controlled, underlying quantum effects detected sufficiently well and their relevance could get revealed [sae9]. This might remain valid for open systems, since the environment coupled to the simulator can be tailored with its impact being suspected to influence significantly the relevant quantum dynamics. Our group is dedicated to build such a model system based on trapped ions (and atoms), to derive and to perform two different classes of experimental quantum simulations: (1) addressing systems that might still be numerically tractable, however, hard or impossible to get realized in the laboratory. (2) addressing systems that remain numerically intractable, but where experimental results might assist in revealing underlying concepts. In the context of class (1), we proposed how to extend our experimental work on quantum walks on non-orthoganal motional states [sae6], collaborating with the group of R. Werner (University of Hannover). In another approach, we discovered how to realize topologically protected defects within Coulomb crystals - in parallel to theoretical work done by B. Reznik and H. Landa (University of TelAviv) revealing the suitability of those defects to simulate solitons in the quantum regime.

Simulating discrete solitons: During the process of crystallization, a system will seek for perfect order (minimal energy). By evolving the phase-transition too fast for communication between different sections of the crystal, sub-ensembles find perfect crystalline order, while becoming incommensurate at their borders (see Fig. 1.8). We demonstrated that these defects can oscillate as trapped quasi particles in their self-induced confining potential within the crystal [sae3]. In close collaboration with theory, we reported about the properties of our experimental findings [sae2], such as, the different species of defects, their coupling to the mesoscopic environment of the crystal, their mutual (coherent) interaction and their potential prospects on accessing the quantum regime, provided by the unique, gapped structure of the related localized motional modes [sae3].

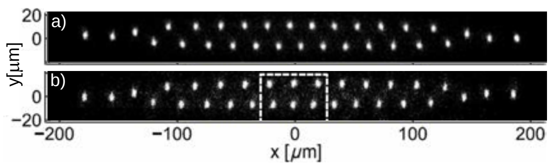


Figure 1.8: 1D-2D Coulomb crystals (31 ions). a) CCD image of fluorescence light of ions in zigzag configuration. b) Only the ions to the left of the centre region (dashed box) form a zigzag structure as in (a), the positions on the right are mirrored about the x-axis. The ions in the centre region are forming an extended topological defect, predicted to feature a discrete soliton.

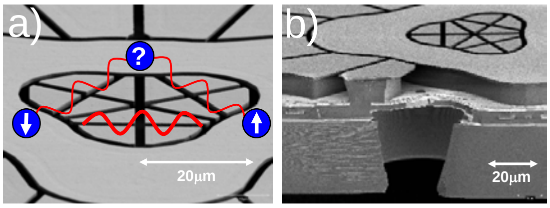


Figure 1.9: Electron-microscopic images of our novel rf-surface traps, a basic 2D array micro-fabricated by SNL. a) Bird's eye view, the gaps isolating between rf and DC patches (ions and individually controllable interactions are animated). Three ions residing in three individual traps are suited to simulate anti-ferromagnetic interactions between three quantum spins. Classically, only two neighbouring 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 tremendously complex state). b) Show case (similar as (a)), however, providing additional insight into the underlying structure, e.g., the electrodes' extensions shielding the insulators and the cross section through a loading hole.

Simulating quantum spin systems: 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, following a proposal by Porras and Cirac, we further extended our simulator in size and dimensionality. Our efforts are two-fold.
(i) Together with our collaborators from the Universities of Ulm, Madrid and Sussex, we further proposed how to extend the experimental toolbox, boosting the strength of interaction by using phonons directly for simulating particles exposed to artificial gauge fields [sae10] and to photo-assist and control the dynamics of their tunneling between neighbouring lattice sites simulated by the ions [sae8]. We additionally study to exploit continuous sympathetic cooling of the phonon modes mediating relevant interaction in the model system, that is, permitting them to provide even more robust coherent (entangling) operations [sae4]. The Fraunhofer Institute for Physical Measurement Techniques (IPM), funded by a private investor, is developing a novel laser concept and supporting us with a pilot system, especially designed for this purpose.
(ii) Supported by our collaborators at the National Institute of Standards and Technology (NIST) and Sandia-National-Laboratories (SNL) we designed and realized a basic, two dimensional array of rf-surface traps (see Fig.1.9). In parallel, we tested a state-of-the-art liner trap that had been fabricated by SNL according to the identical (MEMS) technologies. We recently trapped ions within the fully functional triangular array [sae1].

OPtically trapping Ions and AToms (OPIAT)

Our group had achieved optical trapping of an ion in a dipole trap, recently followed by a 1D-optical lattice [sae5] (see Fig.1.10). There is a long-term prospect for scaling 2D quantum simulations in optical lattices, based on ions or even on ions and atoms. However, our current project of optically trapping an ion within a BEC of atoms is dedicated to overcome fundamental limitations set by micro-motion when combining optical and rf-trapping. We want to study how chemical reactions proceed at lowest temperatures? The classical concept predicts that approaching zero velocity is equivalent to a standstill of any dynamics. On the one hand, deviations can be expected, since the classical model is ceasing to be appropriate when particle-wave dualism is gaining importance. On the other hand, we might see quantum mechanical properties as minor corrections. However, in the regime of lowest temperatures quantum effects dominate and chemistry is predicted to obey fundamentally different rules. As a consequence, quantum chemistry

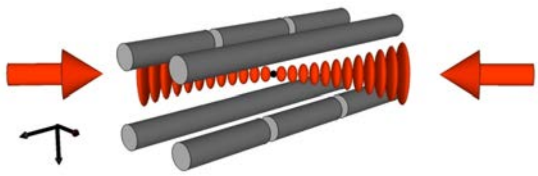


Figure 1.10: Schematic for all-optical trapping. Initially, the segmented, linear rf trap provides a two-dimensional confinement in the radial directions while the axial confinement is featured by dc voltages. After trapping and laser cooling, residual stray fields get compensated before transferring the ion into the optical trap (dipoletrap: rf off, dc on; standing wave: rf and dc off).

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 Warsaw) we aim to study ultra-cold formation of $BaRb^+$ within our optical traps. In a different context, however, developing the basic toolbox for operation, we performed a pump-probe experiment (5fs UV-pulses) on a single molecular ion [sae7]. In collaboration with R. Cote (Univ. of Connecticut) we elaborate on options how to observe a BEC bound to an ion.

1.2.6 Molecular and Nanophysics

The focus of research of the **Molecular and Nanophysics group of F. Stienkemeier and M. Mudrich** lies in understanding the fundamental quantum mechanical properties of atomic and molecular complexes and their interaction with light. The properties of the systems under study and the dynamics of processes are primarily probed by the interaction with electromagnetic radiation. Utilized light sources include spectrally highly resolving laser systems, ultra-short pulse lasers for dynamical studies and facility-based light sources in the XUV range (synchrotron, free-electron-lasers). In order to concentrate on fundamental aspects and to resolve quantum state specific properties, isolated unperturbed atomic and molecular complexes at cold or ultracold temperatures are probed such as gas-phase atomic, molecular or cluster beams, or cluster-isolated molecular complexes. Here, in particular helium nanodroplet isolation techniques at millikelvin temperatures are pursued. On the one hand, we are intrigued by the fundamental properties of superfluid helium nanodroplets and their guest-host interaction for which we use the embedded species as microscopic probes. On the other hand, we utilize the helium nanodroplets as "nano-cryostats" for synthesizing molecular complexes in a cold and weakly interacting matrix. Experiments include the dynamics of aggregation and cluster formation, microsolvation, cold chemical reactions, photo-dissociation and ionization by multi-photon absorption up to the strong-field and collective regimes. Furthermore the dynamics of cold molecular collisions using velocity-tunable molecular beams and laser-cooled scattering targets is studied.

Excitation and energy transfer in molecules and organic nanostructures

The formation of organic complexes and nanostructures isolated in helium nanodroplets and at rare gas clusters allows by means of VIS and UV spectroscopy to characterize electronic and geometric structures both of the chromophores [sti1] and the host clusters [sti2]. The unique synthesis at rare gas clusters by successive pickup of individual constituents provides specific compositions of a host-guest system (Fig. 1.11). Using organic molecules (e.g. PTCDA) we compared the dopant interaction and achievable spectral resolution for different host cluster materials (Ar, Ne, H_2), also in correspondence with bulk matrices, studied in collaboration with the group of Wolfgang Harbich at the EPFL in Lausanne. The quite unresolved bulk spectra could be assigned in comparison to cluster isolated absorption and emission spectra [sti2]. Continuation of this work at higher doping levels even yielded superradiant properties, where the doped organic chromophores collectively and coherently emit fluorescence as evidenced by a lifetime shortening of the excited states. In collaboration

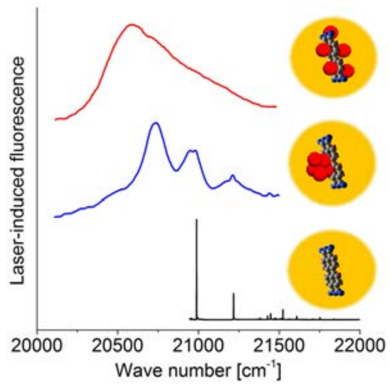


Figure 1.11: Absorption spectra of the polycyclic aromatic pigment molecule PTCDA isolated in He nanodroplets (bottom trace) and complexes of PTCDA with Ar atoms in two different conformations (upper traces).

with the Fraunhofer IAP (Institute for Applied Solid State Physics) a new narrow-band mid-IR VECSEL (Vertical External Cavity Surface-Emitting Laser) has been tested for high resolution vibrational spectroscopy. Sufficient power and narrow bandwidth for overtone spectroscopy of CO_2 could be confirmed; however, the scanning capabilities are not sufficient yet over desirable ranges.

LDM Beamline at FERMI@Elettra - Studies of electronic processes with XUV light sources

Our group has coordinated in an international collaboration (Fig. 1.12) the setup of the Low Density Matter (LDM) endstation at the LDM beamline at the new seeded XUV Free-Electon-Laser (FEL) FERMI@Elettra in Trieste. The major part of the endstation was designed, assembled and tested in Freiburg. It combines a variety of beam sources (pulsed supersonic sources for atomic, molecular, doped cluster and nanodroplet beams, radicals, micro plasma source) with velocity map imaging photoelectron and photoion detection, high kinetic energy ion detection and photon scattering. First results on pure and doped helium clusters revealed a new collective ionization process [sti3, sti4]. Since FERMI is the first seeded XUV FEL with outstanding coherence properties, in particular pump-probe experiments (IR-XUV, UV-XUV, XUV-XUV) are in preparation. Complementary to the experiments

Figure 1.12: LDM Project: Collaboration to setup an endstation for experiments involving atomic molecular and cluster beams at FERMI@elettra.

with XUV FEL radiation, synchrotron radiation has been employed applying photoelectron-photoion-coincidence-spectroscopy (PEPICO) of neutral cluster beams. An inwards/outwards migration process of charges/excitations, respectively, was identified in helium droplets [sti5].

Energy dissipation and coherent processes in cluster-isolated molecular systems

Real-time photodynamics has been studied using femtosecond pump-probe techniques in combination with various detection schemes. One focus lies on the dynamics of molecular rotations and vibrations under the influence of the superfluid He droplet environment. In the cases of alkali metal diatomic and triatomic molecules the system-bath couplings induce slow vibrational relaxation and decoherence on time scales ranging from 10 to 100 picoseconds. This allows to perform precision vibrational spectroscopy of weakly bound high-spin systems which are not accessible by other methods. Furthermore, the analysis of decay and decoherence times in comparison with model calculations done by W. Strunz at the TU Dresden provides fundamental properties of nanometer-sized quantum fluid clusters and their interaction with molecular probes [sti6].

The formation or breakup of chemical bonds can be studied by means of time-resolved mass-spectrometry and by imaging fragment ions or electrons from photoionization. In this way, the formation and stabilization of exotic alkali metal-helium exciplex molecules has been followed in real-time. Probing the desorption process of excited dopant atoms off the helium droplet surface by means of ion imaging spectroscopy reveals the details of the photodynamical response of metal-helium droplet complexes [sti8]. Surprisingly, we find excellent agreement with a simple diatomic model where the metal atom constitutes one atom and the whole helium droplet the other. This work is pursued in collaboration with the theory group of M. Barranco at the University of Barcelona with the goal of reaching a detailed microscopic understanding of solvation and desolvation dynamics. In an active collaboration with A. Baklanov at ICKC in Novosibirsk, Russia, we study the photodynamics of highly excited diatomic molecules prepared in the gas-phase or inside helium nanodroplets using ion imaging detection.

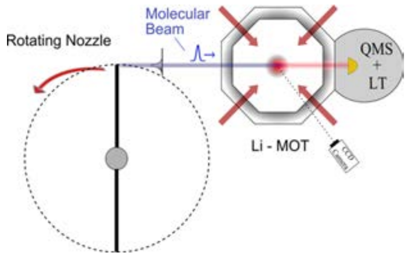


Figure 1.13: Sketch of the experimental setup used for cold collision experiments.

Upon illumination of a helium droplet with intense near-infrared laser pulses, a highly charged nanoplasma is ignited, provided the droplets are doped with a few dopant atoms or molecules which act as seeds. The dynamics of the ignition and expansion of these helium nanoplasmas have been studied in a collaboration with the experimental group of J. Ullrich and R. Moshammer at MPI-K in Heidelberg with the theory group of J. M. Rost and U. Saalmann at MPI-KS Dresden and of T. Fennel at the University of Rostock [sti9].

Cold collisions and cold chemistry

The dynamics of elementary collisions and reactions at very low temperature is governed by quantum mechanical effects. We experimentally investigate reactive and non-reactive collisions between atoms and molecules at tunable scattering energies below 10 K. Our approach combines a magneto-optic trap for ultracold lithium atoms with a setup for producing slow and cold molecular beams from a counter-rotating nozzle (Fig. 1.13). Surprisingly, even elastic atom-atom collisions feature highly structured differential scattering cross sections due to the presence of quantum rainbow features, diffraction oscillations and shape resonances [sti10]. Various techniques of guiding and focusing beams of polar molecules using electrostatic fields have been developed. New methods of generating slow beams of cold molecules using cryogenic pulsed valves, magnetic and electrostatic decelerators are being developed in collaboration with T. Momose at UBC in Vancouver.

1.2.7 Biomolecular Dynamics

The **Biomolecular Dynamics group of G. Stock** is concerned with the theory and computation of biomolecular dynamics and spectroscopy. To describe the structure, dynamics and function of biomolecules in microscopic detail and to account for the various corresponding observables from NMR, EPR, IR and UV spectroscopy, we combine classical molecular dynamics simulations and mixed quantum-classical concepts. All-atom computer simulations as well as state-of-the-art multidimensional experiments on biomolecules generate an enormous amount of data, which require a careful theoretical analysis. The ultimate goal is a truly microscopic understanding of the underlying physics, which usually requires the construction of simple models that explain the essential dynamics of the process. Most of our research projects during the reporting period can be summarized in the three topics listed below.

The *Biomolecular Dynamics* group provides a link between the molecular physics research of the light-matter interactions groups and the biophysics and polymer research of the condensed-matter groups, and also connects to the Physical Chemistry groups of the Chemistry department. From October 2010 to October 2012, G. Stock was Managing Director of the Institute of Physics. Currently he is a Senior Internal Fellow of the Freiburg Institute for Advanced Studies (FRIAS).

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 [sto1]. The resulting low-dimensional probability distribution $P(\{q_i\})$ can then be used to construct the free energy landscape $F = -kTP(\{q_i\})$ 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 [sto2]. 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 [sto3]. During the reporting period we have developed and improved these methods and employed them to study peptide conformational dynamics [sto1], protein folding [sto4] and peptide aggregation [sto5].

As a highlight of this research direction, we mention the recently proposed *most probable path* algorithm which identifies the metastable states of the system, combined with dynamical coring of these states in order to obtain a consistent Markov state model [sto3]. Adopting extensive molecular dynamics simulations of villin headpiece protein (Fig. 1.14), the method facilitates the construction of a dendrogram associated with the folding free energy landscape, which reveals a hierarchical funnel structure and shows that the native state is rather a kinetic trap than a network hub [sto4]. The model is in line with recent experimental observations that the intermediate and native states differ mostly in their dynamics (locked vs. unlocked states).

Moreover we have developed a novel data driven Langevin algorithm, which performs a local 'on the fly' estimation of the multidimensional Langevin vector fields describing deterministic drift and stochastic driving [sto2]. The approach avoids the definition of Markov states as it is defined in coordinate space, it can be derived from a microscopic Hamiltonian using projection techniques, and it contains the temperature as driving force. As the method requires only local information, the input data need not to be Boltzmann weighted in order to warrant that the Langevin model yields correct Boltzmann-distributed results. This property can be used in enhanced sampling methods such as the construction of the overall energy landscape of a system from short trajectories.

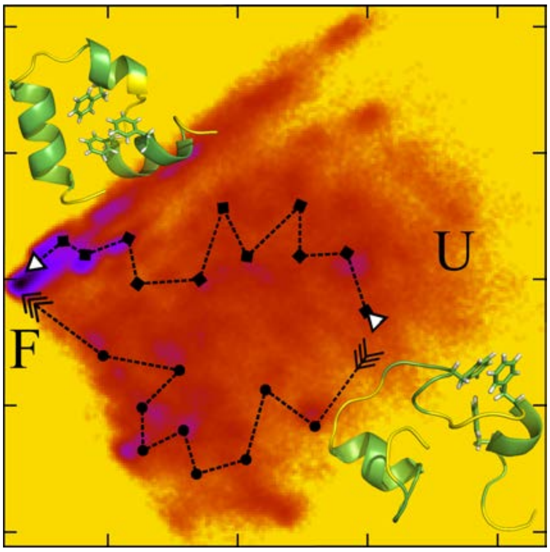


Figure 1.14: Free energy landscapes of the folding of villin headpiece protein [sto4].

Energy and signal flow

The propagation of energy, heat and signal flow through molecular systems has received consider-

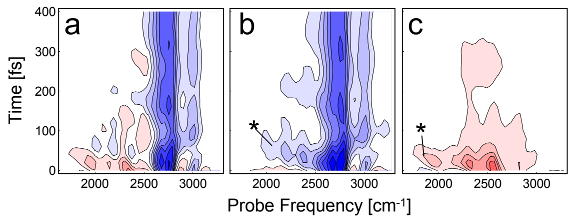


Figure 1.15: Time- and frequency-resolved pump-probe spectrum for a three-mode model of a vibrational conical intersection [sto8]. Shown are the (a) complete signal, (b) bleach and stimulated emission contribution and (c) excited state absorption. Signals of positive and negative sign are colored in red and blue, respectively.

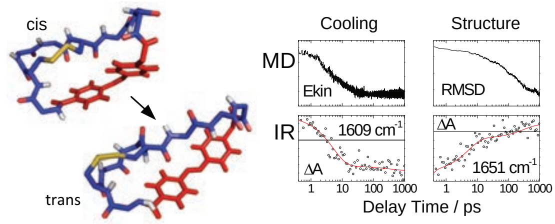


Figure 1.16: Following ultrafast cis-trans photoisomerization of a photoswitchable bicyclic peptide, transient infrared spectroscopy as well as molecular dynamics simulations reveal the cooling of the photoexcited system in the water solvent (5 ps) and the conformational rearrangement of the peptide (300 ps) in real time [sto7].

able interest. In biomolecules, the transport of heat and vibrational energy occurs within (tens of) picoseconds [sto6]. The propagation of conformational change in intramolecular signaling, on the other hand, is believed to occur on a much longer time scale of say, nano- to milliseconds. Interestingly, though, recent experiments and simulations indicate a possible connection between these fast and slow processes, e.g., via the notion that allosteric interactions may be of dynamical nature. To investigate these intriguing phenomena, transient infrared experiments on photoswitchable peptides and proteins (collaboration with P. Hamm, Zürich) are a powerful approach, because they are able to monitor all time scales of interest. Accompanying theses experimental studies, nonequilibrium molecular dynamics simulations allow us to study the mechanisms of energy transport and the transport of conformational change. We have shown that the energy flow in biomolecules is indeed fast and anisotropic, and can affect resides quite distant from the heat source. Transport of conformational change in a photoswitchable PDZ2 domain, on the other hand, is found to occur in various stages from pico- to microseconds, which may reflect elastic deformation, (de-)stabilized interactions and conformational transitions. The simulations have been employed in the interpretation of transient IR spectra reflecting energy transport and conformational change [sto7]. Currently, three further publications are written up on this endeavor. The project is also the topic of G. Stock's Senior Internal Fellowship at the Freiburg Institute for Advanced Studies.

In a somewhat different line of research, we have introduced the concept of vibrational conical intersections as a potential source of ultrafast vibrational energy relaxation, using the coupling between high-frequency OH modes and low-frequency intramolecular hydrogen bonding modes [sto8, sto9]. Adopting malonaldehyde and the water dimer as first examples, we have derived a model Hamiltonian, parameterized it via *ab initio* calculations, and performed time-dependent wave packet calculations of the vibrational relaxation dynamics. A simulation of the corresponding time- and frequency-resolved spectra (Fig. 1.15) revealed that the spectral response of the simple models is qualitatively quite similar to the experimental response of strong intramolecular hydrogen bonds.

Multidimensional time-resolved spectroscopy

In transient infrared (IR) experiments, a molecular system may be photoexcited in a nonstationary conformational state, whose time evolution is monitored via IR spectroscopy with high temporal and structural resolution. As a theoretical formulation of these experiments, we have derived explicit expressions for transient one- and two-dimensional IR spectra and discuss various levels of approximation and sampling strategies [sto10]. Adopting a photoswitchable octapeptide in water as a representative example, nonequilibrium molecular dynamics simulations were performed and the photoinduced conformational dynamics and associated IR spectra are discussed in detail [sto7, sto10]. Interestingly, it has been found that the time scales of dynamics and spectra may differ from residue to residue by up to an order of magnitude. Even when a localized amide I mode is probed (e.g., via isotope labeling), the vibrational frequency shift was shown to depend in a complicated way on the conformation of the entire peptide as well as on the interaction with the solvent (Fig. 1.16). The study clearly reveals the limits of the interpretation of transient IR spectra and conformational dynamics in terms of a few exponential time scales.

1.2.8 Kiepenheuer-Institute for Solar Physics

The **Kiepenheuer-Institut für Sonnenphysik (KIS)** led by O. von der Lühe (experimental solar physics) and S. Berdyugina (theoretical solar physics) 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 three main research foci: Sun, Stars, and Techniques.

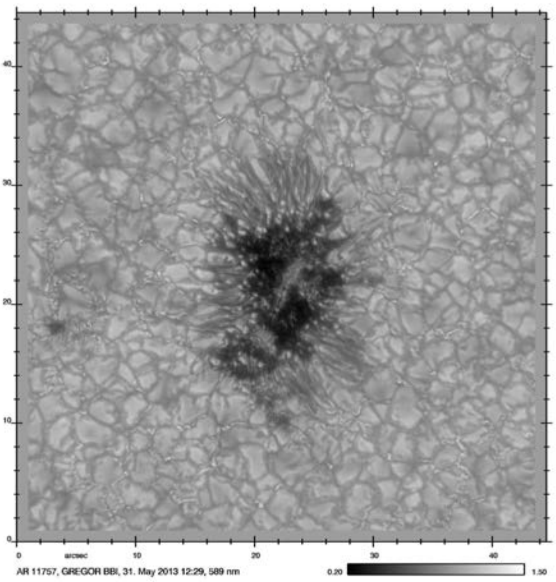


Figure 1.17: A small sunspot observed at GREGOR with a 1 nm pass-band filter at 589 nm with the spatial resolution approaching the telescope diffraction limit of 60 km on the solar surface.

Recent research highlights include:

- observational detection and numerical verification of fine-structure vortex tubes within granules,
- discovery of magnetic tornadoes as new energy channels into the upper atmosphere,
- detection of magnetic field topology variations during a sunspot emergence and numerical and observational studies of wave properties in the solar atmosphere, with implications for the outer solar atmosphere heating,

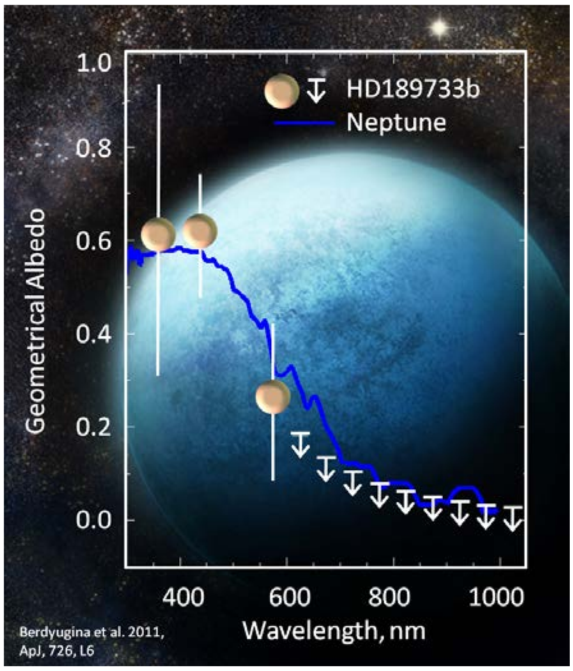


Figure 1.18: The first measurement of the geometrical albedo of an exoplanet reveals its blue color similar to Neptune.

- new helioseismological constraints on the meridional flow, sunspot magnetic field structure and flows below sunspots,
- first detection of the reflected light from an extrasolar planet and determination of its albedo and color.

The institute operates German solar telescopes at the Observatorio del Teide, Tenerife, Spain, including the 1.5-m telescope GREGOR (since 2012), 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 (ATST/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 (ATST, EST, SPRING).

1.3 Important Publications and Conference Talks

1.3.1 Publications

Group Buchleitner

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[abu4] T. Geiger, T. Wellens, and A. Buchleitner, “Inelastic Multiple Scattering of Interacting Bosons in Weak Random Potentials”, Phys. Rev. Lett. **109** (2012) 030601.

[abu5] F. Schlawin, N. Cherroret and A. Buchleitner, “Bunching and anti-bunching of localised particles in disordered media“, Europhys. Lett. **99** (2012) 14001.

[abu6] V. Shatokhin and T. Wellens, “Rigorous derivation of the triple scattering signal from single-atom responses”, Phys. Rev. A **86** (2012) 043808.

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[abu8] J. Zimmermann, R. Mulet, T. Wellens, G. D. Scholes, and A. Buchleitner, “Efficiency scaling of non-coherent upconversion”, J. Chem. Phys. **138** (2013) 134505.

[abu9] S. Sauer, C. Gneiting and A. Buchleitner, “Optimal Coherent Control to Counteract Dissipation”, Phys. Rev. Lett. **111** (2013) 030405.

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Group Gross

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[gro5] D. Gross, V. Nesme, H. Vogts and R.F. Werner, “Index theory of one dimensional quantum walks and cellular automata,” Commun. Math. Phys. **310** (2012) 419.

Group Helm

[hel1] C. Basler, K. Reininger, F. Meinert, P. N. Ghosh, and H. Helm, “Phase control and diagnostic of quantum mechanical superpostition states,” Phys. Rev. A **87** (2013) 013430.

[hel2] S. Welte, C. Basler and H. Helm, “Studies of Berry’s phase and its sign in quantum superposition states of thermal ^{87}Rb atoms,” Phys. Rev. A (2013) submitted.

[hel3] M. Roghani, H. Helm and H.-P. Breuer, “Entanglement dynamics of a strongly driven trapped atom,” Phys. Rev. Lett. **106** (2011) 040502.

[hel4] P. C. Fechner, K. Mozer, and H. Helm, “Profound Isotope Effect in Dissociation of Triatomic Hydrogen,” J. Phys. Chem. A **117** (2013) 9794.

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Group von Issendorff

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[iss2] M. Niemeyer, K. Hirsch, V. Zamudio-Bayer, A. Langenberg, M. Vogel, M. Kossick, C. Ebrecht, K. Egashira, A. Terasaki, T. Möller, B. v. Issendorff and J. T. Lau Spin coupling and orbital angular momentum quenching in free iron clusters Phys. Rev. Lett. **108** (2012) 057201.

[iss3] Kiran Majer, and Bernd v. Issendorff Photoelectron spectroscopy of silicon doped gold and silver cluster anions Phys. Chem. Chem. Phys. **14** (2012) 9371.

[iss4] C. Hock, M. Schmidt, and B. v. Issendorff Low-temperature caloric behavior of a free sodium nanoparticle Phys. Rev. B 84 (2011) 113401.

[iss5] J. T. Lau, M. Vogel, A. Langenberg, K. Hirsch, J. Rittmann, V. Zamudio-Bayer, T. Möller, and B. von Issendorff Highest occupied molecular orbital-lowest unoccupied molecular orbital gaps of doped silicon clusters from core level spectroscopy J. Chem. Phys. **134** (2011) 041102.

Group Schaetz

[sae1] T. Schätz, C. Monroe, T. Esslinger, “Focus on quantum simulation,“ New J. Phys. **15** (2013) 085009.

[sae2] H. Landa, J. Brox, M. Mielenz, B. Reznik, T. Schätz, “Structure, Dynamicss and Bifurcation of Discrete Solitons in Trapped Ion Crystals,“ New J. Phys. **15** (2013) 093003.

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[sae4] A. Bermudez, T. Schätz, M.B. Plenio, “Dissipation-Assisted Quantum Informaton Processing with Trapped Ions,“ Phys. Rev. Lett. **110** (2013) 110502.

[sae5] M. Enderlein, T. Huber, Ch. Schneider, T. Schätz, “Single ions trapped in a one-dimensional optical lattice,“ Phys. Rev. Lett. **109** (2012) 233004.

[sae6] R. Matjeschk, A. Ahlbrecht, M. Enderlein, Ch. Cedzich, A.H. Werner, M. Keyl, T. Schätz, “Quantum walk with non-orthogonal position states,“ Phys. Rev. Lett. **109** (2012) 240503.

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[sti1] J. Roden, A. Eisfeld, M. Dvorak, O. Bünermann, F. Stienkemeier, "Vibronic Lineshapes of PTCDA Oligomers in Helium Nanodroplets," J. Chem. Phys. **134** (2011) 054907.

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[sti6] B. Gruener, M. Schlesinger, P. Heister, W. T. Strunz, F. Stienkemeier, M. Mudrich, "Vibrational relaxation and dephasing of Rb_2 attached to helium nanodroplets," PCCP **13** (2011) 6816.

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[sti9] S. R. Krishnan, Ch. Peltz, L. Fechner, V. Sharma, M. Kremer, B. Fischer, N. Camus, T. Pfeifer, J. Jha, M. Krishnamurthy, C. D. Schroeter, J. Ullrich, F. Stienkemeier, R. Moshammer, T. Fennel, M. Mudrich, "Dopant induced ignition of helium nanodroplets in intense few-cycle laser pulses," Phys. Rev. Lett. **107** (2011) 173402.

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Group Stock

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[sto2] N. Schaudinnus *et al.*, “Data driven Langevin modeling of biomolecular dynamics,” J. Chem. Phys. **138** (2013) 204106.

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[kis4] N. Bello González, F. Kneer, R. Schlichenmaier, “Shear and vortex motions in a forming sunspot. Twist relaxation in magnetic flux ropes”, Astron. Astrophys. **538** (2012) A62.

[kis5] J.M. Borrero, P. Kobel, “Inferring the magnetic field vector in the quiet Sun. II. Interpreting results from the inversion of Stokes profiles”, Astron. Astrophys. **547** (2012) A89.

1.3.2 Conference Talks

Group Buchleitner

1. A. Buchleitner, Transport, disorder and entanglement, International Symposium on Dynamical Control of Quantum Correlations, Heidelberg, January 2011.
2. A. Buchleitner, Transport, disorder and entanglement, Workshop on New Trends in Quantum Dynamics and Quantum Entanglement, Triest, February 2011.
3. A. Buchleitner, Various Aspects of Open System Entanglement Dynamics, Quantum Open System Frontiers: Entanglement, Decoherence and Control, Peking, April 2011.
4. T. Wellens, Efficient and coherent excitation transfer across disordered molecular networks, International Workshop on Noise in Non-Equilibrium Systems: From Physics to Biology, Dresden, April 2011.
5. A. Buchleitner, Transport, disorder and entanglement, 5th Workshop on Quantum Chaos and Localisation Phenomena, Warschau, May 2011.
6. A. Buchleitner, What's complex in quantum optics, ESF-PESC Strategic Workshop on Signatures of Quantumness in Complex Systems, Nottingham, June 2011.
7. T. Wellens, Coherent transport of waves in nonlinear disordered media, Quantum Technologies Conference II, Krakow, Poland, September 2011.
8. T. Wellens, Coherent transport of waves in nonlinear disordered media, 2nd International Conference on Mathematics Information Science, Sohag, Egypt, September 2011.
9. T. Wellens, Optimal networks for excitonic energy transport, Workshop on Engineering and Control of Quantum Systems, Dresden, October 2011.
10. A. Buchleitner, Modeling photosynthetic exciton transport on random graphs, NITheP Research Workshop: Quantum Biology, Durban, South Africa, November 2011.
11. A. Rodriguez, Multifractal fluctuations and scaling at the three-dimensional Anderson transition, Invited topical talk, 76th Annual Meeting of the DPG and DPG spring meeting of the Condensed Matter Division, Berlin, March 2012.
12. A. Buchleitner, Quantum transport in biological functional units: noise, disorder, structure, COST workshop "Fundamental Problems in Quantum Physics", Malta, April 2012.
13. C. Gneiting, Harnessing entanglement: control and detection perspectives, 3rd International Workshop on Entanglement, Decoherence and Quantum Control, Shanghai, June 2012.
14. A. Buchleitner, (Quantum) complexity in biological tissue - why could coherence matter?, SFB-Meeting, Innsbruck, July 2012.
15. T. Wellens, Optimal networks for excitonic energy transport, Quantum Africa 2, Northern Drakensberg, South Africa, September 2012.
16. A. Buchleitner, Multipath quantum interference – from atoms to biomolecules, International Workshop on "Atomic Physics" Dresden, November 2012.
17. A. Buchleitner, (Quantum) complexity in biological tissue - why could coherence matter?, International Workshop on Quantum Biology, IIT Jodhpur, January 2013.
18. T. Wellens, Multiple Scattering of Interacting Bosons in Random Potentials, Nottingham Workshop on Quantum Non-equilibrium Dynamics, February 2013.
19. A. Buchleitner, Robust design principles for quantum enhanced excitation transport, CLEO/Europe-IQEC, Munich, May 2013.

20. A. Buchleitner, Nonmonotonic quantum-to-classical transition in multiparticle interference, 6th Workshop on Quantum Chaos and Localisation Phenomena, Warschau, May 2013.
21. A. Buchleitner, The noise makes the signal – what a small fry should know about stochastic resonance (. . . and quantum “complexity"), Complex quantum systems and their applications, Ackergill Tower, Scotland, May 2013.
22. A. Buchleitner, Optimal coherent control to counteract dissipation, Ultracold Rydberg Physics, MPIPKS Dresden, July 2013.
23. A. Buchleitner, Energy transport in driven helium: localization vs. interaction, CEMAD workshop, Victoria, Canada, July 2013.
24. C. Gneiting, Optimal coherent control to counteract dissipation, Perspectives in Nonlinear Dynamics 2013, Hyderabad, India, July 2013.
25. A. Rodriguez, Multifractal distributions in disordered media, Complex nanophotonics science camp, Cumberland Lodge, Windsor Great Park, Berkshire, UK, August 2013.
26. T. Wellens, Quantum chaotic design principles for photosynthetic light harvesting, Complex Nonlinear Systems: From Basic Science to Applications, Samarkand, Uzbekistan, October 2013.
27. A. Buchleitner, Complex quantum systems in a nutshell, Multi-path interference beyond Shih-Alley and Hong Ou-Mandel, Quantum Information Processing, Communication and Control 2013, KwaZulu-Natal, South Africa, November 2013.
28. T. Wellens, Quantum transport in disordered media with nonlinearity, 8th Conference on Nonlinear Systems and Dynamics, Indore, India, December 2013.
29. A. Rodriguez, Exploiting multifractal fluctuations to characterize the Anderson transition, Workshop “Waves in complex media", Grenoble, France, December 2013.

Group Gross

1. D. Gross, The Complexity of Learning Quantum States, Workshop on Quantum Tomography, Singapore, December 2011.
2. D. Gross, Quantum walks and cellular automata: a coarse view, Workshop on Operator Structures in Quantum Information Theory, Banff, Canada, February 2012.
3. D. Gross, Matrix completion, with a little help from quantum, International Conference on Compressive Sampling, Tianjing, China, June 2012.
4. D. Gross, A survey of quantum marginals, representation theory, and card shuffling, Workshop on Quantum Information, Seefeld, Austria, June 2012.
5. D. Gross, Quantum Marginals & Entanglement Polytopes, International Congress on Mathematical Physics, Aalborg, Denmark, August 2012.
6. D. Gross, Entanglement Polytopes, Quantum Entanglement Detection, Bilbao, Spain, September 2012.
7. D. Gross, Low-rank matrix recovery, with some aid from quantum mechanics, February Fourier Talks, Maryland, USA, February 2013.
8. D. Gross, The complexity of learning quantum states, Mathematical Aspects of Quantum Modeling Conference, Padua, Italy, June 2013.
9. D. Gross, Quantum Information for Optical Microscopy, Mathematical Challenges in Quantum Information Workshop, Cambridge, UK, September 2013.
10. D. Gross, Marginal Entropies for Causal Inference and Quantum Non-Locality, Quantum Marginal Workshop, Cambridge, UK, October 2013.

11. D. Gross, A Partial Derandomization of Phase Retrieval via PhaseLift, Statistical Issues in Compressive Sensing, Conference, Göttingen, November 2013.

12. R. Chaves, Inferring causal structures from entropic information, Workshop on Quantum Correlations and Contextuality, Natal, Brazil, December 2013.

13. D. Gross, A partial derandomization of Phase Retrieval, Matheon Workshop on Compressed Sensing, Berlin, December 2013.

Group von Issendorff

1. v. Issendorff, B., Structure and thermodynamics of pure and doped water clusters Gordon conference on Molecular and Ionic Clusters, Ventura (USA), January 2012.

2. v. Issendorff, B., Structure and Dynamics of Finite Fermi Systems: simple metal clusters and fullerenes, Hauptvortrag DPG Frühjahrstagung, Stuttgart, March 2012.

3. v. Issendorff, B., Gas phase studies of cluster properties: from ultrafast electron dynamics of fullerenes to magnetism of transition metal particles, Kolloquium IPCMS, Straßburg University (France), March 2012.

4. v. Issendorff, B., Structure and thermodynamics of simple metal and water clusters, Kolloquium IPMC, EPFL Lausanne (Switzerland), May 2012.

5. v. Issendorff, B., Structure and thermodynamics of pure and doped water clusters, Kolloquium physical Chemistry department, Göttingen University, June 2012.

6. v. Issendorff, B., Nanoparticle phase transitions: melting, Symposium on size selected clusters, Davos (Switzerland), March 2013.

7. v. Issendorff, B., Water clusters: thermal behavior and electron solvation, XXV International Symposium on Molecular Beams, Prague (Czech Republic) June 2013.

8. v. Issendorff, B., Thermodynamic properties of water clusters, 6th International Symposium Atomic Cluster Collisions, Wuhan (China), July 2013.

9. v. Issendorff, B., Metal Cluster Studies with XUV radiation, Sino-German Center Symposium on VUV FELs in Molecular, Cluster and Surface Science, Dalian (China), September 2013.

Group Schaetz

1. T. Schaetz, "A poor man's quantum computer? the experimental quantum simulator", NIST-Workshop, Boulder, USA, Feb 2011.

2. T. Schaetz, "New ion (+atom) trap concepts for quantum simulations", Workshop on Quantum Simulations, Benasque, Spain, March 2011.

3. T. Schaetz, "Shuttling Magnesium, Barium and molecular ions in radiofrequency and optical traps from Garching to Freiburg", Quantum-Conference, Madrid, Spain, March 2011.

4. T. Schaetz, "Ions (and atoms) for quantum simulations", CAMEL7, Nessebar, Bulgary, June 2011.

5. T. Schaetz, "Single molecular ion vibrational wave-packet dynamics studied by fs-laser pump-probe dissociation spectroscopy", IOTA-Workshop, Sandbjerg Estate, Denmark, Nov 2011.

6. T. Schaetz, "Towards Arrays of Ions (and Atoms) for Quantum Simulations", Conference in Tel Aviv, Israel, March 2012.

7. T. Schaetz, "Towards Arrays of Ions (and Atoms) for Quantum Simulations", Conference ECTI, Obergurgel, Austria, Sept 2012.

8. T. Schaetz, "Towards Arrays of Ions (and Atoms) for Quantum Simulations", Workshop on Quantum Simulations, Bilbao, Spain, Oct 2012.

9. T. Schaetz, “Trapping of Topological-Structural Defects in Coulomb Crystals”, Qion 2013, Quantum conference, Obergurgl, April 2013.
10. T. Schaetz, “Atoms and Ions commonly trapped by light - towards chemistry at the Nano-Kelvin level”, Conference ITAMP 2013, Boston (Cambridge), USA, Sep 2013.
11. T. Schaetz, “Arrays of Ions (and Atoms) for Quantum Simulaltions”, Conference “Quantum simulations”, Benasque, Spain, Sep 2013.
12. T. Huber, COST-IOTA Workshop on Cold Molecular Ions, Arosa, Switzerland, Sep 2013.
13. T. Schaetz, “Atoms and Ions commonly trapped by light - towards chemistry at the Nano-Kelvin level”, Conference “ Iontech II”, Paris, France, Oct 2013.
14. T. Schaetz, “2D Analogue Quantum Simulations Exploiting Ions (and Atoms) in Optical and RF-Traps”, Workshop IQsim13, Brighton, UK, Dec 2013.

Group Stienkemeier

1. F. Stienkemeier, Photoionization of doped helium nanodroplets, Gordon Research Conference (Molecular & Ionic Clusters), Ventura, CA, USA, 2012.
2. F. Stienkemeier, Formation and Dynamics of Nanoplasmas in Doped Helium Nanodroplets, Gordon Research Conference (Electronic Spectroscopy & Dynamics), Lewiston, ME, USA, 2012.
3. F. Stienkemeier, Helium Nanodroplet Isolation: From Collective Excitations in Organic Aggregates to Ultrashort Time Studies at Millikelvin Temperatures, International Conference on “Correllation Effects in Radiation Fields” (CERF2011), Rostock, 2011.
4. F. Stienkemeier, Improved Rotating Nozzle Setup for Producing Slow and Cold Molecules, International Workshop at Ringberg Castle “Cold and Controlled Molecular Collisions”, Tegernsee, 2011.
5. F. Stienkemeier, Helium droplets and other cryogenic matrices: properties and short time dynamics, 482nd Wilhelm and Else Heraeus Seminar, Bad Honnef, 2011.
6. F. Stienkemeier, Experimental study of the reaction Li + HF at collision energies below 80meV, DMC 2011 (Dynamics of Molecular Collisions Conference), Utah (USA), 2011.
7. M. Mudrich, Photoionization spectroscopy of alkali-doped He nanodroplets, Clustertreffen, Burg Rothenfels, 2011.
8. M. Mudrich, Photoionization spectroscopy of alkali-doped He nanodroplets, IMAMPC 2011 Conference, Rennes, France, 2011.
9. M. Mudrich, Fs spectroscopy of alkali-doped He nanodroplets, 482nd Wilhelm and Else Heraeus Seminar, Bad Honnef, 2011.
10. M. Mudrich, on “Helium Nanodroplets - Confinement for Cold Molecules and Cold Chemistry”, International Symposium on Molecular Beams (ISMB 2011), Bordeaux, France, 2011.
11. M. Mudrich, Evolution of helium nanoplasmas, “Hauptvortrag” at DPG Tagung, Stuttgart, 2012.
12. M. Mudrich, Cold collisions and doped He droplets, VIII International Voevodsky Conference, Novosibirsk, Russia, 2012.
13. M. Mudrich, Photodynamics of doped helium nanodroplets, International Conference on Quantum Fluid Clusters 2013, Regensburg, 2013.
14. M. Mudrich, EUV experiments with helium nanodroplets, International Workshop on ATOMIC PHYSICS, MPI-KS Dresden, 2013.
15. A. LaForge, Collective autoionization in helium nanodropelts, International Conference on Quantum Fluid Clusters (QFC2013), Regensburg, 2013.

16. A. LaForge, Collective autoionization in Helium nanodroplets, Clustertreffen, Herzogenhorn, 2013.
17. J. von Vangerow, Imaging photoionisation dynamics of doped helium nanodroplets, International Conference on Quantum Fluid Clusters 2013, Regensburg, 2013.
18. J. von Vangerow, Photoionisation dynamics of doped Helium Nanodroplets, Clustertreffen, Herzogenhorn, 2013.
19. B. Grüner, Seed location dependent plasma ignition in helium nanodroplets, EAS Konferenz, Riezlern, Austria 2013.

Group Stock

1. G. Stock, *Biomolecular Energy Flow*, CECAM Meeting on Spectroscopy and quantum phenomena in large molecular aggregates, Bremen, June 2011.
2. G. Stock, *MD studies of RNA energy landscapes*, Workshop on RNA Dynamics, Telluride Science Research Center, July 2011.
3. G. Stock, *Modeling of transient IR experiments*, Workshop on Vibrational Dynamics, Telluride Science Research Center, July 2011.
4. G. Stock, *Quantum-classical simulation of the energy flow in biomolecules*, Quantum Molecular Dynamics: A Conference in Honor of William H. Miller, Berkeley, Jan. 2012.
5. G. Stock, *Quantum-classical simulation of the energy flow in biomolecules*, Heraeus Workshop on Frontiers in Biomolecular Simulation, Jan. 2012.
6. G. Stock, *Quantum signatures in biomolecular processes*, Black Forest Focus on Quantum Efficiency, Bonndorf, March 2012.
7. G. Stock, *MD Simulation of Photoinduced Protein Conformational Dynamics*, CECAM workshop on Functional Dynamics of Biomolecules - computational and experimental approaches, Lugano, Nov. 2012.
8. G. Stock, *Modeling of transient IR experiments*, ACS Meeting on Infrared Spectroscopy of gas and condensed phase biomolecule, Anaheim, March 2011.
9. G. Stock, *Spectral Signatures of Energy and Signal Transport in Biomolecules*, Joint Meeting of the British & German Biophysical Society, Hünfeld, March 2013.
10. G. Stock, *Nonadiabatic Vibrational Dynamics*, Vibrational Dynamics Workshop, Telluride Science Research Center, July 2013.
11. G. Stock, *Perspectives of Protein Dynamics Simulations*, Black Forest Focus on Protein Dynamics: From Water Hydration to Crowding Effects, Titisee, Sept. 2013.
12. G. Stock, *Data driven Langevin modeling of biomolecular dynamics*, Molecular Kinetics 2013, Berli, Sept. 2013.
13. G. Stock, *Spectral Signatures of Energy and Signal Flow in Biomolecules*, CECAM workshop on Frontiers of computational biomolecular spectroscopy and mass spectrometry, Forschungzentrum Jülich, Oct. 2013.

KIS

1. Schmidt, W., Science with EST, the ATST, and other ground-based facilities, ESPM-13 Meeting, Rhodos, Greece, Sept 12-16, 2011.
2. Steiner, O., Recent Advances in the Exploration of the Small-Scale Structure of the Quiet Solar Atmosphere: Vortex Flows, the Horizontal Magnetic Field, and the Stokes-V Line-Ratio Method, Hinode 5 Workshop, Cambridge, MA, USA, Oct. 10-15, 2011.

1.4 PhD, Diploma and Master Theses

1.4.1 PhD Theses

Group Buchleitner

1. T. Scholak, “Transport and coherence in disordered networks”, 2011. `http://www.freidok.uni-freiburg.de/volltexte/8283/`
2. M. Tichy, “Entanglement and interference of identical particles”, 2011. `http://www.freidok.uni-freiburg.de/volltexte/8233/`
3. H. Venzl, “Ultracold bosons in tilted optical lattices – impact of spectral statistics on simulability, stability, and dynamics”, 2011. `http://www.freidok.uni-freiburg.de/volltexte/8126/`
4. F. Eckert, ”Speckle instabilities in nonlinear disordered media”, 2013.
5. S. Hunn, “Microscopic theory of decaying many-particle systems”, 2013.
6. T. Geiger, “Inelastic multiple scattering of interacting bosons in weak random potentials”, 2013. `http://www.freidok.uni-freiburg.de/volltexte/9140/`
7. D. Hörndlein, “Entanglement benchmarked transport”, 2013. `http://www.freidok.uni-freiburg.de/volltexte/9129/`
8. S. Sauer, “Entanglement in periodically driven quantum systems”, 2013. `http://www.freidok.uni-freiburg.de/volltexte/8953/`

Group Helm

1. Timo Wilbois, Single Ionization of Molecular Hydrogen in Strong Laser Fields, 2011.
2. Maryam Roghani, Vibrational Cooling of a Trapped Atom: its evolution to EIT, the development of the scattered radiation field and signatures of correlation and entanglement, 2011.
3. Hannes Hultgren, Dynamics and Structure of Negative Ions - Photoinduced double detachment on nano- and femtosecond time scales, 2012.

Group von Issendorff

1. Mattias Svanqvist, On the influence of the temperature on radiationless relaxation and electron detachment in free fullerenes, 2011.
2. Raphael Kuhnen, Electron wace packet interference and directed emission of electrons in a two color laser field, 2012.

Group Schaetz

1. Ch. Schneider, Towards Scaling Experimental Quantum Simulations with Ions, 2012.
2. M. Enderlein, Optical Ion Trapping for (Scalable) Quantum Simulations and Ultracold Chemistry Experiments, 2013.

Group Stienkemeier

1. Matthieu Dvorak, Solvation of Atoms and Molecules and Their Interactions with Rare Gas and Hydrogen Clusters, 2011.

2. Christian Giese, Vibrational Structure and Dynamics of triatomic Alkali Molecules and RbHe Exciplexes on Helium Nanodroplets investigated with Femtosecond and Picosecond Pump-Probe Techniques, 2012.
3. Barbara Grüner, Femtosekundenspektroskopie an dotierten Heliumnanotröpfchen: Dissipative Vibrationsdynamik und Charakterisierung eines Nanoplasmas, 2013.
4. Matthias Strebel, Streuexperimente bei tiefen Temperaturen mit einem langsamen Molekularstrahl an ultrakaltem 7Lithium in einer magneto-optischen Atomfalle, 2013.

Group Stock

1. Maja Kobus, Quantenklassische Modellierung mehrdimensionaler IR-Sepktren von Peptiden, 2011.
2. Roman Shevchuk, Water models and hydrogen bonds, 2013.
3. Stefano Mostarda, Network studies of complex systems: from biomolecules to quantum transport, 2013.
4. Abhinav Jain, Modeling the Structural Dynamics of Peptides and Proteins, 2013.
5. Laura Riccardi, Modeling the free energy landscape of biomolecules: small RNAs and peptide aggregation, 2013.

KIS

1. Franz, M., Spectropolarimetry of sunspot penumbrae, 2011.
2. Nutto, C., Numerical experiments on the propagation of waves in a convectively unstable magneto-atmosphere, 2011.
3. Wenzel, R., Sunspot umbra atmospheres (with ETH Zürich, Switzerland), 2011.
4. Waldmann, T., High-resolution spectroscopy with Fabry-Perot filtergraphs, 2011.
5. Schmidt, D., Characterization of the multi-conjugated adaptive optics system for GREGOR, 2012.
6. Schad, A., Space-time analysis of complex processes (with FDM Freiburg), 2013.

1.4.2 Diploma/Master Theses

Group Buchleitner

1. K. Mayer, “Many-particle quantum walks”, 2011.
2. R. Blattmann, “The pump-probe approach to coherent backscattering of intense laser light by cold atoms with degenerate energy levels”, 2011.
3. F. Schlawin, “Propagation of quantum particles in disordered media”, 2011.
4. S. Roerden, “Partial Rates for k-Photon Processes in 1-d Helium”, 2011.
5. J. Zimmermann, “Anderson localization and non-linear scattering in a disordered 1D quantum system”, 2011.
6. T. Zech, “Hidden symmetries of quantum transport in photosynthesis”, 2012.
7. T. Binninger, “Multiple scattering of intense laser light in a cloud of cold atoms”, 2012.
8. V. Neimanns, “One- and two-photon single and double ionization in 1D frozen planet helium”, 2012.

9. J. Schäfer, "Laser stabilization and mode separation", 2012 (External, Univ. of Hamburg, with A. Hemmerich).
10. A. Cocuzza, "ESR-Untersuchungen an BLUF-Domänen", 2013 (External, Physikal. Chemie, Freiburg, with S. Weber).
11. F. Anger, "Disorder effects on interference: from one to many particles", 2013.
12. A. Ketterer, "The diagrammatic pump-probe approach to coherent backscattering of intense laser light by cold Sr atoms", 2013.

Group Gross

1. Panagiotis Papanastasiou: Computational Complexity of Detecting Genuine Entanglement from Local Spectra, 2013.

Group Helm

1. Florian Meinert, Transient Quantum Dynamics of Coherent Population Trapping Resonances, 2011.
2. Alexander Lambrecht, Zeitaufgelöste Spektroskopie an einer Dunkelresonanz von ^{87}Rb, 2011.
3. Faouzi Saidani, Untersuchung und Kontrolle der Resonatorkopplung in THz-Metamaterialien, 2011.
4. Reininger Katrin, Experimentelle Phasensteuerung eines kohärenten Überlagerungszustandes, 2013.
5. Christoph Testud, Charakterisierung elektrisch leitfähiger Mikrostrukturen im Thz-Frequenzbereich, 2013.
6. Jannis Seyfried, Aufbau eines Interferometers zur Messung der Dispersion bei elektromagnetisch induzierter Transparenz, 2013.
7. Jan Hodapp, Entwicklung und Charakterisierung plasmonischer Linsen für radial polarisierte Strahlung im THz-Frequenzbereich, 2013.
8. Christian Grumber, Großflächige und frequenzselektive Terahertz Photo-Dember-Emitter, 2013.
9. Thomas Meyer, Slow Light under the Condition of Electromagnetically Induced Transparency, 2013.
10. Stephan Welte, Experimental and theoretical studies of Berry Phases in an EIT medium, 2013.

Group Schaetz

1. M. Zugenmaier, "Towards Optical Trapping of a single ^{138}Ba^{+} Ion", 2013.

Group Stienkemeier

1. Sebastian Müller, Deposition und Spektroskopie von PTCDA-Molekülen auf einer ultradünnen Glasfaser, 2011.
2. Christoph Schreyvogel, Aufbau und Charakterisierung einer magnetooptischen Falle für 7Li-Atome, 2011.
3. Lutz Fechner, Aufbau eines Velocity-Map-Imaging-Spektrometers und winkelaufgelöste Spektroskopie an Rubidium-dotierten Helium-Nanotröpfchen, 2011.
4. Amon Sieg, Velocity-Map-Imaging an Rubidiumionen, Rubidium-Helium-Exciplexen und Rubidiumdimeren auf Helium-Nanotröpfchen, 2012.
5. Lukas Schäfer, Emissionsspektroskopie an PTCDA in Heliumnanotröpfchen, 2012.

6. Bernhard Ruff, Nachweis von Lithium aus kalten Kollisionen, 2012.
7. Manuel Rometsch, Edelgas-dotierte Helium-Nanotröpfchen in starken Laserfeldern, 2012.
8. Martin Singer, Dotierung eines gepulsten Heliumtröpfchenstrahls mittels Laserverdampfung, 2013.
9. Michael Richter, IR-Spektroskopie an CO2 mit einem schmalbandigen VECSEL, 2013.
10. Dominik Buchta, EUV Ionisation von reinen und dotierten Helium Nanotröpfchen, 2013.
11. Lukas Bruder, Phase-Modulated Wave Packet Interferometry in the Gas Phase and Implementation of an Interlock System for the LDM End-Station, 2013.
12. Steffen Spieler, Manipulation polarer Grundzustandsmoleküle durch einen Mikrowellenresonator und Erzeugung metastabiler Edelgasatome, 2013.

Group Stock

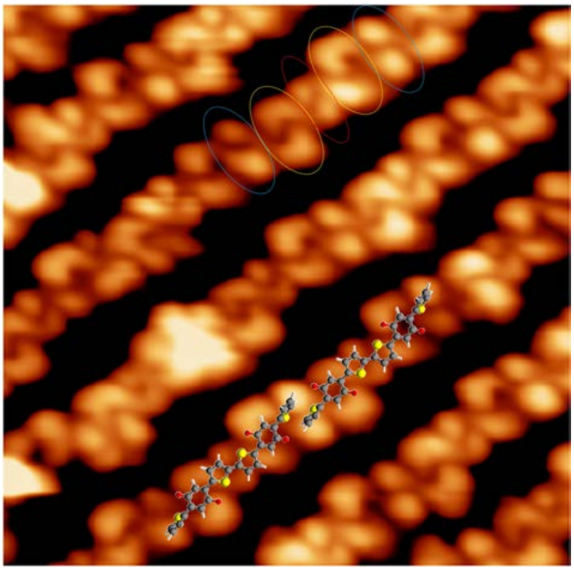
1. Sebastian Waltz, Molecular Dynamics Simulation Study of the Aib Peptide Dynamical Transition, 2011.
2. Paul Brettel, A Study on Vibrational Energy Transfer in Proteins, 2013.
3. Florian Sittel, Statistical Analysis of Protein Dynamics, 2013.

KIS

1. Glogowski, K., Temporal variation of the solar meridional flow, 2011.
2. Herzberg, W., Mass and radius determination of solar-like stars observed by Kepler, 2011.
3. Siegel, D., Excitation of stellar oscillations by gravitational waves, 2011.
4. Thomann, M., Height distribution of refractive index fluctuations in the Earth atmosphere, 2011.
5. Heunoske, D., Time-resolved emission spectroscopy of impact plasmas (with EMI, FhG), 2012.
6. Lange, M., Electrostatic and visual studies of impact plasmas (with EMI, FhG), 2012.
7. Nekuruh, S., Characterization of a high-order deformable mirror for GREGOR, 2012.
8. Ruf, A., Photothermal methods in mid-infrared spectroscopy (with IPM, FhG), 2012.
9. Schwarz, B., The formation of a penumbra observed with SDO/HMI, 2012.
10. Kiefer, R., Seismology of sunspots, 2013.
11. Kiess, Ch., Long-term behavior of sunspot properties, 2013.
12. Böning, V., Interaction of gravity waves with stars, 2013.

Chapter 2

Condensed Matter and Applied Physics



Experimental Physics

- **Prof. G. Reiter**
- **Prof. E. von Hauff**
- **Prof. O. Waldmann**
- **Prof. E. R. Weber (ISE)**

Theoretical Physics

- **Prof. A. Blumen**
- **Prof. H. Grabert**
- **Prof. M. Moseler**
- **Prof. J. Timmer**

- **Prof. A. Aertsen (Biology, co-opted)**
- **Prof. J. Hennig (Medicine, co-opted)**
- **Prof. A. Rohrbach (Engineering, co-opted)**

Chapter caption: Scanning tunneling microscopy (STM) image showing chains of 2TBT and 3TBT oligomeric molecules, which consist of TBT units, a central dialkoxybenzene core (B) having octyl groups attached laterally and connected to two thiophene rings (T).

2.1 Overview

The research area 'Condensed Matter and Applied Physics' comprises six groups located at the Institute of Physics working on Theoretical Polymer Physics (**A. Blumen**, **O. Mülken**), Theoretical Condensed Matter Physics (**H. Grabert**, **H.-P. Breuer**, **D. Bercioux**, **L. Mühlbacher**), Organic Photovoltaic and Electronics (**E. von Hauff**), Functional Nanosystems (**M. Moseler**, **M. Walter**), Experimental Polymer Physics (**G. Reiter**, **W. Stille**), Dynamic Processes in Life Sciences (**J. Timmer**), and Nanophysics and Molecular Magnetism (**O. Waldmann**), one group located at the Fraunhofer Institute of Solar Energy - ISE (**E. R. Weber**), and the three groups of the coopted members of the Physics Institute (**A. Aertsen**: Neurobiology and Biophysics, Faculty of Biology, **J. Hennig**: Faculty of Medicine **A. Rohrbach**: Bio- and Nanophotonics, Department of Microsystems Engineering - IMTEK). Since 2007 H. Grabert serves as director of the Freiburg Institute of Advanced Studies (FRIAS). From 2009 to 2013 J. Timmer was Co-Director of the School of Life Sciences 'LifeNet' of FRIAS, and since 2012 he is Executive Director of the Freiburg Centre for Systems Biology.

Research-wise the Condensed Matter and Applied Physics research area aims at exploring the classical and quantum physical phenomena, functional principles, and technological applications of systems, which are build of a network of interacting nano- or microscale objects as building blocks. The physical properties of the building blocks are typically well understood as well as the short-range interactions between them; the targets of the research interest are hence the emerging complex structures, dynamics, transport and functions.

The systems investigated 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, such as chemical bonding, vibrational, Coulomb and entropic forces, super exchange, charge and spin transport, directional diffusion and biological signal transduction. The systems therefore span all length scales from molecular to biological, and the usual research questions arise, such as the crossover from quantum to classical, and microscopic to macroscopic. Here an obvious connection and scientific overlap with the research undertaken by the groups in the research area 'Atomic, Molecular and Optical Sciences' exists. The focus in the Condensed Matter and Applied Physics research area is however 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, as they can be observed and realised in advanced or biological materials, both of artificial and natural origin. Figure 2.1 aims at sketching this richness in systems and materials investigated in the Condensed Matter and Applied Physics research area.

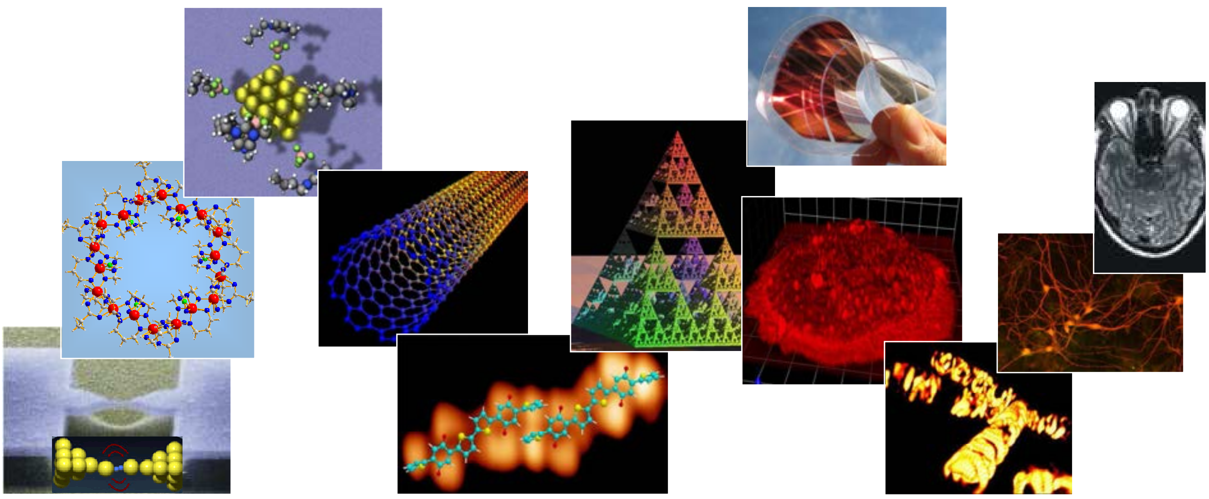


Figure 2.1: Sketch of the variety of condensed and soft matter materials investigated by the research groups in the Condensed Matter and Applied Physics section. They range from nanoscopic systems involving a dozen or so of interacting units to macroscopic ensembles of units and networks.

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 divided into one or the other. The research activities presented in Section 2.2 primarily focus on advanced quantum mechanical phenomena (beyond electronic structure) in low-dimensional systems, such as complex quantum many-body states and excitations, quantum tunneling, environmental effects such as dissipation, decoherence and relaxation in open systems, and the role of topology. The considered materials range from one and two dimensional carbon based materials, nano and micro structured semiconducting and optical materials, 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 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 biological cells, proteins and their interactions, bio-mimetic systems and synthetic cell systems and ensembles of neurons and the brain. They focus on understanding the statistical mechanics relevant to such 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 exemplarily be highlighted here:

The interaction of open systems with a complex, structured environment often induces an involved quantum dynamical behavior featuring strong memory effects. In collaboration with a team in Turku (Finland), the Grabert/Breuer group has developed the first general non-Markovian quantum theory based on the exchange of information between the open system and its environment. The predictions have been fully confirmed by an experiment at the Key Laboratory of Quantum Information in Hefei (China), allowing the control of the transition from the Markovian to the non-Markovian regime. The results were published in *Nature Physics* [gra8].

Despite many unsuccessful attempts by other groups before, the Reiter group was able to grow large single crystals of long conjugated polymers by employing a highly controlled self-seeding approach. Such large single crystals comprised of highly ordered semiconducting chains having the same molecular conformation over many length scales represent valuable model systems for molecular devices. The results were published in *Angewandte Chemie* [rei6].

It has been a fifty-years old mystery that a certain photoreceptor in plants exhibits its maximum absorption at 667 nm, but its maximum action at 715 nm where its absorption is close to zero. By mathematical modeling of the signalling pathway the Timmer group was able to resolve this mystery. They could demonstrate that the surprising behavior is a dynamical non-equilibrium property of the pathway that applies certain pathway motifs. The results were published in *Cell* [tim8].

2.2 Transport and Dynamics in Matter

2.2.1 Theoretical Condensed Matter Physics

The **Theoretical Condensed Matter Physics group of H. Grabert** is studying the dynamics and transport processes of complex many-body systems with particular emphasis on quantum mechanical effects of relevance for novel technological devices on the molecular and nanoscales. Keywords characterising the area of research include quantum dissipation and decoherence, quantum correlations and entanglement, quantum information and computation, electronic correlations, topological phases, and fermionic atoms in optical lattices. Hermann Grabert is released from teaching and administrative duties since he serves as a director of the Freiburg Institute for Advanced Studies (FRIAS). He is substituted by H.-P. Breuer. The main lines of research can be subsumed under the following themes:

Dirac Fermions in two-dimensional nanostructures. The low-energy physics of electrons in graphene, a single layer of carbon atoms on a honeycomb lattice, is described by a Dirac Hamiltonian with the speed of light replaced by the Fermi velocity. It is also possible to design lattices where the low-energy description corresponds to particles with an effective spin larger than 1/2. These systems can be created by means of fermionic cold atoms placed in optical lattices and they lead to novel physical phenomena such as super Klein tunneling [gra1, gra2].

Carbon nanotubes. Carbon nanotubes can be viewed as a stripe of graphene rolled to form a hollow cylinder. Their electronic properties, semiconducting or metallic, are uniquely determined by the width and angle of the cut-out stripe. Nanotubes represent a prototype of one-dimensional conductors or quantum wires, which display remarkable transport properties [gra3].

Topological insulators. The quantum Hall effect is a seminal phenomenon of modern solid state physics because it leads to a quantized conductance whose value is robust against external perturbations. Topological insulators display similar effects even in the absence of an external magnetic field. These materials have a high potential as dissipation-less building blocks of electronic devices with very low power consumption [gra4].

Quantum theory of dissipation and decoherence. The theory of open, dissipative quantum systems plays an important role in many developments of modern quantum mechanics. It provides answers to numerous problems ranging from fundamental questions to predictions for technological applications. Our team studies general properties of open quantum systems and basic features of their dynamical behavior as well as applications to challenging questions of experimental relevance such as the entanglement dynamics of strongly driven trapped atoms in laser cooling and the detection of quantum correlations by local operations [gra5, gra6].

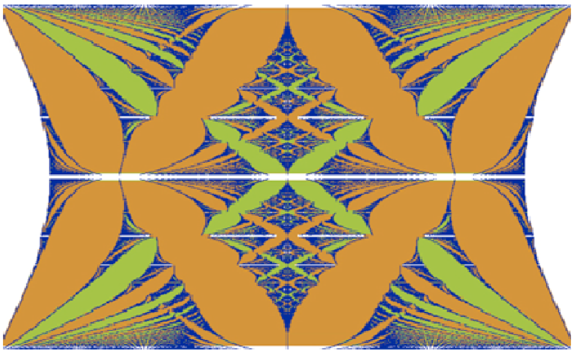


Figure 2.2: Phase diagram for the honeycomb lattice subject to a synthetic gauge field (vertical axis) in dependence on the Fermi energy (horizontal axis). The dark regions represent the energy spectrum. The gaps are colored according to the Z2 index; green: $\nu = 0$, orange: $\nu = 1$. Figure taken from [gra4] featured in Physical Review A, Kaleidoscope.

Quantum memory and dynamics of correlations. The standard approach to the dynamics of dissipative quantum systems presupposes a memoryless time evolution. However, many realistic systems are influenced by strong system-environment correlations and involved quantum memory effects. The recent technological progress allows high-precision experiments which measure the degree of such effects using, e.g., photons moving in polarisation-maintaining optical fibers or in birefringent materials. We have developed theoretical tools and models to analyse these experiments which are important for applications in future quantum technologies [gra7, gra8].

Quantum Monte Carlo simulations. Since analytical tools are frequently limited to simplified models, quantitative studies of experimentally relevant systems often require advanced numerical methods. The Monte Carlo technique provides a powerful yet flexible approach to access the exact quantum dynamics. Based on a stochastic sampling of the underlying configurations, it can be used to calculate equilibrium and transport properties of molecular and nanostructures in the presence of dissipative environments [gra9].

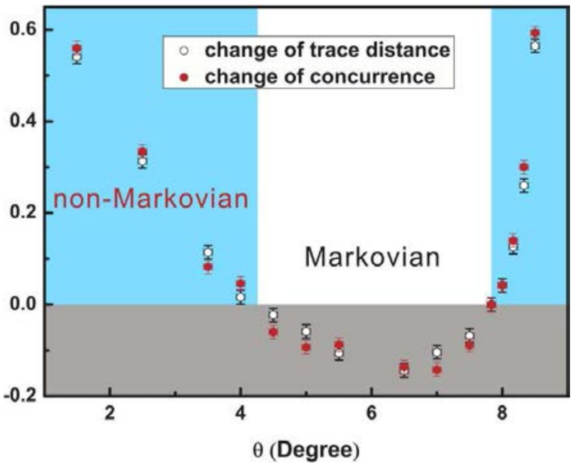


Figure 2.3: Experimental measurement of the transition from Markovian to non-Markovian quantum dynamics. The plot shows the non-Markovianity measure for the polarisation degree of freedom of photons as a function of a control parameter. Figure taken from [gra8].

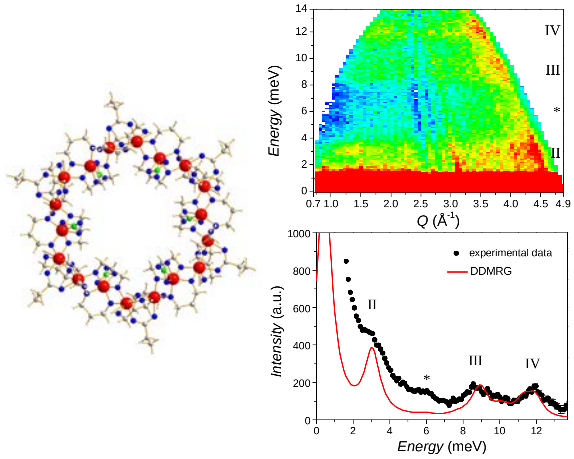


Figure 2.4: Left: Crystal structure of a Fe_{18} molecular wheel. The red balls represent Fe^{III} centers, which carry a spin of $s = 5/2$. The other balls represent C, N, and O atoms; H atoms are omitted. Right: Inelastic neutron scattering data on Fe_{18} and dynamic density matrix renormalisation group (DDMRG) simulation (red line in bottom panel) [wal4].

Energy transfer in light harvesting systems. The highly effective mechanism of resonant energy transfer along networks of bacteriochlorophylls is a major incentive for improving the efficiency of dye and organic solar cells. Burning issues are the influence of the surrounding protein structure and the conditions for optimal energy transfer. Combining the quantum theory of open systems with quantum Monte Carlo simulation techniques, we have aim at a detailed microscopic understanding of the underlying dynamical processes on the femtosecond timescale [gra10].

2.2.2 Nanophysics and Molecular Magnetism

The **Nanophysics and Molecular Magnetism group of O. 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. 2.4. The ligands play a three-fold 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 single-molecule magnets containing highly-anisotropic metal ions such as Co(II) and Lanthanides are investigated. Experimentally the group applies spectroscopic techniques such as inelastic neutron scattering and, since recently frequency-domain Fourier-transform THz (FDFT THz) electron spin resonance, and thermodynamic techniques such as in-house built micro hall magnetometers and ac susceptometers.

Nano-size 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-dimension 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. $s > 1$, and it in fact turns out that these systems are of more interest than the $s = 1/2$ cases. Connections to the physics observed in extended spin lattices exist. For instance, in the molecular wheels, in which the metal ions are arranged on nearly perfect rings as in the Fe_{18} molecule (Fig. 2.4), the low-energy excitations can be described by finite versions of spin-wave theory, and Anderson's tower of states or quasi-degenerate joint states can be experimentally observed. Inelastic neutron scattering experiments in the relevant energy range could be performed in cooperation with Christou's synthetic chemistry group (Gainesville, FL, USA), and in cooperation with Schnack's theory group (Bielefeld), could be fully interpreted [wal4]. This is remarkable considering that the dimension of the Hilbert space of Fe_{18} is a staggering 10^{14}. In the molecular chains, in which the metal ions are arranged linearly (Fig. 2.5), a peculiar even-odd effect was observed. A detailed investigation of the spin excitations in this class of compounds for varying chain lengths and spin lengths using exact diagonalization, classical simulations, and, in cooperation with Eggert's theory group (Kaiserslautern), quantum field theory techniques [wal1]. As the most far-reaching result it could be demonstrated that the finite spin lattices are fundamentally distinct from the extended lattices, and that in fact a crossover boundary exists which separates the two (Fig. 2.5). It was also found that current field theoretic methods do not extend to the finite lattices.

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, and the systems in fact usually exhibit two or even more relaxation regimes and their origin remained speculative and highly controversial. The Waldmann group has recently, in cooperation with Powell's synthetic chemistry and Chibotaru's quantum chemistry groups, made important progress. They could show by experimental means that the two relaxation regimes observed in a Co_2Dy_2 single-molecule magnet can be unambiguously assigned to an exchange-based relaxation mechanism at low temperatures and a Dy-single-ion base relaxation mechanism at intermediate temperatures, see Fig. 2.5 [wal6].

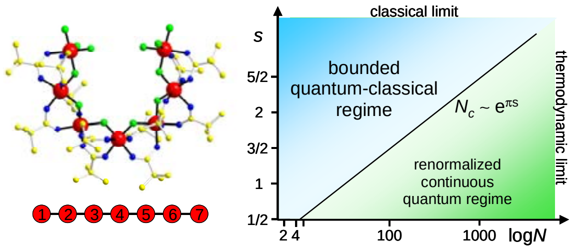


Figure 2.5: Left: Crystal structure of a Cr_7 molecular chain. The red balls represent Cr^{III} centers, which carry a spin of $s = 3/2$. The other balls represent C, N, and O atoms; H atoms are omitted. The sketch below shows the exchange coupling paths. Right: Properties of the antiferromagntic Heisenberg chain in the parameter space spanned by spin magnitude s and chain length N in an s-$logN$ plot, showing the different regimes [wal1].

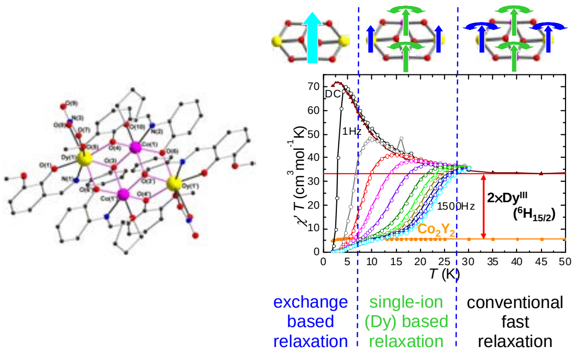


Figure 2.6: Left: Crystal structure of a Co_2Dy_2 single molecule magnet. The yellow and pink balls represent Co^{II} and Dy^{III} centers, respectively. The other balls represent C, N, O, and H atoms. Right: DC and in-phase AC susceptibility demonstrating different magnetic relaxations mechanisms [wal6].

2.2.3 Theoretical Polymer Physics

The research in the **Theoretical Polymer Physics group of A. Blumen** has two main directions. On the classical side it focuses on understanding the dynamic properties of artificial and biological macromolecules, while on the quantum mechanical side it studies the topological influence on quantum trans-

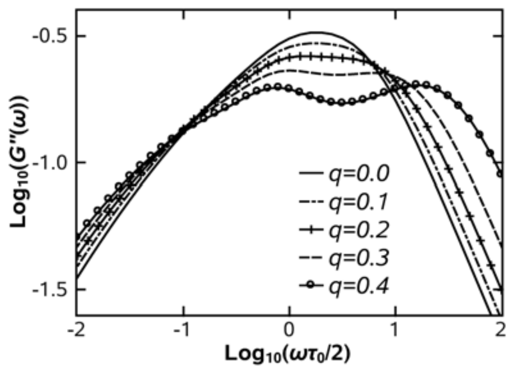


Figure 2.7: Influence of the stiffness represented through the parameter q on the mechanical relaxation loss moduli for dendrimers of eighth generation.

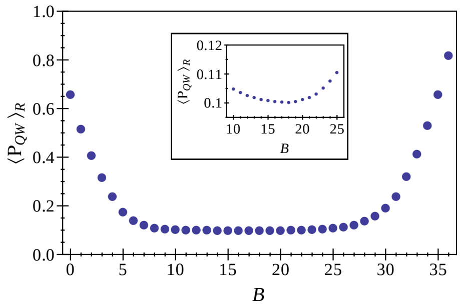


Figure 2.8: Transition form star graph to complete graph.

port properties. In both cases the systems of interest are modeled by networks of interacting nodes.

Polymer Dynamics. One research direction of the group is the relation between (complex) polymer architectures and their static and dynamic properties. Thus in the last three years especially semiflexible macromolecules were studied [blu1, blu2, blu3, blu4, blu5]. The group put forward a new analytic model for semiflexible polymers with arbitrary, treelike architectures, see [blu1]. Based on this model, a large set of branched macromolecular structures, in particular dendrimers [blu2] and regular hyperbranched polymers were treated [blu3]. The group succeeded in studying analytically the eigenmodes of semiflexible hyperbranched macromolecules belonging to different universality classes [blu2, blu3], as well as to assert the fundamental role of stiffness on the dynamics of (hyper)branched structures [blu1, blu2, blu3], see e.g. Fig. 2.7 for dendrimers.

While the model [blu1] allows to treat treelike macromolecules under arbitrary branching and stiffness conditions, treelike structures are devoid of loops. In order to study systems with loops first the maximum entropy principle to semiflexible ring polymers was applied [blu4]; it was found that closing the chain to a ring considerably changes the behavior under semiflexible conditions. Recently the model was extended [blu1] by including dihedral interactions [blu5], a fact which leads to new dynamical properties, especially to a change in the scaling behavior of the mechanical relaxation moduli [blu5].

Now, semiflexibility corresponds to *internal* constraints on the orientations of the macromolecular building blocks. Confined environments, such as nanotubes or porous media, lead to *external* constraints, which were also studied.

Quantum Transport on Networks. In the last three years the group has extended its research of quantum mechanical transport properties of complex networks. The methods of choice are Continuous-Time Quantum Walks (CTQW). The work has focused on the implications of complex network topologies on dynamical properties, and has been summarised in a review article in Physics Reports [blu6]. While the classical counterparts, the Continuous-Time Random Walks (CTRW) are fairly well understood, the knowledge of CTQW is rather limited and a clear classification scheme, depending, e.g., on the fractal or spectral dimension of the network is still lacking.

The group studied CTQW in different settings, such as ordered systems, which become topologically disordered by either adding or removing bonds. The transport efficiency is quantified by the probability to return or remain at the original node. This measure is meaningful both for CTRW and for CTQW and allows to compare the two models [blu6]. The transition from a star graph (SG) to the complete graph (CG) was thus considered [blu7]. Now, CTQW both over the SG and the CG are very inefficient, due to eigenstates strongly localised over small subsets of nodes. By randomly inserting additional bonds into the SG, the CTQW transport efficiency is enhanced, see Fig. 2.8, an effect which may seem counter-intuitive given that random networks also show localisation [blu7]. In a second example the group studied regular two-dimensional networks (lattices) with randomly placed bonds and with different aspect ratios [blu8]. It was found that square networks have the highest CTQW performance, while landscape as well as portrait configurations lead to less efficient transport, see Fig. 2.9, a fact which differs from classical CTRW findings.

In a related study the effect of the environment on the transport through networks was investigated. Here, the dynamics follows a quantum master equa-

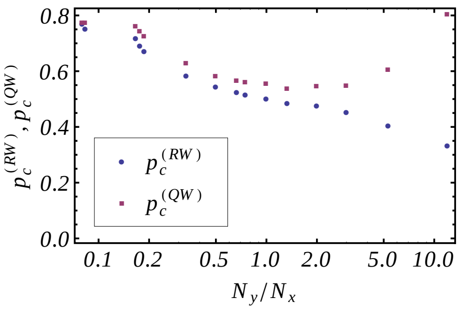


Figure 2.9: Transport efficiency for networks of different aspect ratios.

tion of Lindblad type, leading to a quantum stochastic walk (QSW) citeSCHIJ:2012a. Now, the QSW allows for a parametric transition from CTQW to CTRW. It was found that already a very small coupling to the environment is sufficient to overcome the (quantum) localisation effect in a system consisting of seven nodes [blu9].

Motivated by works on coupled quantum dots the group also considered a system in a source-network-drain setting, consisting of three coupled two-level systems arranged on a chain where the end nodes are coupled to the source and the central node is coupled to a drain/trap. Such a system has a dark state which can block the transport. Now, depending on whether the two initially excited nodes are correlated, the transport may be enhanced by avoiding the dark state [blu10].

2.3 Functional Materials

2.3.1 Experimental Polymer Physics

Research of the **Experimental Polymer Physics group of G. 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, which to some extent are inspired by processes found in nature.

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 organisation and structure formation. Polymer physics represents a fundamental pillar in terms of fundamental and conceptual issues in an interdisciplinary approach of innovative materials research.

The Reiter group follows a 'bottom-up' approach: molecular interactions and their control on a sub-nanometer scale determine the hierarchical organisation 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:

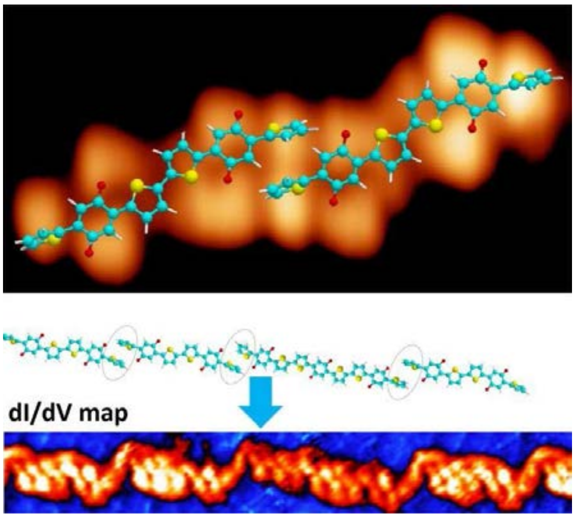


Figure 2.10: An example of a supra-molecular pathways with a continuous density of states established by physically linked molecules.

Molecular interactions and structure formation: Self-assembly of supra-molecular systems on graphene. In cooperation with research groups from Mulhouse, Montpellier and Pau (France) we demonstrated that conjugated 2,5-dialkoxy-phenylene-thienylene-based oligomers can self-assemble on epitaxial monolayer graphene to form long supra-molecular pathways exhibiting a continuity in the electronic density of states across individual molecules physically linked by π-π-interactions of their end-groups. The use of graphene as substrate provided high sub-molecular resolution of electronic orbitals, which were identified with the help of density functional theory calculations. The combination of intra- and inter-molecular non-covalent interactions, together with a weak adsorption on the substrate, provided sufficient stability of the molecular arrangement and so improved the conjugation of electrons along and even across molecules within a chain (see Fig. 2.10).

This work represents one facet of our activities of linking molecular features with optoelectronic properties. Relevant publications: [rei1, rei2, rei3, rei4].

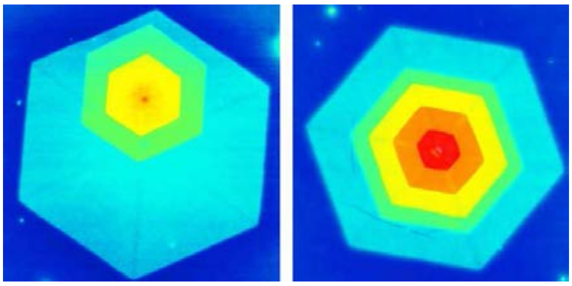


Figure 2.11: Two examples of typical atomic force microscopy topography images of stacks of lamellar polymer crystals, all in registry with the underlying crystal, as demonstrated by the hexagonal symmetry and the unique orientation of all hexagons.

Phase transitions in complex systems: Polymer lamellar crystal growth in three dimensions. Systematical investigations polymer single crystals grown in ultrathin films led to a general concept of a nucleation induced insertion mechanism, allowing to generate secondary lamellar crystals on amorphous fold surfaces, which are in registry with an underlying single crystal. Thus, the order of the crystal unit cell can be propagated not only in the lateral but also in the vertical direction of the lamellar crystal. The dependence of the number density of secondary lamellae on the width of the side branches of the underlying crystal suggests that nucleation of secondary lamellae was controlled by the morphology of the underlying crystal which, in turn, could be tuned by crystallisation temperature and film thickness (see Fig. 2.11).

This work is based on general concepts of polymer crystallisation derived from collaborations with groups in Dresden (Germany), Strasbourg (France), Beijing, Nanjing and Shanghai (China). Relevant publications: [rei5, rei6, rei7, rei8].

Polymers at interfaces and in thin films: Segmental relaxations have macroscopic consequences in glassy polymer films. Together with researchers from the Institut Charles Sadron, Strasbourg (France), the University of Cambridge (UK), and the National Tsing Hua University, Hsinchu (Taiwan) we investigated the consequences of physical aging in thin spin-coated glassy polystyrene films through detailed dewetting studies. A simultaneous and equally fast exponential decay of dewetting velocity, width and height of the rim with aging time was

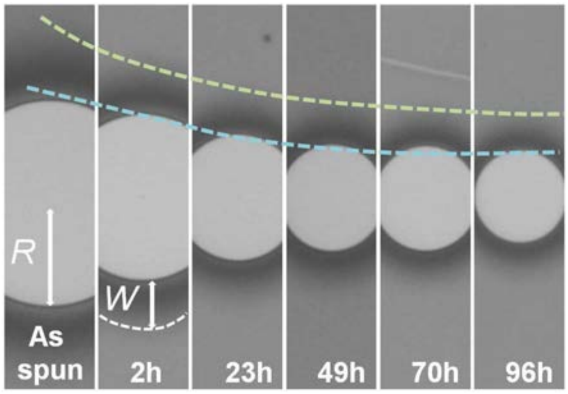


Figure 2.12: Typical examples for dewetting holes in unstable polymer films aged for varying periods of time.

observed, which is related to a reduction of residual stresses within such films. The temperature dependence of these decay times followed an Arrhenius-behaviour, yielding an activation energy on the same order of magnitude as values for the β-relaxation of polystyrene and for relaxations of surface topographical features. Our results suggest that rearrangements at the level of chain segments are sufficient to partially relax frozen-in out-of-equilibrium local chain conformations, i.e., the cause of residual stresses, and they might also be responsible for macroscopic relaxations at polymer surfaces (see Fig. 2.12).

This work is an example of our longstanding activities on properties of thin polymer films. Relevant publications: [rei9, rei10]

2.3.2 Functional Nanosystems

The recent modeling and simulation activities of **Functional Nanosystem group of M. Moseler** aim at a mechanism-oriented understanding of the functions of complex nanoscale material systems, such as free, supported [mos6, mos7] or protected [mos5, mos10] clusters and nanoparticles, nanotubes, nanowires,[mos2] graphene,[mos4] nanoscale compounds, polymers, coatings [mos3] and nanotribological contacts [mos8, mos1, mos3]. The group uses and develops a whole spectrum of methods to explain and predict structures and processes in nanoscale materials. Massive parallel density functional theory calculations are performed to study the electronic structure and nuclear equilibrium structures of nanomaterials [mos7]. Large scale quantum and classical [mos9] molecular dynamics simulations give insights into the complex atomistic dynamics in nanoscopic systems. Processes on longer time and length scales are studied with coarse

Figure 2.13: Artistic view of the mechano-chemistry during diamond polishing.

grained dynamics such as discrete element methods and smooth particle hydrodynamics.

The following examples highlight the most important results from the last three years:

Mechanochemistry and triboinduced phase transformations in carbon hard coatings. Nano- and micron-sized sp^3 carbon films made of diamond or diamond-like carbon (DLC) are extremely important for friction reduction and wear protection in many industrial applications (for instance for CO_2 reduction in the automotive industry). Downsizing in engines results in increasing loads and therefore even these hard coatings show wear. This wear has been studied by classical molecular dynamics simulations using a bond-order potential [mos9]. For diamond [mos8] the formation of a soft, mainly sp_2 hybridized amorphous carbon (a-C) nanolayer is observed that is not stable with respect to mechanical plowing or oxidative etching by ambient air [mos6]. The phase transformation is governed by the mechanical extraction of carbon atoms from the diamond surface. Thus mechanochemistry plays a crucial role in the wear of diamond. The velocity of the diamond/a-C interface depends on the diamond surface orientation with the highest speed found for (110) surfaces that are rubbed in the (001) direction, while the lowest interface speed was observed for the diamond

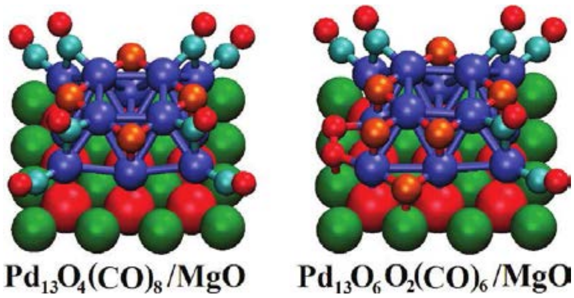


Figure 2.14: CO adsorption on Palladium-oxide nanoclusters supported by MgO.

(111) surface. These finding are in perfect agreement with a 600 years old experimental knowledge of diamond polishers who experience this anisotropy in the wear rate for different gem stone orientations (see Fig. 2.13 for the cover related to the article [mos8]). Also hydrogen-free DLC films show such a mechanochemical phase transition to an a-C [mos3].

Magnesia-Supported Palladium Oxide Nanocatalysts. Although many industrial catalytic processes take place on metal nanoparticles that are oxidized during the reaction, a detailed knowledge of the influence of the oxidation state on their catalytic activity is still lacking. Therefore, we used density functional theory in order to explore the dependence of the reaction temperature of catalysed carbon monoxide oxidation on the oxidation state of $Pd_1 3$ clusters deposited on MgO surfaces [mos7]. It is shown that molecular oxygen dissociates easily on the supported Pd_{13} cluster, leading to facile partial oxidation to form $Pd_1 3O_4$ and $Pd_1 3O_6$ clusters (see Fig. 2.14). The calculations reveal that the reaction barriers on the two oxides are markedly different in agreement with temperature programmed reaction experiments. Such nanooxides play a crucial role in the catalysed combustion of CO to CO_2 in car catalytic converters.

Interactions of polymers with reduced graphene oxide. Graphene can be used to strengthen polymers. Stability of the resulting nanocomposits is only achieved if the graphene sheets bind sufficiently to functional groups of the polymer (e.g. to aryl functions). In order to explore the stability of polymer graphene nanocomposites, we studied the interaction of benzene molecules with various defects in graphene [mos4]. We find that the binding strength of benzene to the various defects is governed by steric hindrance. Our first principles calculations in combination with a simple model predict decreased stabilities of polymer graphene nanocomposites made of reduced graphene oxides depending on the defect density.

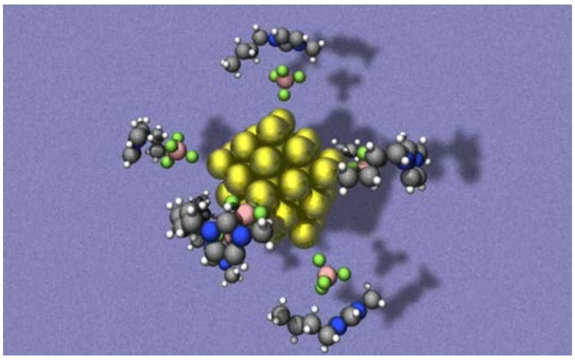


Figure 2.15: Model of the gold cluster surrounded by an ionic liquid.

A 58-electron superatom-complex model for the famous Schmid-gold cluster. Ligand protected gold clusters are of high interest due to their extraordinary stability even under harsh conditions. The electronic reason for stability is explained by the Superatom-Complex (SAC) model applicable irrespective on the ligand type. We have re-investigated the famous gold-phosphine-halide Au:PR_3:Cl compound of 1.4 nm dimension (Schmid gold), where the SAC model guided us to the $[Au_{69}(PR_3)_{20}Cl_{12}]$ anion that is energetically and chemically far superior to the standard $Au_{55}(PR_3)_{12}Cl_6$ model in the literature [mos10].

Gold clusters in ionic liquids show quantised charging. Gold clusters can not only be stabilised by ligand monolayers, but also in ionic liquids. The latter are molten salts at room temperature with fascinating properties. Their high conductivity and vanishing vapor pressure enables them to be used as powerful solvents. In a joint collaboration with the experiment [mos5] we investigated the unexpected quantized charging of IL stabilised gold clusters. We were able to explain the observed unusual capacitance behavior by the charge dependent re-arrangement of the IL-pairs in the first shell around the cluster (see Fig. 2.15 for the model used).

2.3.3 Organic Photovoltaic and Electronics

Research in the group **Organic Photovoltaic and Electronics** led by **E. von Hauff** focusses on the understanding of fundamental processes in organic and nanostructured semiconductors and heterostructures for applications in electronics. A bottom-up approach is used to correlate the electrical, optical and structural properties with device performance in solar cells, transistors, diodes and sensors.

Organic photovoltaics. Organic solar cells are based on donor-acceptor systems for the absorption of light, separation of charge and transport of photocurrent. The most commonly investigated kind of organic solar cell is the polymer:fullerene bulk heterojunction (BHJ). The active layer consists of a soluble conductive polymer derivative blended with a soluble fullerene derivative. The extended donor-acceptor interface in the two component active layer facilitates efficient electron transfer between the polymer and fullerene. Controlling the complex morphology of the donor-acceptor system is crucial for producing reliable and efficient photovoltaics. We systematically studied mechanisms which influence electron transfer, the primary step in photovoltaic energy conversion. Using optical spectroscopy to monitor recombination processes, we were able to elucidate the intricate relationship between molecular structure and morphology of the organic active layer and carrier recombination at the donor-acceptor interface [vH1]. To reduce recombination losses over this channel we investigated novel strategies such as molecular doping to fill trap states in amorphous low bandgap polymers, and thereby increase carrier mobility. We demonstrated that this results in increased photocurrents and efficiencies in doped BHJ devices [vH3, vH4]. In addition to efficiency, the stability of organic solar cells has becoming an increasingly important topic in the community. We use transient and steady state optical and electrical tools to investigate changes in the nature of photoexcited states of the active layer after exposure to oxygen under UV illumination, as well as changes to material interfaces. We were able to correlate a loss in photogenerated excitons in the active layer with a loss in the photocurrent in the solar cell. With impedance spectroscopy we reconstructed the electronic density of states in the solar cell and demonstrated the emergence of trap states induced by ageing [vH2]. We extended this work by developing an equivalent circuit model for the BHJ solar cell [vH7] in which the circuit elements could be correlated to specific materials and interfaces in the device. The model serves as a diagnostic tool to identify and locate changes in the electrical properties of the solar cell due to ageing. We applied this model to correlate the charge extraction efficiency in the solar cell with device stability [vH9]. Additionally we have investigated novel solar cell architectures, including inverted structures with stable ZnO window electrodes [vH6].

Organic-inorganic hybrid structures for solar energy conversion. Although power conversion efficiencies of purely organic photovoltaics has increased rapidly in the last years, solar cell performance is inherently limited by the high energetic dis-

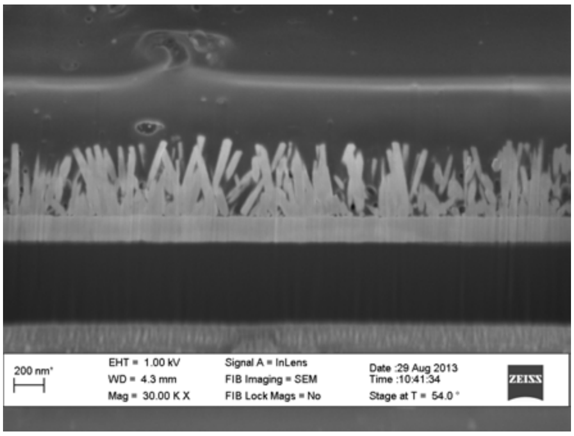


Figure 2.16: Scanning electron microscopy (SEM) cross section image of ZnO nanorod array/PPV interface. Image M. Scherer, InnovationLab GmbH.

order and poor electrical properties of the organic active layer. Combining organic semiconductors with inorganic nanostructures offers the possibility to go beyond these limitations by maximising both the optical and electrical response of the solar cell active layer. Wide band gap semiconductors such as zinc oxide and titanium dioxide are particularly interesting for solar energy applications due to their electronic and optical properties. Additionally, these materials can be synthesised to form a wide variety of structures including thin films and nanostructures. We explore using vertically aligned ZnO nanorods which are coated with an organic absorber. Light absorption results in photoinduced electron transfer from the organic semiconductor to the inorganic nanostructure. The large surface area of the extended hybrid interface facilitates charge separation, and the well-ordered nanostructure array promotes efficient electron collection from the solar cell. Figure 2.16 shows a cross section of a ZnO nanorod array coated with the polymer poly(p-phenylene vinylene) (PPV), which was processed from choloroform, spin coated onto the substrate and subsequently annealed. The electron microscopy images were taken in cooperation with the Innovation Lab in Heidelberg.

Plasmonic structures for solar energy conversion The light absorption in hybrid active layer is limited by the absorption capabilities of ZnO and the the thin organic film. To increase the light harvesting properties we developed plasmonic nanohybrid structures. ZnO nanopyramids were colloidally synthesised and functionalised with gold particles. By photoexciting the ZnO structures with UV illumination, gold particles form via a photocatalytic process at the tips of the pyramids. The result is Au capped ZnO nanopyramids, shown in Fig. 2.17. The controlled implementa-

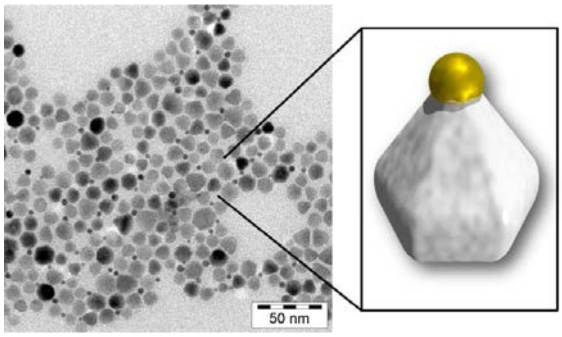


Figure 2.17: Transmission electron microscopy (TEM) image of Au-functionalised ZnO nanopyramids. The inset shows a schematic of the structure.

tion of plasmonic particles on semiconducting structures has potential for photovoltaic and solar water splitting applications, these structures are interesting for use in solar water splitting.

2.3.4 Solar Energy

The **Solar Energy group of E. R. Weber** works on silicon and on organic solar cells. The research is focused on the identification of the factors limiting the power conversion efficiency in these devices. The aim is to develop better and cheaper solar cells by creating new cell and module concepts. The basis for this work is a thorough understanding of the underlying processes. This is achieved by extensive characterization in combination with numerical simulations.

In ***Silicon Material Characterization and Process Modelling*** the Weber group had as one of its major activities the coordination of as well as scientific contributions to the research cluster SolarWinS. The project investigates incorporation of impurity elements from the crucible and the crucible coating into the silicon during crystallization of multicrystalline silicon ingots. The group developed, in close co-operation with Fraunhofer ISE, a detailed understanding of the incorporation and re-distribution of the main impurity iron during the crystallization process and the successive solar cell processing steps. A complete numerical model with the simulation tool Sentaurus Process was developed accounting for the detailed temperature history, and requiring no other input than impurity concentrations in crucible and coating as measured at partner institutes in the consortium [web3]. The prominent impurities found experimentally and treated in the simulations were Fe, Co and Cr. Major progress was concerned with the incorporation of the crystalline inhomogeneity of multicrystalline silicon, and the incorporation of a realistic description of the kinetics of precipitation of metals

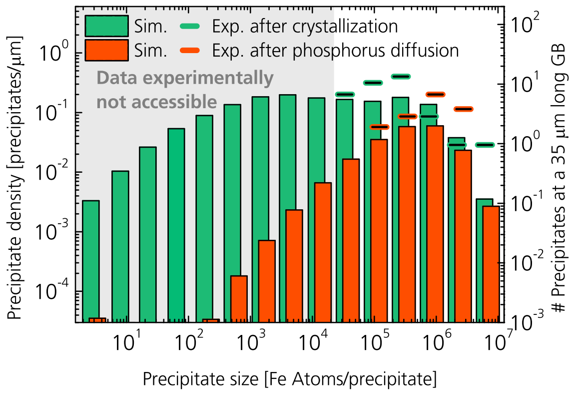


Figure 2.18: Comparison of the simulated and measured line densities of different iron-silicide precipitate sizes before and after emitter diffusion. During emitter diffusion mainly small and medium precipitates are gettered.

using a Fokker-Planck equation. The distribution of the impurity atoms in the interstitial state and a size distribution of precipitates are obtained as illustrated in Fig. 2.18.

As a further step, a new model of the recombination activity of precipitates of different cluster sizes was established. With these models, the quantitative information on interstitial iron distribution over the full block height experimentally obtained from photoluminescence images as well as the combined recombination activities of interstitial and precipitated species could be described very well. Among other topics also upgraded metallurgical silicon was investigated. The scientifically most interesting contribution concerns the development of an improved empirical model for the charge carrier mobilities in silicon. It has been noticed already before that in compensated silicon the commonly accepted models predict higher mobilities than measured. These deviations were attributed to increased scattering by the additional ionized impurities in compensated silicon: screening of ionized scattering centers by the mobile carriers as included in the previous modeling was overestimated. An improved parametrization model for the doping concentration dependence allows an excellent description of all available data and is presently already used as the state-of-the-art mobility model.

The research on ***Organic Solar Cells*** covers many different physical and technological aspects. It spans from deepening our understanding of the fundamental working principles of organic solar cells to the development of cell and module concepts relevant for production. We test and characterize new organic semiconductors and analyse their efficiency potential on the basis of characterization data and optical and electrical modeling. Electrical modeling also enables the application specific dimensioning and optimization of different module structures. Novel cell and module concepts with high potential for cost reduction are developed in the lab and realized in a roll-to-roll process.

The widely used Indium Tin Oxide (ITO) is expected to be one the major cost driving factors for organic solar cells and so one of the group's focus points is to develop ITO-free cell architectures. The setup based on an Al/Cr electron contact in combination with a PEDOT:PSS/metal grid hole contact is comparably well suited for the standard photoactive layers prepared from P3HT:PCBM. It showed promising long term stability [web1] and was used to realize modules comprising 11 cells connected in series on a flexible substrate. These modules reached very good fill factors of up to 65% [web9]. Although the deposition of a metal grid on top of the hole conductor PEDOT:PSS was achieved with Aerosol and screen printing it is always critical for the underlying photoactive material if an inorganic material in solution is deposited on top of it and subsequently annealed. From the point of view of an easy and cost-effective deposition it is much more beneficial to use techniques such as sputtering which however can usually not be performed on top of organic layers without damaging the latter. Recently the group could show that it is possible to use two separately deposited electrodes on two different substrates process organic layers and to merge the two subcells at an organic/organic interface by simple roller lamination [web2]. The three

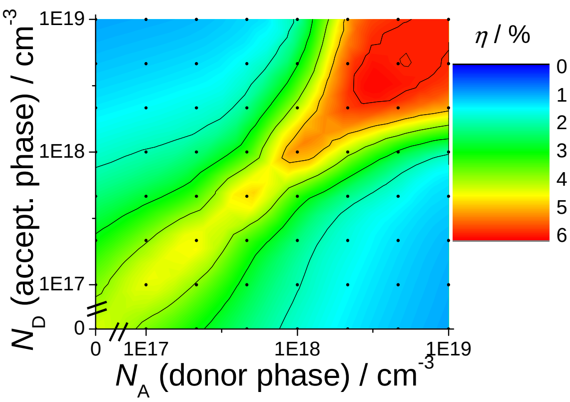


Figure 2.19: Efficiency of a bulk-heterojunction organic solar cell as a function of doping concentrations in the donor and acceptor phase.

most striking differences between organic and typical crystalline inorganic solar cells are the roughly six orders of magnitude lower charge carrier mobilities in the photoactive organic layers, the low dielectric permittivity of the organic materials and their comparatively high absorptivity. The last property is necessary to compensate for the poor charge carrier transport which allows only for very thin photoactive layers in the range of 50-300 nm. As a consequence of the low dielectric permittivity the initial photoexcitation does usually not lead to the creation of (quasi-)free charge carriers but rather to strongly bound excitons. To overcome their binding energy and to create free charge carriers, the photoactive layer of organic solar cells consists of two components, a donor and an acceptor phase between which a very fast electron transfer is observed. Inorganic solar cells use doping to increase the conductivity of one type of charge carrier. To understand the consequences of doping in the case of organic solar cells we carried out simulations based on a 2-dimensional donor/acceptor model. This allowed for simultaneous and individual doping of the different phases. Interestingly, doping only either the donor (p-type) or the acceptor (n-type) phase leads to a decrease in the current density of the device. However, a simultaneous doping of both phases can significantly improve the transport properties and thus increase the fill factor as can be seen in Fig. 2.19 [web7].

2.4 Biological Systems

2.4.1 Dynamic Processes in Life Sciences

The Dynamical Processes in the **Life Sciences group of J. Timmer** aims at transferring the quantitative and predictive approach of physics to the life sciences. During the reporting period, until October 2013, Timmer's teaching duties were taken over by Th. Filk as Timmer served as Co-Director of the School of Life Sciences 'LifeNet' of the Freiburg Institute for Advanced Studies (FRIAS). FRIAS was funded 2008 in the frame of the German Excellence University Initiative as the central measure of the 'Vision for the future' concept of the University of Freiburg.

Modelling in cell biology. The largest part of the group works on systems biology of cellular signal transduction, i.e. the information processing of external stimuli by cells finally leading to altered gene expression. A lot is known about the involved proteins 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 contains unknown parameters. We de-

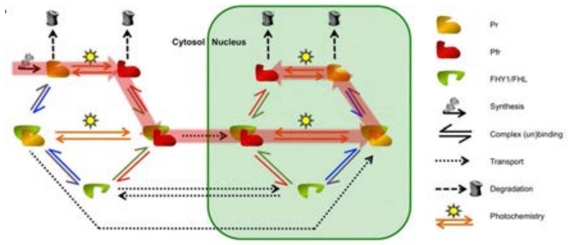


Figure 2.20: Scheme of the phythocrome A photoreceptor signalling pathway. The path enabling the counter-intuitive behavior of the pathway is highlighted.

veloped methods to estimate these parameters from time-resolved measurements of the involved proteins [tim2]. Special attention was payed to correctly propagate the uncertainty of the experimental data to the uncertainty of the estimated parameters and in turn - to the uncertainty of the predictions [tim4]. Thus, we deal with modeling and parameter estimation in nonlinear, partially observed, stiff, sparse, noisy dynamical systems. Application during the reporting period range from plant biology [tim8] via cancer research [tim10], erythrogenesis and immunology to synthetic biology [tim3].

Time series analysis in neurology. The second line of research is about time series analysis in neurology. Here, it is the central topic to decipher neural networks based on time-resolved measurements of brain activity. Since explicit models are not adequate for the brain, we work with semi-parametric models, i.e. over-parameterized linear stochastic models. Based on the fitted models, we infer the network topology and interactions strengths by applying ideas from Granger-causality. We have shown that the approach is able to obtain correct results also for typical cases of non-linear, even chaotic, systems [tim5]. We generalized the modeling approaches for the non-stationary and the noisy case. During the reporting period, the main applications were in the fields of epilepsy,[tim7] tremor [tim9] and stroke research [tim6].

In both lines of research, the strategy of the group consists in four steps. First, we aim to establish longterm collaborations with biological or clinical groups. We then typically first apply methods that are already known. Third, we try to extract new, generic, methodical challenges from the specific projects, solve them with the goal to publish these achievements in the high-ranked theoretical journals. Finally, we apply them within the projects with the aim to publish the results in the high-ranked biological or clinical journals and iterate this strategy. During the reporting period, we published one paper in Science and one in Cell. Due to this research strategy, a Ph.D. thesis typically consists of two parts, a first theoretical and second application part.

Helioseismology. Apart from these main topics of the group, we have a long-term tradition to be involved in extraterrestrial projects. During the reporting period, in cooperation with the Kiepenheuer Institute for Solar Physics, we developed methods to reconstruct flows within the sun from observed oscillations at the surface. By these methods, we were able to reconstruct the meridionial flow roughly for the whole convection zone of the sun improving established methods by a factor of 15 of accessible depth [tim1].

2.4.2 Bio- and Nano-Photonics

The **Bio- and Nano-Photonics group of A. Rohrbach** (Department of Microsystems Engineering - IMTEK) 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 modeling 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 coupling between two particles, can reach interaction lengths of even several particle diameters [roh10] and often control time-variant effects such as reactions kinetics or synchronization in biological processes. In the last couple of years we used line scanning optical tweezers to trap two or more diffusing particles in a confined optical potential [roh5] to increase their collision rate(see Fig. 2.21). Using coherent light scattering of the trapping laser [roh6] we were able to track several particles in 3D with nanometer precision at 10 kHz. These results confirmed the hypothesis that inside living cells a dynamic change of the size of

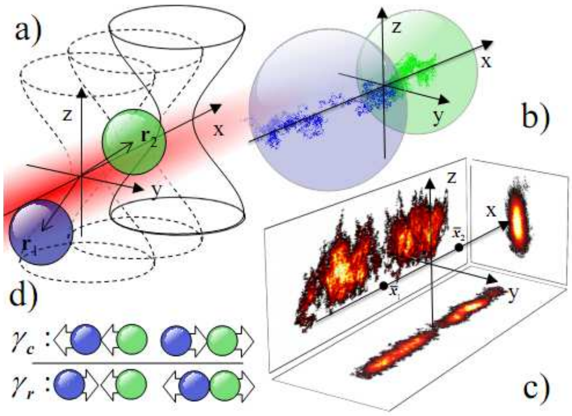


Figure 2.21: A scanned laser trap generates an elongated optical potential. b) Recovered trajectories. c) 3D position histograms of 2 diffusing beads in a single potential. d) Particle diffusion by collective (drag γ_c) and relative motion (drag γ_r).

membrane compartments controls the collision rate between particles and thereby reaction efficiencies.

Bio-mimetic systems. The second class subserves 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 [roh10]. 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) to study phagocytosis, where particle uptake into the artificial cell (GUV) is induced and measured with optical traps.

Living cell 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 100 nm spatial resolution which was used to investigate the molecular motor driven dynamics of the cytoskeleton protein MReB inside rod-shaped bacteria (B. Subtilis) [roh1, roh2].

Furthermore we investigated ultra-small, deformable, helical bacteria (S. Melliferum) which were oriented in object adapted optical traps(see Fig. 2.22). 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 kHz [roh7]. In another large project we investigate the nano-

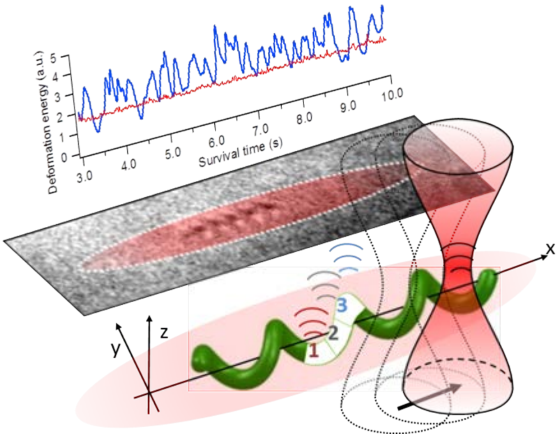


Figure 2.22: A 200 nm thin helical bacterium undergoes fast shape changes in an object adapted optical optical trap. Coherently scattered light allows fast 3-D super resolution imaging and to analyse the switching between mechanical energy states.

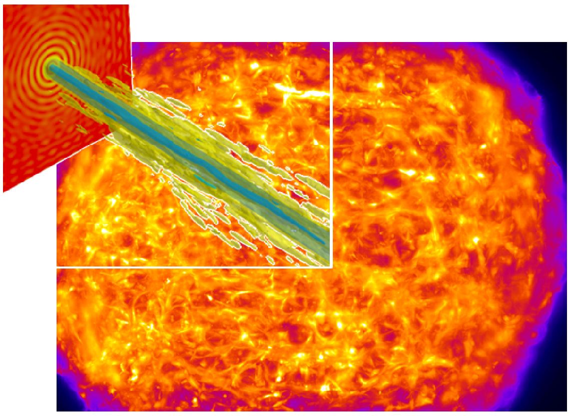


Figure 2.23: A fluorescently labeled cancer cell cluster of 230 μm diameter illuminated with self-reconstructing Bessel beams.

mechanics at the periphery of macrophages, which use complex mechanism based on cytoskeleton reorganization and collaborative work of molecular motors to uptake particles or bacteria either by thin cell protrusions or flat membranes. Using feedback controlled optical traps [roh8] and 3D interferometric tracking in the MHz range help to reveal the physical laws that influence phagocytosis.A system of much further complexity are clusters of thousands of cells, where cellular components are fluorescently labeled (Fig. 2.23) and scanned by holographically shaped, self-reconstructing illumination beams forming a light sheet [roh3, roh4, roh9]. 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.

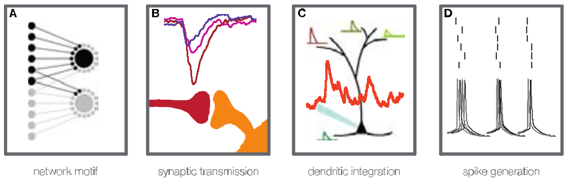


Figure 2.24: Steps of information transmission in neuronal networks. From [aer5].

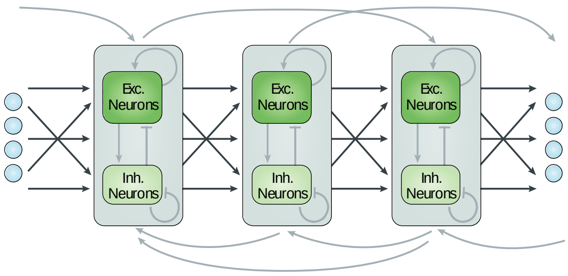


Figure 2.25: The feedforward network as a model of information processing in the brain. From [aer10].

2.4.3 Neurobiology and Biophysics

The **Neurobiology and Biophyics group of A. Aertsen** (Faculty of Biology) studies mechanisms of higher brain function. Modern approaches in this research area are increasingly concerned with neuronal dynamics. The task of organizing perception and behavior in a meaningful interaction with the external world prompts the brain to recruit its resources in a properly orchestrated manner. Contributions from many elements, ranging from individual nerve cells and networks of cells to entire brain areas, need to be coordinated in time and space.

The research goal is to understand how this organization is brought about, and how coordinated activity of ensembles of neurons is used by the brain. To this end we study the spatio-temporal organiza-

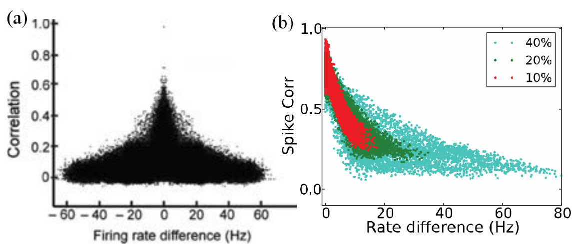


Figure 2.26: Spike correlations between neurons as a function of spike rate in experimental data (a: mitral cells) and model simulations (b). From [aer2].

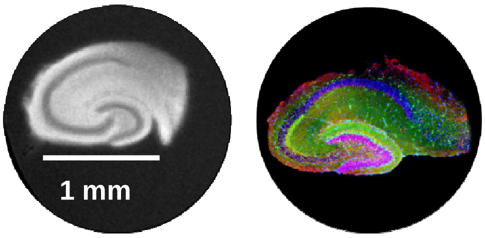


Figure 2.27: MicroMR of a slice preparation of a hippocampal slice of a mouse brain (l) compared with a microscopic view(r).

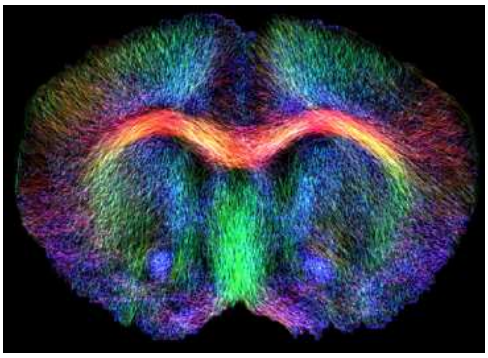


Figure 2.28: In vivo measurement of the neuronal fibres of a mosue brain using diffusion tensor MRI.

tion of brain activity at multiple scales simultaneously. Rules governing this organization and underlying mechanisms are brought to light by complementary approaches of physiological experimentation (multiple intra- and extracellular single-neuron recordings, local field potential and epicortical field potential recordings), advanced data analysis and neuronal network modeling, see Figs. 2.24, 2.25, and 2.26.

This multi-disciplinary approach has been instrumental in founding the new field of Computational Neuroscience: What are the theoretical foundations and computational mechanisms of brain function? How can this knowledge be applied in the development of neural prostheses and interfaces that directly connect to the nervous system? Thus, our research is at the core of the research programmes in Computational Neuroscience at the Bernstein Center Freiburg (BCF) and in Neurotechology (Brain-Machine Interfacing) in the Excellence Cluster BrainLinks-BrainTools.

2.4.4 Medical Physics

Biomedical Imaging techniques allow the investigations of living systems in vivo. Technological developments in all imaging modalities are extremely fast.

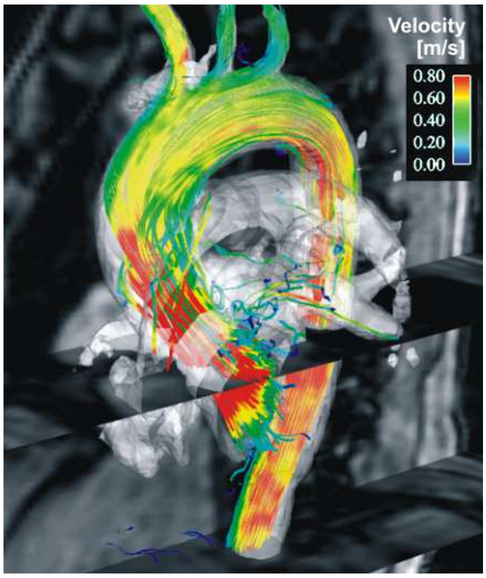


Figure 2.29: Quantitative measurement of blood flow in the aorta.

The **Medical Physics group of J. Hennig** (Department of Radiology) is active in the development of new methods and technologies specifically for magnetic resonance imaging (MRI) and their application in basic, preclinical, and clinical science as well as for clinical applications. The research ranges from the development of new measurement methods to data analysis and processing to hardware development of gradients, RF coils and other devices to improve and increase morphological, functional, metabolic, and physiological MR-measurements on all scales, see Figs. 2.27, 2.28, and 2.29. The activities are dedicated to develop MRI on all scales, from microMR on cell ensembles and tissue preparations to small animal imaging to MRI in humans. Key areas of applications are

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

Current research highlights include the development of an ultrafast technique for whole brain functional imaging at 10 fps and - very recently - a method for continuous hyperpolarization, which increases the MR signal of specific marker molecules by a factor of several thousands.

2.5 Important Publications and Conference Talks

2.5.1 Publications

Group Aertsen

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[blu2] F. Fürstenberg, M. Dolgushev, A. Blumen Analytical Model for the Dynamics of Semiflexible Dendritic Polymers J. Chem. Phys. 136 (2012) 154904.

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[blu7] A. Anishchenko, A. Blumen, O. Mülken, Enhancing the Spreading of Quantum Walks on Star Graphs by Additional Bonds, Quantum. Inf. Process. 11 (2012) 1273.

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2.5.2 Conference Talks

Group Aertsen

1. A. Aertsen, Computational Neuroscience - Experiments and Theory on a journey together. Keynote talk at NevroNor Conference ”Future visions in Neuroscience”, The Research Council of Norway, Oslo, November 29, 2011.

Group Blumen

1. O. Mülken, Quantum walks on networks: Dynamics - dissipation - decoherence Workshop on the dynamics and asymptotics in the Dicke model and quantum networks May 04, 2012 Matrahaza, Hungary.
2. A. Blumen, Modeling Semiflexible Behavior in Hyperbranched Macromolecules and in Polymer Networks 7th International Symposium Molecular Mobility and Order in Polymer Systems June 6-10, 2011 St.Petersburg, Russia.
3. A. Blumen, Continuous Time Random Walks and Continuous Time Quantum Walks XVI Conference on Statistical Physics and Complex Systems June 22-24, 2011 Parma, Italy.
4. A. Blumen, Continuous Time Random Walks and Continuous Time Quantum Walks The 5th IFAC Symposium on Fractional Differentiation and Its Applications, May 14-17, 2012 Nanjing, China.
5. A. Blumen, Coherent Transport and Trapping in the Continuous Time Quantum Walk Formalism, RKCM 2012: Reaction Kinetics in Condensed Media, September 11-16, 2012 Lochow, Poland.
6. A. Blumen, From Continuous Time Random Walks to Continuous Time Quantum Walks New Challenges in Complex System Physics, May 20-24, 2013 Samarkand, Uzbekistan.

Group Grabert

1. L. Mühlbacher, From quantum dots to light harvesting: Real-time quantum Monte Carlo for charge and energy transfer in dissipative quantum systems, Quantum Transport in Nanoscale Molecular Systems, August 2011, Telluride, USA.
2. H.-P. Beuer, Quantification and control of non-Markovianity in open quantum systems, Workshop SMQS-IP2011, 17.-19. Oktober 2011, Jülich Supercomputing Centre.
3. D. Bercioux, Pseudo-spin-dependent scattering in carbon nanotubes, International Workshop on Carbon-based Spintronics, October 2011, Dresden, Germany.
4. H. Grabert, Quantum transport in defected carbon nanotubes, Sasha Gogolin Memorial Meeting, November 2011, Trieste, Italy.
5. D. Bercioux, Quantum transport in defected carbon-nanotubes, 7th Annual IEEE International Conference on Nano/Micro Engineered and Molecular Systems, March 2012, Kyoto, Japan.
6. D. Bercioux, Spin-Resolved Transport Properties of Inhomogeneous Graphene Nanostructures, Graphene Conference 2012, April 2012, Brussels, Belgium.
7. H.-P. Breuer, Foundations and Measures of Quantum Non-Markovianity, Quantum Twin Workshop, 30. May-2. June 2012, Favignana, Sicily, Italy.
8. H.-P. Breuer, Quantum measures for non-Markovianity, Capri fall School on non-equilibrium processes and fluctuation-dissipation theorems, 9.-16. September 2012, Capri, Italy.
9. D. Bercioux, Flat bands in quasi-one-dimensional and two-dimensional lattices, International Workshop on Flat Bands: Design, Topology and Correlations, March 2013, MPIKS Dresden, Germany.

10. H.-P. Breuer, Foundations of Quantum Non-Markovianity in Open Systems, 534. WE-Heraeus-Seminar Quantum Many-Body Dynamics in Open Systems, 2.-5. April 2013, Bad Honnef, Germanyk.
11. H.-P. Breuer, Nonequilibrium Quantum Dynamics of Open Systems, Quantum Many-Body Systems out of Equilibrium, 12.-30. August 2013, MPIKS, Dresden, Germany, Plenary talk.
12. H.-P. Breuer, Quantum dynamics of open systems: Non-Markovianity, initial correlations and nonlocal memory effects, QCCC Symposium Frontiers in Quantum Dynamical Systems, 17.-18. Oktober 2013, Institute of Advanced Study, TU München, Germany.
13. H. Grabert, Mesoscopic electrons and Cooper pairs, Quantum Superconducting Circuits and Beyond, Yale, New Haven, CT, USA, December 2013.

Group Hennig

1. J. Hennig, Tsungming Tu Award Lecture: Visualize and Quantify Living Biological Systems: Present and Emerging Magnetic Resonance Imaging Technologies, National Sun-YaTsen University, Kaoshiung, Taiwan, 29. Jan. 2011.
2. J. Hennig, Einstein Lecture: Magnetic Resonance Imaging: Visions of Life, Chinese Academy of Science, Hefei, 6. Nov. 2011.
3. J. Hennig, Investigation of Brain Dynamics with Fast Functional MRI, 17th International Biophysics Congress (IUPAB), Beijing, China, Oct. 30th - Nov. 3rd, 2011.
4. J. Hennig, Molecular Imaging with small animal MR, Opening Lecture, International Meeting on Small Animal Imaging, Kaohsiung, Taiwan, 10.-11. Feb. 2012.
5. J. Hennig, Fast Dynamic Measurement of Brain Physiology with MR-Encephalography(MREG), Annual Meeting OHBM (Orgaization for Human Brain Mapping), Beijing, 10.-14. June 2012.
6. J. Hennig, Sir Peter Mansfield Lecture: Challenges and Opportunities for MR - A scientists perspective, ESMRMB (European Society for Magnetic Resonance in Medicine and Biology), Lisbon, 2012.
7. Hennig J., William Mong Lecture: Visualize and Quantify Living Biological Systems: Present and Emerging Magnetic Resonance Imaging Technologies, Hongkong University, 18. Nov. 2013.

Group Moseler

1. M. Moseler, Multiscale materials modelling as a tool for the optimisation of resource efficiency in technical systems, 1st International ECEMP Colloquium, 25.01.2011, Dresden.
2. M. Moseler, Diamonds arenı́ forever: atomistic insights into wear of the hardest material on earth, International Nanotribology Forum (INF), 22.05. - 03.06.2011, Hoi An, Vietnam.
3. M. Moseler, Atomistic insights into the tribology of diamond materials and the growth of carbon nanotubes, Specialist Meeting on Carbon, 26.9.2011, Puerto Vallarta, Mexico.
4. M. Moseler, The mechanochemistry of wear in diamond, Tribochemistry 2011, 26 Oct. 2011, Hagi, Japan.
5. M. Moseler, Atomistic Insights into the Tribological Properties of Diamond and Gold Coatings. International Tribology Conference, October 30 - November 3, 2011 Hiroshima, Japan.
6. M. Moseler, Atomistic/continuum multiscale coupling Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations, International Workshop March 26 - 29, 2012 Dresden.
7. M. Moseler, Towards an atomistic understanding of tribo-induced phase transitions Gordon Research Conference on Tribology July 2012 Waterville, Maine.

8. M. Moseler, Atomistic understanding of wear in carbon tribomaterials Wear of Materials 2013, 14.-18.3.2013, Portland.
9. M. Moseler, Atomistic modeling of nanostructure formation via cluster deposition, Gordon Research Conference on Clusters, Nanocrystals, and Nanostructures,4.-9.8.2013, Mount Holyoke College.
10. M. Moseler, Towards an atomic scale understanding of wear in carbon coatings and metals Leeds-Lyon-Symposium on Tribology, 4.-6.9.2013, Lyon.

Group Reiter

1. G. Reiter, Probing Properties of Polymer in Thin Films Workshop Thin Films 3.-14. August 2012 Hsinchu, Taiwan.
2. G. Reiter, Propriétés de Polymères en Films Minces Réunion du GT Surfaces, Journee 'Surfaces Fonctionelles du Groupe de Travail Surfaces', 6. November 2012 Paris, France.
3. G. Reiter, Formation of Hierachically Structured Single Crystals World Polymer Congress 2012 24.-29. June 2012 Blacksburgh, Virginia, USA.
4. G. Reiter, Single Crystals of Conjugated Polymers Supramolecular Functional Materials for Organic Electronics Conference 26.-28. June 2013 Strasbourg, France.
5. G. Reiter, Single Crystals of Conjugated Polymers International Physics Congress 2.-5. September 2013 Istanbul, Turkey.

Group Timmer

1. J. Timmer, Quantitative Modelling of Signalling Pathways, Integrated Pharmacology: Signaling from Cells to Systems, 23.02.11, Bonn.
2. J. Timmer, Systems Biology of the Epo-Receptor, Proteomic Forum 2011, 07.04.11, Berlin.
3. J. Timmer, From the Identifiability of Models via Key Systems Properties in Cancer Signaling Pathways to Predicting Cellular Behavior, Conference on Translational and Systems Medicine, 21.06.11, Stockholm, joint talk with U. Klingüller.
4. J. Timmer, Joining Forces of Bayesian and Frequentist Methodology: A Study for Inference in the Presence of Non-identifiability, Signal Processing and Inference for the Physical Science, 26.03.12, Royal Society, London.
5. J. Timmer, Systems Biology in Cancer Research, Meeting of the "Hinterzartener Kreis", 04.05.13, Como, Italy.

Group von Hauff

1. E. von Hauff, Improving Photovoltaic Performance in Low Bandgap Polymer:Fullerene Solar Cells by Molecular Doping, International Conference on Flexible Electronics (ISFOE), July 11-13, 2011, Thessaloniki, Greece.
2. E. von Hauff, Issues related to efficiency and stability in polymer based solar cells, African Network for Solar Energy (ANSOLE), February 17-19, 2012, Yaounde, Cameroon, Keynote.
3. E. von Hauff, Issues related to efficiency and stability in polymer solar cells, European Society for Quantum Solar Energy Conversion (QUANTSOL), March 11-16, 2012, Bad Gastein, Austria.
4. E. von Hauff, Controlling recombination and improving the photocurrent in polymer:fullerene blends with molecular doping, SPIE Photonics Europe, 16-19 April, 2012, Brussels, Belgium.

5. E. von Hauff, Lifetime issues in polymer photovoltaics, The Sino-German Symposium on Organic Photovoltaic Materials and Organic Solar Cells, May 27-31, 2012, Chengdu, China.
6. E. von Hauff, The role of contact interfaces on the efficiency and lifetime of organic solar cells, Electronic Structure and Processes at Molecular-Based Interfaces (ESPMI), April 28-May 3, 2013, Weizmann Institute, Rehovat, Israel.
7. E. von Hauff, Material interfaces in organic solar cells, SPIE Optics & Photonics, 25-29 August 2013, San Diego, USA.
8. E. von Hauff, Molecular doping to tune opto-electronic properties in organic semiconductors, European Conference on Molecular Electronics (ECME), September 3-7, 2013, London, England.

Group Waldmann

1. O. Waldmann, Molecular Nanomagnets: A Challenge for Quantum Many-body Physics in "Small" Spin Systems, 504. WE-Heraeus-Seminar Quantum Magnetism in Low Spatial Dimensions April, 2012, Bad Honnef, Germany.

Group Weber

1. E. R. Weber, The Role of Material Science for Future Photovoltaics, German Polish Conference on Crystal Growth (GPCCG), 14.-18. March 2011, Frankfurt (Oder), Germany, Plenary Talk.
2. E. R. Weber, Progress in Materials for Solar Energy Conversion, American Physical Society (APS) Conference, 21.-25. March 2011, Dallas, USA, Plenary Talk.
3. U. Würfel, Investigation of Degradation Mechanisms in P3HT:PCBM Solar Cells by Means of Impedance Spectroscopy, CELIV and Modeling ISOS 4 - 4th International Summit on Organic Photovoltaic Stability, 5.-6. December 2011, Golden, USA.
4. E. R. Weber, New Materials and Processes for Photovoltaics, Manufacturing Society of Vacuum Coaters SVC Tech Conference 2012, 30. April 2012, Santa Clara, CA, USA, Keynote speech.
5. E. R. Weber, The Future of Crystalline Silicon Photovoltaic Technology, IEEE Photovoltaic Specialists Conference, 05.-08. June 2012, Austin, TX, USA, Plenary Talk.
6. B. Zimmermann, Application Specific Design of Organic Solar Cells and Modules Large-area, Organic and Printed Electronics Convention (LOPE-C) 2012, 19.-21. June 2012, Munich, Germany.
7. U. Würfel, Activities on Organic Solar Cells at Freiburg Materials Research Centre and Fraunhofer ISE, 2012 Global Organic Photovoltaic Conference (GOPV2012), 09.-12. September 2012, Suzhou, China.
8. B. Zimmermann, Application Specific Design of Organic Solar Cells and Modules ISOS 5 - 5th International Summit on Organic Photovoltaic Stability, 06.-07. December 2012, Eindhoven, The Netherlands.
9. E. R. Weber, Defect Control in Photovoltaic Technology 27th International Conference on Defects in Semiconductors (ICDS) 2013, 25. July 2013, Bologna, Italy, Plenary Talk.
10. E. R. Weber, The Global Energy Transformation, International Solar Energy Society (ISES) Solar World Congress 2013, 04. November 2013, Cancun, Mexico, Keynote speech.

2.6 PhD, Diploma and Master Theses

2.6.1 PhD-Theses

Group Blumen

1. M. Dolgushev, Theoretical Investigations of Semiflexible Branched Polymers, June 2011. http://www.freidok.uni-freiburg.de/volltexte/8455/
2. G. Berezovska, Monte Carlo Study of Semiflexible Polymers, November 2011. http://www.freidok.uni-freiburg.de/volltexte/8601/

Group Grabert

1. Prathan Srivilai, Quantum Monte Carlo study of the metallic single electron pump, June 2012.
2. Klaus Ferdinand Albrecht, Nonequilibrium charge transport through quantum dots with electron-phonon interaction, November 2013.
3. Bruno Leggio, Quantum fluctuations and correlations in equilibrium and nonequilibrium thermodynamics, November 2013.
4. Lucia Lenz, Spin-orbit interactions in carbon based materials, October 2013.

Group Hennig

1. S. Baumann, Time-of-flight-Magnetresonanzangiographie mit kontinuierlich bewegtem Patiententisch, January 2011.
2. B. Zahneinsen, Funktionelle Magnetresonanztomographie mit stark unterabgetasteten Trajektorien, February 2011.
3. T. Hugger, Mehrkanal-Bildrekonstruktion bei Unterabtastung in der funktionellen Magnetresonanztomographie, Mai 2011.
4. S. Bauer, Entwicklung und Analyse von Beschleunigungsmethoden für die funktionelle Untersuchung des kardiovaskulären Systems mit Magnetresonanztomographie, October 2011.
5. D.N. Splitthoff, SENSE Shimming (SSH): Fast detection of B0 Field inhomogeneities in Magnetic Resonance Imaging, December 2011.
6. G. Schultz, Magnetic Resonance Imaging with nonlinear Gradient fields: Signal encoding and image reconstruction, April 2012.

Group Reiter

1. N. Basu, Investigation of Melting and Re-Crystallisation Behavior of Polyethylene Nanocrystals, August 2012. http://portal.uni-freiburg.de/exppolymer/abstracts/2012-5-rei
2. M. Chowdhury, Thin Polymer Films Out of Thermodynamic Equilibrium, August 2012. http://portal.uni-freiburg.de/exppolymer/abstracts/2012-6-rei
3. K. Jahanshahi, Reversible Crystallization and Dissolution of Poly(γ-benzyl L-glutamate) in Thin Film Solutions via Addition and Removal of a Nonsolvent, August 2013. http://portal.uni-freiburg.de/exppolymer/abstracts/2013-8
4. R. Shokri, Self-Assembly of Supra-Molecular Systems on Graphene or Graphite, April 2013. http://www.freidok.uni-freiburg.de/volltexte/8990/pdf/thesis_Roozbeh.pdf

5. K. Rahimi, Controlling the Crystal Growth and Morphology of Conjugated Polymers, April 2013. `http://www.freidok.uni-freiburg.de/volltexte/8980/pdf/thesis_khosrow_v5.pdf`

Group Rohrbach

1. Lars Friedrich, Surface scanning using optically trapped probes, 2011.
2. Florian Fahrbach, Microscopy with self-reconstructing beams, 2012.
3. Philipp von Olshausen, Total internal reflection microscopy: super-resolution imaging of bacterial dynamics and dark field imaging, 2012.
4. Markus Grießhammer, Interferometrisches Tracking und Manipulation von Nanorods mit optischen Pinzetten, 2013.
5. Felix Kohler, Photonic force based investigations of filopodial dynamics and coupled molecular motors, 2013.
6. Benjamin Tränkle, Interaktionsdynamik kolloidaler Partikel in beschränkten Volumina, 2013.

Group Timmer

1. B. Greese, Study of the Mechanisms Underlying Trichome Initiation using Mathematical Modelling, 2011.
2. C. Kreutz, Statistical Approaches für Molecular and Systems Biology, 2011. `http://www.freidok.uni-freiburg.de/volltexte/8404`
3. A. Raue, Quantitative Dynamic Modeling - Theory and Application to Signal Transduction in The Erythropoietic System, 2013.
4. A. Schad, A new approach for the global helioseismic investigation of the solar meridional flow, 2013.
5. L. Sommerlade, Time-resolved estimation of direct directed influences, 2013.

Group Waldmann

1. Joscha Nehrkorn, Exploring Molecular Nanomagnets with Spectroscopic Techniques: Spin Exchange Coupling and High Anisotropy, 2012. `http://www.freidok.uni-freiburg.de/volltexte/8710/`
2. Alexander Sundt, AC and DC magnetization Studies on Heterometallic 3d-4f Molecular Nanomagnets, 2012.

Group Weber

1. S. Schäfer, Organic solar cells based on vacuum processed small molecules, April 2011.
2. J. Haunschild, Lumineszenz-Imaging - Vom Block zum Modul, March 2012.
3. U. Jäger, Selektive Laserdiffusion für Hocheffiziente Solarzellen aus Kristallinem Silicium, October 2012.
4. F. F. Stelzl, 2-dimensionales Donator/Akzeptator-Modell für organische Solarzellen und experimentelle Untersuchungen mittels Nanoelektroden, December 2012.
5. J. Greulich, Mehrdimensionale Simulation und Charakterisierung von neuartigen, mit industrierelevanten Methoden hergestellten Silicium-Solarzellen, February 2014.

2.6.2 Diploma/Master Theses

Group Blumen

1. M. Schuler, Quantum Stochastic Walk auf offenen Netzwerken, March 2013.
2. P. Liebermann, Energietransfer und Dekohärenz im Phasenraum, February 2012.
3. M. Bauer, Exzitonendynamik auf Netzwerken im Nichtgleichgewicht, April 2011.
4. B. Berger, A Generalized Master Equation Approach for the Excitation Transport and Trapping on Quantum Networks, November 2011.
5. J. Kohlberger, Dissipative Exzitonendynamik auf kleinen Netzwerken, September 2011.

Group Grabert

1. Linnéa Schätzle, Spin-dependent properties of bilayer graphene, November 2013.
2. Juliane Klatt, A numerical study of the phononic properties of molecular junctions subject to vibronic coupling, October 2013.
3. Han Xiao, Exact master equation for a bosonic many-body system coupled to a bosonic bath, October 2013.
4. Andreas Inhofer, Time-dependent quantum dot coupled to the edges of a two-dimensional topological insulator, August 2013.
5. Steffen Wißmann, Characterization of optimal quantum states with maximal memory effects, December 2012.
6. Michael Schulze, Adiabatic quantum pumping on quasi one-dimensional lattices, April 2012.
7. Stefan Fischer, Coherence in a network of two-level systems coupled to a bosonic field, December 2011.
8. Govinda Clos, Information flow in the dynamics of the spin-boson model: Quantifying non-Markovianity, October 2011.
9. Manuel Gessner, Initial correlations in open quantum systems, September 2011.

Group Hennig

1. W. Buchenberg, Entwicklung eines hybriden US-MR Systems zur Beurteilung der Herzfunktion während freier Atmung, October 2011.
2. A. Ruh, Modellierung und Messung des H2O-NMR Spektrums von Blut vor dem Hintergrund der “Effective-Medium” Theorie, 2011.
3. R. Borowiak, Aufbau einer Niederfeld NMR-Detektionseinheit zur Kalibrierung eines PASADENA-Hyperpolarisators, April 2012.
4. R. Sostheim, Charakterisierung von suszeptibilitätsinduzierten MR-Signalstörungen für die Anwendung in der MRT, May 2012.
5. T. Fredrich, Statistical Aspects of the Global Tracking Algorithm, August 2013.
6. F. Lippus, Perfusionsgewichtete Magnetresonanztomographie: Entwicklung einer integrierten, kontinuierlichen Arterial Spin Labeling Methode, June 2013.

Group Moseler

1. Matthias List, Molekulardynamik-Simulationen zur Untersuchung des Scherverhaltens mesogener Flüssigkeiten, 2013.
2. Ruth von Waldenfels, Schwingungsspektren des erste elektronischen Übergangs von Molekülen mit delokalisiertem p-Elektronensystem, 2013.

Group von Hauff

1. H. Beh, ZnO nanopyramids for organic-inorganic hybrid photovoltaics, October 2013.
2. S. Illner, Investigation of optical properties of copper phthalocyanine layers modified by plasmonic nanoparticles, October 2013.
3. S. Meisenheimer, Ordered Silver Nanoparticles for Silicon Solar Cells:Simulation and Fabrication, October 2013.
4. Raphael Präg, Eigenschaften des Ladungstransports organischer Halbleiter in feldabhängigen Dünnschichtstrukturen, November 2013.

Group Reiter

1. T. Maier, Untersuchung der zeitlichen Änderung der Grenzflächeneigenschaften von Polymerlaminaten, June 2013.
2. A. Skilitsi, Total Internal Fluorescence Microscopy: Fluorescence Probability of Fluorescent proteins in Living Cells, October 2013.

Group Rohrbach

1. Martin Glasstetter, Untersuchung der intrazellulären Dynamik von Phagosomen und des umgebenden Zytoskeletts mittels kohärenter Lichtstreuung, 2013.
2. Andreas Meinel, Mechanische und energetische Konzepte der phagozytischen Partikelaufnahme synthetischer Zellen, 2013.
3. Hoda Mousavi, Wavefront Correction for Bessel Beams Propagating Through Scattering Media, 2013.
4. Julian Roth, Kohärente Abbildungen der Dynamik des helikalen Bakteriums Spiroplasma melliferum und Analyse seiner Nanomechanik, 2013
5. Marc Blattmann, Optisches Fangen kolloidaler Partikel - Oberflächenstrukturierung und plasmonische Kopplung, 2012.

Group Timmer

1. R. Ramb, Graphical Models in Time Series: From Basic Concepts to Latent Variables, 2011.
2. B. Steiert, Identifiability Analysis and Experimental Design of Non-linear Dynamical Systems, 2012.
3. J. Ortmann, Uni- and bivariate analysis of imaging data and its application in neurology, 2012.
4. M. Schelker, Parameter Estimation in Non-autonomous Dynamical Systems, 2012.
5. B. Bastian, Spatial and temporal patterns in biology, 2013.
6. C. Tönsing, Optimal Experimental Design for Ordinary Differential Equation Models: New Insights into the Origin of Sloppiness, 2013.

7. K. Klawitter, Simulation und Analyse von ereigniskorrelierten Daten, 2013.

Group Waldmann

1. Pascal Wendler, Aufbau eines AC-Suszeptometers zur Untersuchung magnetischer Moleküle bis 100 kHz, February 2013.

Group Weber

1. D. Walter, Lebensdaueruntersuchung an kristallinem Silicium-Dünnschichtmaterial, January 2011.
2. J. Richter, Optimierung nichtlinearer dynamischer Systeme am Beispiel eines inselfähigen Stromnetzes mit erneuerbaren Energien, February 2011.
3. F. Schindler, Materialeigenschaften von alternativ aufgereinigtem multikristallinem Silicium, February 2011.
4. K. Dreyer, Bonding- und Lift-Off-Techniken zur Herstellung von III-V-Solarzellen auf "modifizierten" Substraten, February 2011.
5. A. Kimmerle, Herstellung und Charakterisierung hochohmiger Emitter für Hocheffizienzsolarzellen, February 2011.
6. S. Werner, Herstellung und Charakterisierung von Emittern für Emitter Wrap-Through Solarzellen, April 2011.
7. O. Höhn, Dreidimensionale photonische Kristalle - Simulation und Erzeugung, May 2011.
8. G. S. Kutscheidt, Untersuchung und Modellierung der Strahlaufweitung an Oberflächen von Spiegeln solarthermischer Kraftwerke, May 2011.
9. P. Faubert, Evaluation des Potentials von Metallfolien zur rückseitigen Kontaktierung von Solarzellen mit Laser-legierten Kontakten, October 2011.
10. N. Wöhrle, Optische Simulation von rückseitenpassivierten Silicium-Solarzellen, November 2011.
11. J. Posdziech, Herstellung und Charakterisierung von Fortgeschrittenen Fluoreszenzkonzentratoren, November 2011.
12. J. Eckert, Influence of mounting scenarios on crystalline silicon photovoltaics module operating temperature for roof mounted home systems, November 2011.
13. H. Steinkemper, Untersuchung der Hochkonversion zur Effizienzsteigerung von Solarzellen, February 2012.
14. A. Witzky, Elektrische und optische Charakterisierung von Silicium-Carbid-Schichten mit eingebetteten Silicium-Nanokristallen für Silicium-basierte Solarzellen mit hoher Bandlücke, March 2012.
15. T. Rist, Modellierung und Charakterisierung von Fluoreszenzkonzentrator- und Hochkonvertersystemen, April 2012.
16. J. Frank, Simulation von Bifacialen Solarzellen für Photovoltaiksysteme mit Hochkonvertern, June 2012.
17. N. Milenkovic, Simulation und Charakterisierung epitaktischer Emitter für Wafer-Solarzellen, July 2012.
18. D. Schuldis, Passiviermechanismen extrem dünner mittels ALD abgeschiedener AL2O3-Schichten, August 2012.
19. B. Bremen,Untersuchung von SF6-O2-Plasmen zur maskenlosen Texturierung kristalliner Siliciumoberflächen, August 2012.

20. I. Geisemeyer, Rückwärtsdurchbrüche in multikristallinem Silicium im Modulbetrieb - Thermische Simulation, September 2012.

21. D. Impera, Charakteriesierung von amorph-kristallinen Silicium-Hetero-Solarzellen mit multikristallinem Absorber, September 2012.

22. K. Krauß, Verlustanalyse von Solarzellen aus umg-Silicium, September 2012.

23. M. Tondorf, Entwicklung eines Inline-Verfahrens zur optischen Kontrolle der Qualität von Oberflächentexturen und Anti-Reflex-Beschichtungen in der Solarzellenfertigung, November 2012.

24. S. Wasmer, Lebensdauerkalibrierung ortsaufgelöster Photolumineszenz-Aufnahmen zur Bewertung multikristalliner Silicium-Wafer und Analyse des lokalen Durchbruchverhaltens von Solarzellen, February 2013.

25. L. Ogrodowski, Untersuchung lokaler Metall-Halbleiter-Kontakte für industrielle PERC-Solarzellen, February 2013.

26. S. Schröer, 2-Dimensionale Simulation von amorph/kristallinen Silicium-Hetero-Solarzellen, February 2013.

27. M. A. Fischer, Untersuchung organischer Solarzellen mit numerischen Simulationen und CELIV, March 2013.

28. H. Lindner, Inline-Detektion von Hot Spots auf kristallinen Silicium-Solarzellen durch Infrarot-Thermographie, March 2013.

29. J. Löffler, Photonische Vielschichtsysteme für Fluoreszenzkonzentratoren, March 2013.

30. J. Schmidt, Qualitätskontrolle in der PV-Produktion and Analyse verschiedener Defekte in umg Cz-Silicium, March 2013.

31. S. Rappl, Passivierung von plasmageätzten Siliciumoberflächen, April 2013.

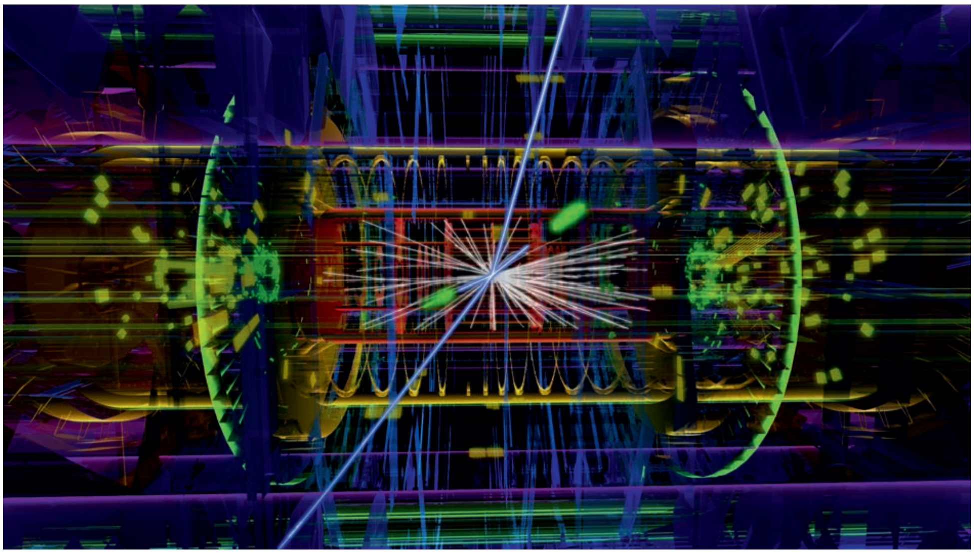
32. S. Wolf, Photonische Strukturen zur Effizienzsteigerung der Hochkonversion, April 2013.

33. T. Welschehold, Evaluation von Charakterisierungsmethoden zur Inline-Detektion von Mikrorissen in Siliciumwafern und deren elektrische und mechanische Bewertung, April 2013.

34. B. Fröhlich, Charakterisierung von Hochkonvertermaterialien für die Photovoltaik, August 2013.

Chapter 3

Particles, Fields and Cosmos



Experimental Physics

- **Prof. G. Herten**
- **Prof. K. Jakobs**
- **Prof. K. Königsmann**
- **Prof. M. Schumacher**

Theoretical Physics

- **Prof. S. Dittmaier**
- **JProf. H. Ita**
- **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.

Today's experimental activities are focussed on CERN with participation in the ATLAS experiment at the LHC with groups led by **G. Herten, K. Jakobs and M. Schumacher** and in the COMPASS experiment with the group of **K. Königsmann**. The permanent faculty members **H. Fischer, U. Landgraf, U. Parzefall, C. Weiser and S. Zimmermann** contribute in leading roles to these experiments. Since April 2013 **P. Jenni**, who led the ATLAS Collaboration as spokesperson from 1995 to 2009 and had a leading role during the initialization and realization of the experiment, works as a guest scientist at our institute. In December 2013 the University of Freiburg awarded a Honorary Professorship to him. The experimental activities are accompanied by strong activities in theory led by **S. Dittmaier, J. van der Bij and H. Ita**. They 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 has contributed right from the beginning 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 2004 the Freiburg group (M. Schumacher) operates a so-called ATLAS Tier-2 Grid-centre for high performance computing. Today the group 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 research and development for the upgrade of the ATLAS experiment towards the High-Luminosity LHC (HL-LHC). The work of more than twenty years culminated in 2012 in the discovery of the long-sought Higgs boson by the ATLAS and CMS experiments. The Freiburg group contributed significantly to this discovery.

The COMPASS (COmmon Muon and Proton Apparatus for Structure and Spectroscopy) experiment allows for a detailed investigation of the structure of hadrons with the aim to improve our understanding of QCD in the non-perturbative regime. In particular, the goal of the experiment is to disentangle the individual contributions of quarks and gluons to the spin of the nucleon. The main contributions of the Freiburg group concern the analyses of muon scattering data on longitudinally and transversely polarised nucleons, hardware developments and construction of the readout of the detector.

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" level (and beyond) and applied in cutting-edge calculations where existing techiques 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. One example is the *LHC Higgs Cross Section Working Group*, which was led by S. Dittmaier from 2010-2012. A further example, where both experimental and theoretical physicists are involved, is the EU Training network *HiggsTools* which will start at the beginning of 2014.

The Freiburg particle physics groups have also strong involvements in detector physics and are members of important Research and Development 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)*. For the COMPASS experiment digitisation and trigger electronics have been developed. This concerns high-speed and high resolution transient recorders, time-to-digital converters and trigger processors, all programmable to adapt to different applications.

The activities in the ATLAS experiment are embedded in a *Collaborative Research Centre* of the German Ministry for Education and Research (BMBF Forschungsschwerpunkt FSP-101 ATLAS), where 13 German Universities, the Deutsche Elektronen Synchrotron (DESY) and the Max-Planck-Institute for Physics in Munich (MPP), collaborate. During the present funding period (2012 - 2015) the University of Freiburg has 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” (2007-2014), a national research network comprising 18 universities, two Helmholtz Centres (DESY and KIT) and the MPP.

Particle physicists from Freiburg are also very visible in the German high energy physics community. At present, Gregor Herten is the chair of the particle physics section within the German Physical Society (DPG), Stefan Dittmaier is one of two representatives of theory in the German committee for particle Physics (KET) and Markus Schumacher is a member of the management board of the Helmholtz Alliance.

To offer an excellent environment for education and research for PhD students and to foster closer collaboration between theory and experiment, the particle physics groups have successfully established the Research Training Group “Physics at Hadron Colliders” (2005 - 2014), funded by the Deutsche Forschungsgemeinschaft (DFG). This programme was 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. During the past five years 21 PhD students graduated as members of this programme. The topics covered within the school span the entire range of activities on theory and data analysis in the ATLAS and COMPASS experiments.

The future activities of particle physics in Freiburg are directed towards further studies of the profile of the Higgs boson and the search for physics beyond the Standard Model. The successful cooperation between experiment and theory are planned to be continued within a new Research Training Group “Mass and Symmetries after the Higgs boson discovery” for which an application has been put forward.

3.2 Analysis of LHC Data - ATLAS Experiment -

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 the Higgs boson and 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 τ leptons, in the tagging of b-quarks and in the reconstruction of electrons. In addition, they have contributed to important detector simulation projects. Scientists from Freiburg have held leading and visible roles in the collaboration, *e.g.* run coordinator, collaboration board chair and co-convenors of performance and physics groups.

3.2.1 The Search for the Higgs Boson

Since the beginning of the data taking, a large fraction of our analysis activities (groups of K. Jakobs and M. Schumacher) was focussed on the search for the Standard Model Higgs boson in the decay modes $H \to WW^{(*)} \to \ell\nu\ell\nu$, $H \to \tau\tau$ and $H \to b\bar{b}$. Whereas via the decay mode $H \to WW^{(*)}$ we were directly contributing to the discovery of the Higgs boson in the year 2012, the detailed and more challenging investigations of the $H \to \tau\tau$ and $H \to b\bar{b}$ decay modes are essential to probe fermionic couplings of the Higgs boson and thereby to establish its profile. The decay modes A/H $\to \tau\tau$ and $H^{\pm} \to \tau\nu$ were also used to search for heavy neutral and charged Higgs bosons in supersymmetric models (MSSM).

H $\to$ WW$^{(*)}$: The $H \to WW^{(*)}$ channel has its highest sensitivity for Higgs boson masses around 160 GeV, where decays into two real W bosons dominate. Already in Summer 2011, first sensitivity in this mass range was reached by the ATLAS collaboration. The existence of the Standard Model Higgs boson in the mass range from 145 - 206 GeV could

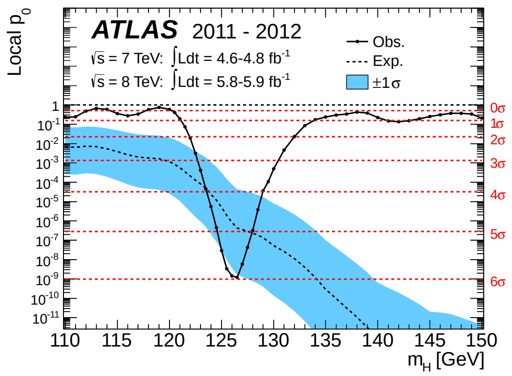


Figure 3.1: The observed (solid) local p_0 (see text) as a function of m_H for the combination of the $H \to \gamma\gamma$ $H \to ZZ^* \to 4\ell$ and $H \to WW^* \to \ell\nu\ell\nu$ search channels. The dashed curve shows the expected p_0 under the hypothesis of a Standard Model Higgs boson signal at that mass with its $\pm 1\sigma$ band. The horizontal lines indicate the p-values corresponding to significances of 1 to 6σ.

be excluded at the 95% confidence level (CL).

With the increase of the centre-of-mass energy in 2012 from $\sqrt{s}$ = 7 TeV to $\sqrt{s}$ = 8 TeV and much higher integrated luminosities, the observation of the Higgs boson became possible. In July 2012, both the ATLAS and CMS Collaborations announced the discovery of a new boson with a mass around 126 GeV [jak1]. The significance of this discovery was largely based on the observation of signals in the high-resolution $H \to \gamma\gamma$ and $H \to ZZ^* \to 4\ell$ channels, with contributions from the $H \to WW^* \to \ell\nu\ell\nu$ channel. The combined discovery significance of the three channels was 5.9σ. In Figure 3.1 the observed local probablility p_0, *i.e.* the probability that the background can produce a fluctuation greater than or equal to the excess observed in data, is shown.

Our group made significant contributions to the $H \to WW^*$ analysis, with focus on the optimization of the selection criteria, the understanding of the reconstruction efficiencies for electrons (see Section 3.2.4) and on the estimation of the important background from non-resonant WW production. The analysis activites in this channel have been pursued ever since. During 2013 our major activities were on studies of the spin and CP properties of the new resonance and on the separation of the important production processes, *i.e.* production via gluon fusion or vector-boson fusion (VBF). This separation is important for the determination of the couplings of the Higgs boson to fermions and W and Z bosons. Important results on these aspects -with significant contributions from our group- were published recently [jak2, jak3], using the full data sample collected by the ATLAS experiment in 2011 and 2012, corresponding to integrated luminosities of 20.7 fb^{-1} at $\sqrt{s}$ = 8 TeV and 4.6 fb^{-1} at $\sqrt{s}$= 7 TeV.

In Ref. [jak3] the Standard Model spin-parity $J^P = 0^+$ hypothesis is compared with alternative hypotheses using the Higgs boson decays $H \to \gamma\gamma$, $H \to ZZ^* \to 4\ell$ and $H \to WW^* \to \ell\nu\ell\nu$, as well as the combination of these channels. The data are found to be compatible with the Standard Model $J^P = 0^+$ quantum numbers for the Higgs boson, whereas all alternative hypothesis studied, namely some specific $J^P = 0^-, 1^+, 1^-$, and 2^+ models, are excluded at confidence levels above 97.8%. The data thus provide evidence for the spin-0 nature of the Higgs boson, with positive parity being strongly preferred. Our group took a leading role in the spin studies in the $H \to WW^*$ channel by setting up multivariate discriminants based on boosted decision trees and contributed to the spin analysis in the $H \to \gamma\gamma$ channel.

In Ref. [jak2] results on the measurement of Higgs boson production and couplings in the di-boson final states were published. In Figure 3.2 the distribution of the transverse mass is shown for $H \to WW^*$ candidate events passing the final selection criteria. A clear excess of events relative to the background-only expectation is observed in the data. For m_H=125.5 GeV, a signal significance of 3.8σ is observed, in agreement with the expectation for a Standard Model Higgs boson.

The events in the various sub-categories in the $H \to WW^*$ channel (binned by the number of jets) have been used together with similar categories in the other bosonic decay channels to fit for the signal strengths separated for the gluon fusion and vector-boson fusion production. A fit of the VBF signal strength normalized to the signal strength in gluon fusion and associated ttH production yields

$$\mu_{\mathrm{VBF}}/\mu_{\mathrm{ggF+ttH}} = 1.4^{+0.4}_{-0.3}(\mathrm{stat})^{+0.6}_{-0.4}(\mathrm{syst}).$$

It provides first evidence -at the 3.3σ level- that a fraction of Higgs boson production occurs through VBF.

H $\to \tau\tau$: In order to fully establish the Higgs mechanism of the Standard Model, the predicted couplings of the Higgs boson to fermions has also to be demonstrated. Until recently, however, evidence for Higgs boson decays into fermionic final states was not conclusive. Due to the proportionality of the coupling strength of the Higgs boson to mass and due to the experimental identification capabilities, fermions of the third generation, *i.e.* $H \to \tau\tau$ and $H \to b\bar{b}$ decays, are preferred. However, their detection re-

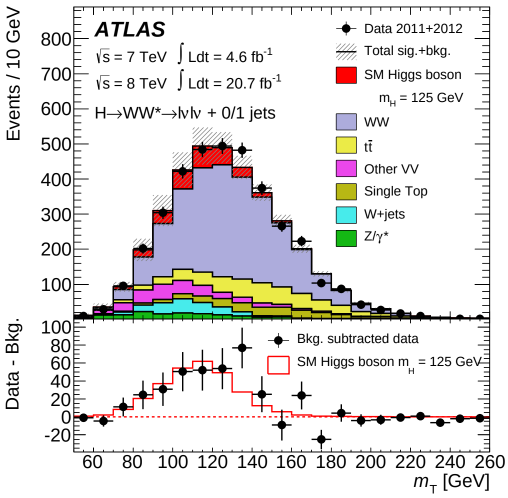


Figure 3.2: The transverse mass distributions for events passing the full selection of the $H \to WW^* \to \ell\nu\ell\nu$ analysis summed over all lepton flavours for final states with $N_{\text{jet}} \leq 1$. The signal is stacked on top of the background. In the lower part of the figure the residuals of the data with respect to the estimated background are shown, compared to the expected m_{T} distribution of a Standard Model Higgs boson.

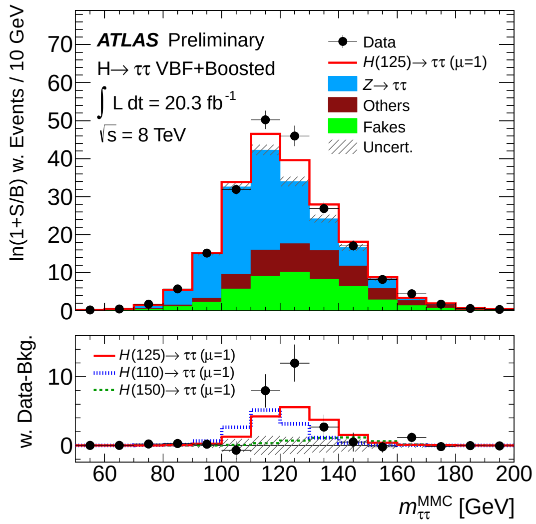


Figure 3.3: Distribution of the reconstructed $\tau\tau$ invariant mass, $m_{\tau\tau}^{MMC}$, where events are weighted by $\ln$ (1 + S/B) for all channels. The bottom panel shows the difference between weighted data events and weighted background events. The distributions for the predicted excess in data over the background are shown for alternative Higgs boson mass hypotheses with m_H = 100 GeV and m_H = 150 GeV.

mains a formidable task given the challenging signal-to-background conditions.

With a branching ratio of 6.3%, $H \to \tau\tau$ is among the leading decay modes for a Standard Model Higgs boson with a mass around 125 GeV. In November 2013 the ATLAS collaboration has presented preliminary results which show clear evidence for such decays [jak4]. The analysis, to which the Freiburg groups contributed significantly, is based on the full data set collected at $\sqrt{s}$ = 8 TeV during 2012. The search is performed in three different final states, according to the decay of the τ lepton: $H \to \tau_{\text{lep}}\tau_{\text{lep}}$, $H \to \tau_{\text{lep}}\tau_{\text{had}}$, and $H \to \tau_{\text{had}}\tau_{\text{had}}$, where τ_{lep} and τ_{had} denote leptonically and hadronically decaying τ leptons, respectively.

A boosted decision tree (BDT) multivariate analysis technique is used to discriminate the signal from the large backgrounds and the BDT output distribution is used as a final discriminant. The events are categorized to enhance signal topologies, where VBF-like topologies (with two additional jets in the forward regions of the detector) and a $\tau\tau$ system recoiling with large transverse momentum against a jet (boosted system) have the highest sensitivity.

The final result of the analysis shows a $H \to \tau\tau$ signal with a significance of 4.1σ, compared with an expected significance of 3.2σ. The excess above the Standard Model backgrounds is shown in Fig. 3.3, where the reconstructed invariant $\tau\tau$ mass distribution is shown. The excess of events in this mass distribution is consistent with the expectation for a Standard Model Higgs boson with m_H = 125 GeV. The ratio of the measured signal strength to the Standard Model expectation is found to be $\mu = 1.4^{+0.5}_{-0.4}$. This constitutes direct evidence of the decay of the Higgs boson to fermions.

The groups from Freiburg have contributed significantly to the optimization and definition of the event categorization (VBF category, boosted category) and to the estimation of important backgrounds. In particular, they played a leading role in the estimation of the dominant and irreducible $Z \to \tau\tau$ background using the so-called embedding technique, where this background is estimated using $Z \to \mu\mu$ events in real data.

Also searches for $H \to b\bar{b}$ decays have been performed using the full dataset recorded by the ATLAS experiment [jak5]. The processes considered are associated $W/Z)H$ production, with $W \to \ell\nu$, $Z \to \ell\ell$ ($\ell = e, \mu$) and $Z \to \nu\bar{\nu}$ decays. No significant excess is observed above the Standard Model background. The ratio of the measured signal strength to the Standard Model expectation is found to be $\mu = 0.2 \pm 0.5(\text{stat}) \pm 0.4\,(\text{syst})$. The analysis procedure is validated by a measurement of the yield of di-boson $((W/Z)Z)$ production, with $Z \to b\bar{b}$, from which the ratio of the observed signal strength to the Standard Model expectation is found to be $\mu_{VZ} = 0.9 \pm 0.2$. The distribution of the invariant mass of the $b\bar{b}$ system, after subtraction of all backgrounds except for the di-boson process, is shown in Fig. 3.4.

Also to this analysis the Freiburg group has contributed significantly. The focus of the activities was on the study of the $WH \to \ell\nu\, b\bar{b}$ channel, where we contributed to the optimization of the selectrion criteria and to the estimation of various backgrounds in a combined fit. At present we are working on analysis improvements by setting up a multivariate analysis to better exploit different correlations in signal and background events.

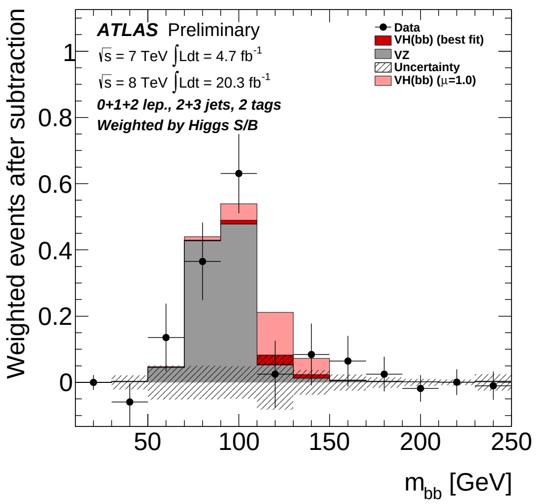


Figure 3.4: Distribution of the invariant mass of the $b\bar{b}$ system, $m_{b\bar{b}}$, after subtraction of all backgrounds except for the di-boson process.

An important question is whether the observed Higgs boson is indeed the Standard Model Higgs boson or whether it shows properties that would indicate physics beyond the Standard Model. Based on the full data set collected so far, the ATLAS collaboration has measured important properties, like signal strengths for the various decay modes and coupling factors to bosons and fermions. So far all properties agree -within the present experimental and theoretical uncertainties- with the predictions of the Standard Model. As an example, the fitted signal strengths separated for the individual bosonic and fermionic channels as well as for the combination of the bosonic channels are summarized in Fig. 3.5.

The continuation of such measurements and the precise determination of the profile of the Higgs boson will be a main focus of analyses in the upcoming Run-2 at the LHC, which is scheduled to start at a

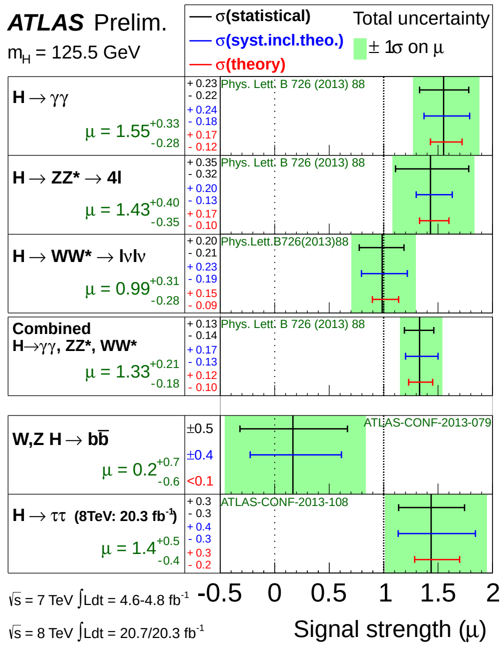


Figure 3.5: The measured production strengths normalized to the Standard Model expectations, for the $H \to \gamma\gamma$, $H \to ZZ^* \to 4\ell$, $H \to WW^* \to \ell\nu\ell\nu$ final states and their combination together with the preliminary signal strength measurements for the $H \to b\bar{b}$ and $H \to \tau\tau$ final states. The measured production strengths are at mH=125.5 GeV.

higher centre-of-mass energy of $\sqrt{s}$ = 13-14 TeV in 2015.

$A/H \to \tau\tau$ and $H^+ \to \tau\nu$: Based on the expertise on the τ performance, the groups of K. Jakobs and M. Schumacher were able to contribute already in the early phase of data analysis to the search for heavy neutral and charged Higgs bosons with decays into final states with τ leptons. The data were found to be compatible with the expectations from Standard Model processes and important cross-section limits and limits in the MSSM parameter space could be set [msch1, msch2, msch6, msch8].

In the search for $A/H \to \tau\tau$ already with the data collected in the year 2010 the limits superseded those obtained at the Tevatron ([msch1]) and they could be improved significantly with the inclusion of more data collected in 2011 ([msch6]). Also the search for $H^+ \to \tau\nu$ based on data collected in 2011 improved the limits obtained at the Tevatron significantly [msch2]. The data collected at $\sqrt{s}$= 8 TeV in 2012 allowed to improve the exclusion and for the first time probe charged Higgs boson masses larger than the top-quark mass [msch8]. Our group contributed to all aspects of the analyses in particular to the estimation of the dominant backgrounds using the embedding technique.

3.2.2 The Search for Supersymmetry

Besides the study of the mechanism for electroweak symmetry breaking, a second focus in the data analysis is 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 resolves 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 in 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. The approach taken in Freiburg is to follow three main analysis strategies.

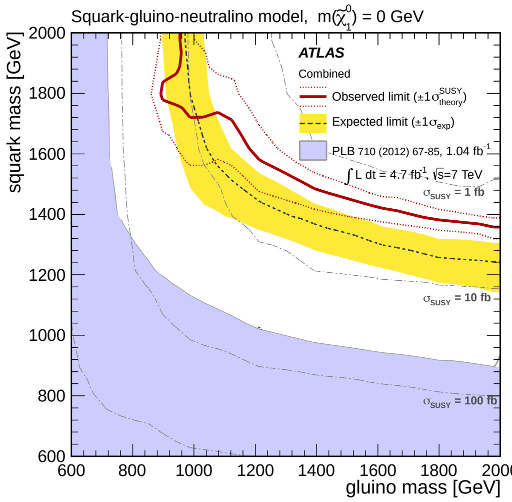


Figure 3.6: The 95% CL exclusion limits on the ($m_{\tilde{g}}$, $m_{\tilde{q}}$)-plane in a simplified MSSM scenario with only strong production of gluinos and first- and second generation squarks, with direct decay to jets and neutralinos [her8]

The first strategy uses inclusive searches based on a generic signature with leptons, jets and missing transverse momentum [her1, her2], 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 1st and 2nd 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 and with additionally one lepton or two leptons with the same electric charge [her4, her5]. 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.

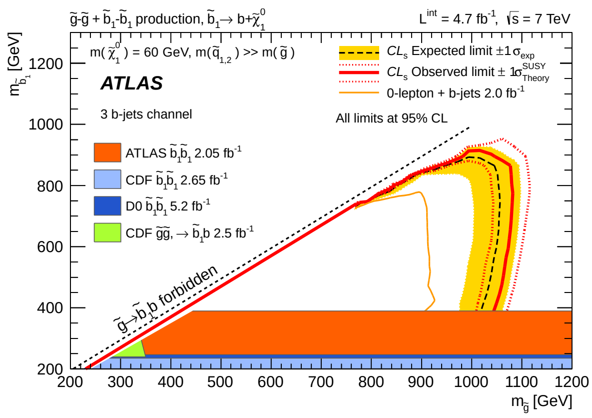


Figure 3.7: Exclusion limits in the ($m_{\tilde{b}} - m_{\tilde{g}}$)-plane for the gluino-sbottom model. The dashed black and solid bold red lines show the 95% CL expected and observed limits respectively [jak10].

As an example, Fig. 3.6 shows the published ATLAS result for the event category with jets and missing transverse momentum [her8] based on data corresponding to an integrated luminosity of 4.7 fb^{-1} collected at a centre-of-mass energy of 8 TeV. The red line shows the 95% exclusion limit in the ($m_{\tilde{q}}, m_{\tilde{g}}$)-mass plane. In the model considered, gluino and squark masses below 860 GeV and 1320 GeV, respectively, are excluded. This analysis alone excludes many SUSY models, which have been proposed before the start of the LHC. The inclusive searches using leptons obtain similar limits. They offer an additional sensitivity for cases where the gluino decays further into lighter supersymmetric particles, like 3rd generation sbottom ($\tilde{b}$) and stop quarks ($\tilde{t}$), which are expected to be light in several scenarios due to quark-mixing effects.

This interesting scenario of light stop masses is addressed in Freiburg in more detail using a search for events with one or more jets containg b-quarks, which are expected from sbottom and stop decays. The specific expertise in Freiburg in b-tagging is utilised to optimise this search strategy, resulting in many contributions to various ATLAS publications [jak6, jak7]. As an example Fig. 3.7 shows the results of a specific search for events containing three b-jets and missing transverse momentum. No excess of events is observed and the measurement is interpreted in a model which assumes gluino pair production with a subsequent decay into sbottom or stop quarks. The red line in the diagram shows the 95% exclusion limits for sbottom and gluino masses, which are much improved compared to previous results from the ATLAS experiment and from the Tevatron experiments.

Since no signal is observed in the channels via the strong production of gluinos and 1$^{\rm st}$ or 2$^{\rm nd}$ generation squarks, the second search strategy performed in Freiburg aims at direct production of sbottom and stop quarks [jak7]. The cross sections are typically one order of magnitude smaller than for gluino pair production. Depending on the squark masses a large spectrum of final states has to be considered to cover the full parameter space. A systematic search approach has been undertaken in the ATLAS collaboration, in which the Freiburg team has contributed in several channels in the low and high sbottom and stop mass regime and for decays into neutralinos or charginos [her6]. A summary of ATLAS results in these searches is presented in Fig. 3.8, with decays into charginos on the left and into neutralinos on the right side. These results were the highlight of many scientific conferences and have triggered a lot of interest of theorists. Stop mass limits up to 650 GeV have been set in these channels and an intensive research is ongoing how to address the diagonal regions in the figure, where the decay products have small kinetic energies and are therefore difficult to separate from the background.

In the third search strategy in Freiburg a model-independent general search is explored to investigate many different final states. Systematically, final states with various combinations of leptons, jets, missing transverse momentum and photons have been categorised and searched for excesses compared to the Standard Model expectations. Although this search method is less sensitive to specific models than dedicated searches, it provides a model-independent approach to detect something unexpected. As an example, Fig. 3.9 presents the results for event classes with electrons and photons [her10]. The black crosses show the measured number of event classes with a given p-value, which is in good agreement with the Standard Model expectation. So far, no new class of events has been observed in these searches. The current research activities in Freiburg and in the ATLAS collaboration in general concentrate on improving the published results using the full data set corresponding to an integrated luminosity of of $\sim$ 20 fb^{-1} at $\sqrt{s}$ = 8 TeV and applying improved selection and reconstruction algorithms. The aim is to publish the results based on the full dataset in early 2014. Following that, the search strategies will be modified and applied to the upcoming LHC data taking at $\sqrt{s}$ = 13-14 TeV. This substantial increase in collision energy will provide a new window to search for physics beyond the Standard Model.

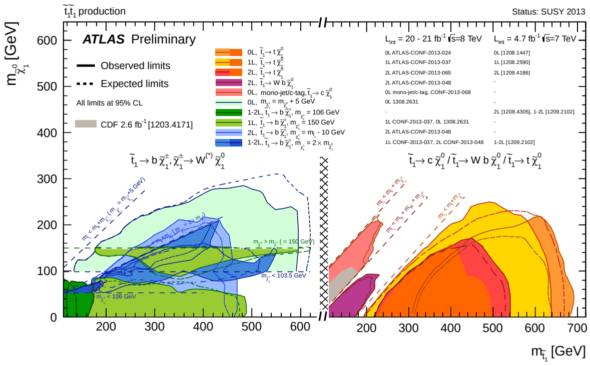


Figure 3.8: Exclusion limits at 95% CL from several searches for direct stop production in the $(m_{\chi_1^0} - m_{\tilde{t}_1})$-mass plane. The dashed and solid lines show the expected and observed limits, respectively.

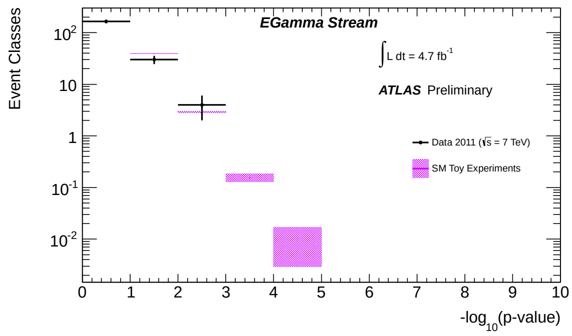


Figure 3.9: The observed and expected number of classes in the e/γ stream having a given range in -log10(p-value). The band for the Standard Model (SM) toy experiments represents the uncertainty, due to the statistics of the toy experiments, on the mean expected number of classes [her10].

3.2.3 Tests of the Standard Model

Another focus in the data analysis lies in the measurement of important Standard Model processes and thereby in precise tests of theoretical predictions (group K. Jakobs). All processes considered are in the area of W and Z boson production, where both electroweak as well as QCD aspects can be tested. The understanding of these processes is also of high relevance for the searches for Higgs bosons and supersymmetric particles.

The Freiburg group contributed significantly to precise measurements of production cross sections of W bosons [jak8]. After the inclusive measurement based on early data collected in 2010, we participated in the improved measurements of differential cross sections, as a function of the pseudorapidity η_ℓ of the lepton during 2011 [jak8]. The major contributions were in the estimation of the background from multijet production via QCD processes and in the important unfolding of detector effects. The results for the differential cross section dσ / d$|\eta_\ell|$ for W^+ production are shown in Fig. 3.10. They are compared to NNLO theory predictions using various parametrizations of the parton distribution functions. The ratio of theoretical predictions to data is also shown.

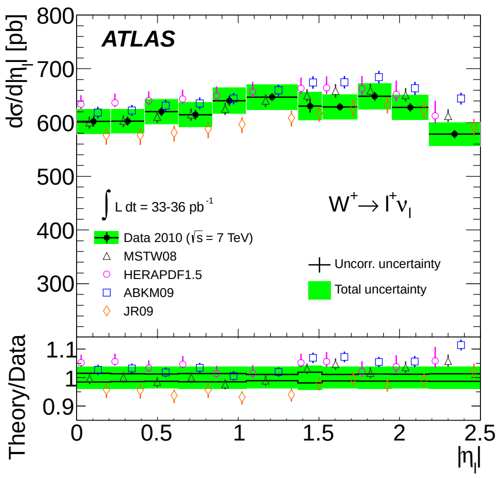


Figure 3.10: The measured differential cross section dσ / d$|\eta_\ell|$ for $W^+ \to \ell^+ \nu$ compared to the NNLO theory predictions using various parametrizations of the parton distribution functions.

These measurements are also important to constrain the parton distribution functions. Further measurements, which were carried out in our group in this domain, are the measurement of the charge asymmetry in W production, i.e. $(\sigma(W^+) - \sigma(W^-))/(\sigma(W^+) + \sigma(W^-))$, and the associated production of W bosons with jets, in particular with jets from heavy quarks. At present we are about to finalize a publication on the associated production of W bosons with c quarks. This measurement will provide further important constraints on the s quark contribution in the proton.

Another publication which was entirely made by our group and which attracted much attention in the theory community of Monte Carlo experts, constitutes the first measurement of the k_T cluster splitting scales in W boson production at a hadron collider. It provides important information for the building of tuning of Monte Carlo generators for LHC physics.

During the early phase of the data-taking, before sensitivity in the $H \to \tau\tau$ search was reached, we contributed in a leading role to the first measurement of $Z \to \tau^+\tau^-$ production (groups of K. Jakobs and M. Schumacher). A cross section consistent with those measured in the electron and muon decay modes and with NNLO theory predictions was measured [msch10].

3.2.4 Detector Performance and Simulation

The Freiburg groups have also contributed in many aspects to the so-called combined performance groups in ATLAS. The work in these groups concerns the understanding and optimization of the reconstruction and identification of the basic detector signatures (e, μ, τ, jets and missing transverse energy as well as b-tagging) which are essential for any analysis. The major contributions to the performance are briefly summarized in the following:

- Contributions to the reconstruction algorithms of τ leptons and the determination of the τ energy scale;
- Calibration of the calorimeter energy scale using E/p matching for single hadrons;
- Measurement of the electron reconstruction efficiency and calorimeter shower shapes using the so-called tag-and-probe method for $Z \to e^+e^-$ events;
- Contributions to b-tagging, with the development of the so-called Jet-Fitter algorithms and to the calibration of b-tagging algorithms with real data;
- Major contributions, partially in leading roles, to the fast detector simulation program ATLFAST. In particular the parametrization of electromagnetic and hadronic showers in the ATLAS calorimeters were carried out in Freiburg.
- Development and testing of the embedding method for $Z \to \tau\tau$ and $t \to b\tau\nu$ events.

3.3 Analysis of COMPASS Data

The COMPASS detector is a fixed target spectrometer situated at an extraction beam line of the CERN SPS. The main aim of the experiment is a detailed investigation of the spin structure of the nucleon. Polarised muons are scattered off *longitudinally* or *transversely* polarised ammonia (NH_3) or deuterated lithium (LiD) targets with high degrees of polarisation. Scattered muons and in the reaction produced photons, electrons and hadrons are detected with an open, two-stage spectrometer and are identified with muon filters, calorimeters and a ring-imaging Cerenkov counter (RICH).

The main physics topics which have been addressed by the Freiburg group within COMPASS are experiments with muon beams. Our analyses concern:

- the helicity structure of the longitudinally polarised nucleon with emphasis on its decomposition into quark helicities and gluon polarisation,
- the transverse spin structure of the transversely polarised nucleon with emphasis on its decomposition into quark transversity distributions,
- measurements of the exclusive production of photons or ρ^0 mesons in the final state (Deeply Virtual Compton Scattering, or Hard Exclusive Meson Production), and finally
- an investigation of hadron multiplicities in scattering off unpolarised nucleons for a better understanding of fragmentation functions.

In addition, hadron beams (typically consisting of 97% pions and 3% kaons) have been used for diffractive and central production with the aim of studying meson and baryon spectroscopy and eventually providing evidence for exotic hadrons, and for a determination of the polarisabilities of the pions and kaons.

In the following those results of the COMPASS collaboration are presented and discussed, to which our group in Freiburg has contributed substantially. For our hardware contributions to the experiment we refer to Section 3.5.

Since the early 1980ies it became apparent that the quark spins do not account for the total spin $\hbar/2$ of the nucleon, as anticipated in the naive constituent quark model, see Fig. 3.11. In the last decade COMPASS has precisely determined the total helicity contribution of quarks to the nucleon spin to be $\Delta\Sigma = (31 \pm 4)\%$, thus not saturating the sum rule $J/\hbar \equiv 1/2 = \Delta\Sigma/2 + \Delta G + L_q + L_g$, where ΔG ist the gluon polarisation and L_i are possible angular momentum contributions from quarks and gluons.

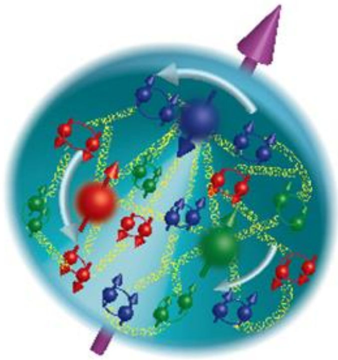


Figure 3.11: Artists view of quarks in a nucleon. Depicted are the three valence quarks in red, green and blue with the spin of the red quark accounting for the nucleon spin. In this picture quark-antiquark pairs and gluons do not contribute to the nucleon spin.

The next important step was clearly the determination of the **Gluon Polarisation in the Nucleon**. The measurement [koe1] of two hadrons with large transverse momenta in the final state yields a (in x_g differential) gluon polarisation of $\Delta g/g = 0.13 \pm 0.06 \pm 0.06$ for gluon momentum fractions $0.04 < x_g < 0.27$, with no significant dependence on x_g observed, see Fig. 3.12, where the data points are split for different regions in x_g. It should be noted that for this analysis a proper understanding of the p_T spectra is mandatory in order not to rely too heavily on Monte Carlo simulations. Therefore a detailed comparison between measured p_T spectra and perturbative QCD calculations was performed in Ref. [koe2].

A second extraction [koe3] of the gluon polarisation was performed by analyzing open-charm production, i.e. D and D* mesons, resulting in $\Delta g/g = -0.06 \pm 0.21 \pm 0.08$ for $0.06 < x_g < 0.22$, see Fig. 3.12. This analysis was performed at leading order in QCD, where the only process producing open-charm is photon-gluon fusion. At next-to-leading-order more processes contribute. Nonetheless, the extracted gluon polarisation, $\Delta g/g = -0.13 \pm 0.15 \pm 0.15$ for $0.12 < x_g < 0.33$, is in good agreement with the leading order result, indicating no significant modification of the gluon polarisation from higher orders in QCD.

Including the latter value of ΔG in a NLO QCD fit to the world data on polarised parton distributions results in [koe3] $\Delta G = 0.24 \pm 0.09$ integrated over the full range of x_g. Therefore, all analyses of the gluon polarisation indicate that it is rather small,

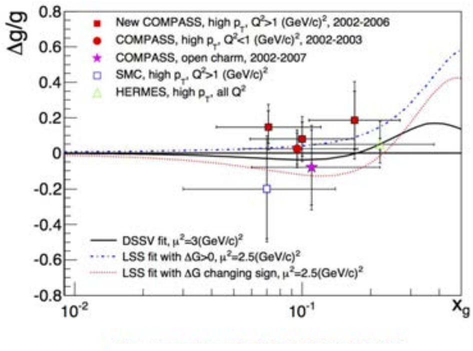


Figure 3.12: A compilation of gluon polarisation measurements. The red star denotes the result of the COMPASS open charm analysis, obtained at LO accuracy. Full red squares denote COMPASS results for high-p_T hadron production for $Q^2 > 1$ (GeV)^2 while a full red circle corresponds to an analysis with $Q^2 < 1$ (GeV)^2. The horizontal bars mark the range in x_g for each measurement, the vertical ones give the statistical precision or the total uncertainties.

$|\Delta G| \lesssim 20\%$. Adding this value to the quark helicity contributions does not saturate the nucleon spin. Thus angular momentum contributions are necessary.

One possibility to access **Orbital Angular Momentum Contributions** to the nucleon spin is a measurement of the so-called Sivers asymmetry with transversely polarised targets: The $\sin(\Phi_{\text{Hadron}} - \Phi_{\text{Spin}})$ modulation of the transverse target spin asymmetry is found to be positive for positively charged hadrons [koe4]. This constitutes a clear indication of a spin-orbit coupling of quarks inside a transversely polarised hadron. Another measurement [koe5, koe6] sensitive to angular momenta is the hard exclusive production of ρ_0 mesons off a transversely polarised target. The same sinusoidal modulation of the measured asymmetry is here sensitive to a Generalised Parton Distribution, which is related to the orbital angular momentum of quarks in the nucleon. Unfortunately, the current experimental precision of this measurement does not constrain the orbital angular momenta of quarks.

Measurements with transversely polarised targets provide the means to determine the **Transverse Quark Spin Contributions** [koe7, koe8]. It turns out that the u- and d-quark distributions are non-zero in the valence quark region and that they are similar in shape but only half as large as the corresponding helicity distributions, as determined for a longitudinally polarised nucleon. In a non-relativistic proton both distributions are expected to be the same, since boost and rotation operators commute. Their different size directly points to the importance of relativistic effects. Due to angular momentum conservation, gluons do not contribute to the transverse spin of the nucleon. Thus the remainder of $1 - 0.5\,\Delta\Sigma \simeq 85\%$ must be carried by the angular momentum of quarks. The determination of the latter quantity will be one of the main challenges for the future of COMPASS.

During the last three years our engagement in the CAST Collaboration had come to an end. The **Search for Axions** arising in the inner core of the sun was extended by using ^{3}He as buffer gas in the bore of a LHC magnet. With gas, coherence in the axion-to-photon conversion can be restored and the sensitivity can be extended to higher axion masses with respect to previous searches with vacuum in the bore. Final results [koe9, koe10] from this campaign set upper limits on the axion-to-photon coupling constant of $g_{a\gamma} < 3 \times 10^{-10}$ GeV^{-1} at 95% CL for axion masses $0.39 < m_a < 1.17$ eV. The region below 0.4 eV was already excluded by the previous CAST measurements with vacuum in the magnet bore. With the new results part of the parameter space of axion models could be excluded for the first time ever. More importantly, this search finally closes the window on axions as candidates for hot dark matter, which requires axions to have a mass $m_a < 0.9$ eV.

3.4 Theory

3.4.1 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, the frontier in predictions at NLO (one-loop level) involves 4 to 6 particles at hadron colliders, depending on the level of complexity of the process. This is the situation after the previous five years, in which the field of perturbative calculations experienced tremendous progress, often called the “NLO revolution”. The groups of S. Dittmaier and H. Ita contributed to this development 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, double precision would not lead to sufficiently precise results in certain regions of phase space.

The group of H. Ita took part in novel developments of unitarity techniques aimed to deal with these challenges (see Ref. [ita6]). These approaches restructure computations using tree amplitudes as the minimal building blocks as opposed to individual Feynman diagrams. This packaging allows to exploit numerically stable and effective tree algorithms at an early stage of the computation. In a second step universal field-theory properties (factorization and unitarity) are used to assemble the final result. In an international collaboration the group achieved one of the first numerically stable implementations of the new methodology with the BLACKHAT program. Since then the effectiveness of the methods has been demonstrated in cutting-edge phenomenological studies of the $pp \to V + (n \leq 5)$-jets processes [ita10, ita7, ita2] including NLO QCD effects. The $pp \to V + 5$-jets process is one of the most complicated ones done so far at NLO in QCD. Moreover, the group provided predictions of $(n \leq 4)$-jet production [ita4].

These computations are not only phenomenologically important, but also serve as a proof-of-principle of the methodology in the high-multiplicity regime. By now the preparatory work towards the automation of non-standard assembly of loop amplitudes could be concluded [ita5]. A broad automation of the approach for generic process signatures is well within reach.

Alternative to the novel approaches employing unitarity cuts of amplitudes, the Dittmaier group refined and further advanced the more traditional Feynman-diagrammatic approach in various directions. Completing earlier work on the fast and numerically stable evaluation of one-loop tensor integrals, Ref. [dit10] presents explicit results of the most general regular and singular 4-point scalar functions with complex internal masses, which are required for the description of unstable particles (resonances). These results are the most complicated analytic building blocks in one-loop amplitudes, both in Feynman-diagrammatic and unitarity-based approaches. They were, in particular, essential in the (diagrammatic) calculation [dit9] of NLO QCD corrections to the process of off-shell top-quark pair production, $pp \to WWb\bar{b} \to \ell\nu\ell'\nu' b\bar{b}$, which represents the first NLO calculation of $2 \to 4$ type with resonances at the LHC.

Finally, phenomenological issues in particle physics often touch upon conceptual problems of quantum field theory. For instance, this is the case in all processes involving unstable particles appearing as resonances whose proper treatment requires perturbative resummations, i.e. some mixing in the perturbative counting, which jeopardize the gauge invariance of the final results, and thus its self-consistency. A few convincing procedures for different situations exist, such as the “complex-mass scheme” for fixed-order NLO calculations, proposed by A. Denner, S. Dittmaier et al. some years ago, but we do not yet have a fully practicable quantum field theory of unstable particles. For instance, resummations potentially involve non-perturbative uncertainties due to tachyonic poles in renormalon calculations. Such resummations have been studied in the van der Bij group [vdb8].

3.4.2 Electroweak Symmetry Breaking and Higgs Physics

Since many years the group of S. Dittmaier contributes to precision calculations for the production and decay of the Higgs boson in the Standard Model 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. The group was co-chaired by S. Dittmaier from 2010 to 2012. 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 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 [dit8, dit4] and were already used in the experimental analyses leading to the discovery of the Higgs boson in 2012.

Exemplarily, Fig. 3.13 illustrates some results of Ref. [dit5] on Higgs-strahlung, i.e. on Higgs-boson production in association with a weak gauge boson W or Z, decaying into different leptonic final states. Specifically, the transverse-momentum distribution of the Higgs boson and the corresponding relative electroweak radiative corrections are shown, as obtained with the Monte Carlo program HAWK, which is developed within a team in which Freiburg particle theory plays a key role. The electroweak corrections mod-

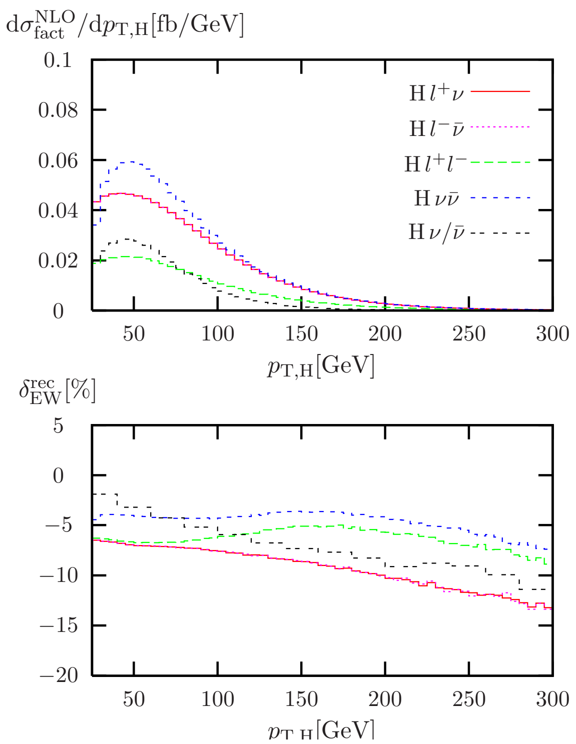


Figure 3.13: Transverse-momentum distribution of the Higgs boson (upper plot) produced via Higgs-strahlung at the LHC, $pp \to WH/ZH \to ll/l\nu/\nu\nu + H$, and corresponding electroweak corrections (lower plot). (Taken from Ref. [dit5].)

ify the cross section at the level of $5-15\%$, which is to be compared to an overall theoretical uncertainty of a few percent, and turn out to depend both on the shape of the distribution and on the specific leptonic gauge-boson decay. These features underline the importance of dedicated higher-order calculations properly taking into account particle decays and full kinematic information. Corrections of the strong interaction (not shown here) modify the Higgs-strahlung cross section additionally at the order of $\sim 30\%$. Even loop-induced contributions from gluon–gluon fusion, which we have investigated at the two-loop level in Ref. [dit2], contribute about $\sim 5\%$ to the cross section.

Alternatives to electroweak symmetry breaking as implemented in the Standard Model via the Higgs mechanism are worked out and investigated in the group of J. van der Bij. The discovery of a Higgs boson at the LHC in 2012 completes the particle spectrum of the Standard Model and essentially excludes the existence of a fourth generation of matter fermions (see e.g. Ref. [dit6]). With the properties of the Higgs boson reasonably well measured and also taking into account that the LHCb measurements give no indication of new flavour physics, extensions of the scalar sector are seriously limited. Within these limits it is, however, important to study possible extensions that could explain features of Nature. We focus on extensions that preserve to a large part the fundamental structure of the Standard Model, in particular singlets and inert triplets.

Pure singlet extensions have been studied in Refs. [vdb3, vdb9, vdb10]. In the first of these papers we showed that in the presence of an extra singlet field the Higgs potential gets stabilized in contrast with the pure Standard Model, for which the vacuum is unstable, given the measured Higgs-boson mass. Interestingly this can be achieved with four-dimensional singlets, but also with higher-dimensional singlet fields without spoiling renormalizability. These so-called HEIDI (=High-D(imension)) models were extensively classified in Ref. [vdb10]. They have an interesting feature: Besides the ordinary Higgs field, which has a somewhat reduced production cross section compared to the Standard Model, they contain another Higgs boson with a small cross section that is invisible. This signal of an invisible Higgs boson with a cross section of about 10% of the Standard Model is undetectable at the LHC and its possible upgrades. They could, however, be studied at the recently proposed TLEP accelerator [vdb4]. Combining precision measurements with the Higgs measurements at the LHC, it was shown that strongly interacting physics cannot be present in the Higgs sector [vdb9] in a way that could be studied in any foreseeable collider.

In a more conventional extension with a singlet and an inert triplet [vdb1], motivated by grand unification, we constrained the parameter range by dark-matter search experiments. The signal of such a dark-matter candidate at the LHC can be quite subtle, consisting of missing energy and a soft pion.

3.4.3 Precision Physics with Electroweak Gauge Bosons and Jets

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. Hence, those processes allow for precision studies of properties of the W and Z bosons, in particular, of their non-Abelian self-interations 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 S. Dittmaier calculates electroweak 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. The recently published results on Z+jet [dit7] and W-pair production [dit1] underline the importance of those effects, which impact observables in the TeV range, where new-physics effects are potentially expected, at the level of some $\sim 30\%$.

Similarly, but to some lesser extent in precision, the physics of jets offers precision QCD studies and has to be controlled as background to searches as well. As another ingredient of precision, we are conducting the calculation of electroweak corrections to jet production, with first results published in Ref. [dit3]. The NLO electroweak corrections turn out to be of the expected size of the currently calculated next-to-next-to-leading-order QCD corrections, reaching the 10% level in the interesting TeV range.

3.4.4 QCD Corrections to Many-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 to the reach of searches for new-physics signals.

In the recent years we could contribute theory predictions to a number of process signatures including $pp \to t\bar{t} \to WWbb \to \ell\nu\ell'\nu'bb$ [dit9], pure multi-jet signatures as well multi-jet production in association with vector bosons [ita10, ita7, ita4, ita2] including NLO QCD corrections. With our computations we could push the state-of-the-art of NLO computations several times providing the first computations for $2 \to 4$ particle scattering (2005 for e^+e^-, 2009 for pp scattering, both by S. Dittmaier et al.), then including five [ita7, ita5] and most recently six final-state objects [ita2].

Proton-proton collisions are multi-layered processes running through a number of physical stages such as the proton break-up, hard scattering, subsequent showering and hadronization, particle decays and, finally, the particle detection. We have been focusing on the theoretical description of the central hard scattering part of the collision using a first principle parton-level description. These computations are a central ingredient in the full event simulation and have been a bottleneck to reducing the theoretical uncertainties. Moreover, we work on the implementation of our results on the hard scattering into Monte Carlo programs which simulate the full sequence of the particle reaction including hadronisation.

Parton-level predictions are valuable on their own right for dedicated observables such as extrapolations from jet-production ratios [ita2], conversion factors (see e.g., Ref. [ita3]), polarization correlations [ita9], and charge asymmetries which help to directly probe new physics. NLO effects are important for quantitatively reliable predictions in the high-multiplicity range, where large powers of the coupling constants appear. In this case the inclusion of NLO effects has been demonstrated to reduce theoretical uncertainties (combined factorization and renormalization variation) from 100% effects to about 20% [ita2]. For our work we implemented key process classes in the NLO matrix element generator BLACKHAT. The physical results are obtained by interfacing the BLACKHAT program with the SHERPA Monte Carlo program. A comparison of our vector-boson-plus-jets predictions to data is shown in Fig. 3.14. These results show an impressive match between first-principle computations and ATLAS measurements.

In addition to a number of explicit physics analyses, we have directly provided our results to the experimental collaborations. First of all, we helped physics analyses providing conversion and transfer factors in a supersymmetry analysis [ita8, ita3]. Furthermore, we developed an event file format [ita1] for supplying simulated data effectively to experimenters allowing them to adapt jet-parameters, phase-space, couplings, cuts, etc., to their setups.

3.4.5 Standard Model Extensions

The measurements at the LHC put strong limits on possible extensions of the Standard Model. In the group of J. van der Bij we therefore focused on minimalistic extensions where no large classes of new particles have to be introduced and the fundamental structure of the Standard Model is only minimally modified. Such models tendentially are able to explain a number of cosmological anomalies, such as the presence of dark matter or the number of light particle species. They are therefore of interest beyond pure accelerator-based physics.

In Ref. [vdb2] we focused on extensions in the neutrino sector. Because the Higgs boson mass is now known, all predictions of the Standard Model are now definite. As a consequence, the indirect tests (loop effects) can be performed with a higher precision than before. Indeed at the level of per mille effects, we found that the Standard Model does not provide a good fit to the data and found some evidence for the

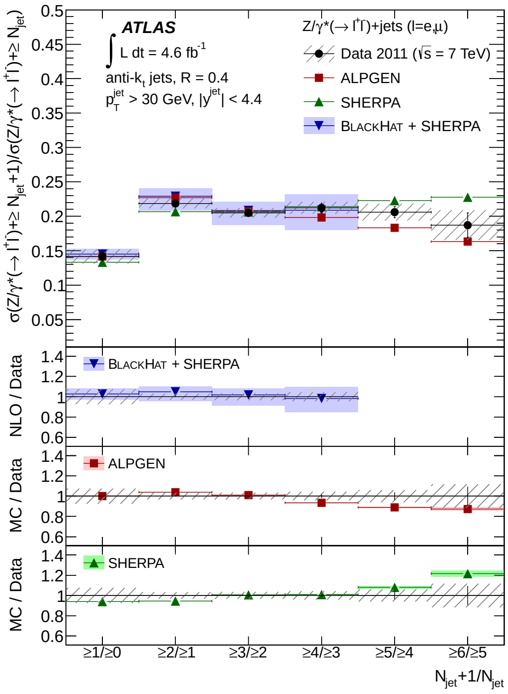


Figure 3.14: Ratio of cross sections for successive inclusive jet multiplicities in $Z(\to \ell\ell)$+jets events. The data are compared to NLO QCD predictions from BLACKHAT+SHERPA and the ALPGEN, SHERPA event generators. The error bars indicate the statistical uncertainty on the data, and the hatched (shaded) bands the uncertainties on data (prediction). For the NLO computations the scale variation dependence is shown which is suppressed in the other predictions. (Taken from `http://arxiv.org/abs/arXiv:1304.7098`.)

presence of sterile neutrinos beyond the three generations of the Standard Model. For this analysis, data from a large number of experiments, also at lower energies, were used. The ongoing improvement of these experiments can make the conclusions more definite.

In Ref. [vdb5] we constructed a simple model with triplet fermions and a singlet Higgs field that can explain a possible excess in the two photon channel in the Higgs signal. Further measurements at the LHC are needed to check whether such an excess is there.

The spectrum of the fermion masses is essentially a mystery. In particular, it is difficult to understand why the neutrinos are so light. For this purpose so-called see-saw mechanisms are postulated, one of which is the so-called inverse see-saw. In Ref. [vdb7] a model was constructed where the inverse see-saw takes place in an automatic way due to the choice of representations. For this an extra Z' boson is needed. There is a subtle interplay between anomaly freedom and the quantum number of the particles. The model can explain the cosmological anomalies and it is fairly unique, containing fermions with fractional lepton number. It can be challenged at the LHC, as Z' bosons and Higgs bosons with masses around the $3-5$ TeV scale are predicted. In Ref. [vdb6] it was shown that unification of coupling constants is possible without supersymmetry in a very simple way, by having a Dirac **24** representation in the theory. In previous work (2007) it was shown that, on the basis of a gravitational anomaly, the gauge group of Nature should be SU(5), including precisely three generations. Supersymmetry would not be allowed. Therefore, the question of unification became urgent. The addition of a Dirac **24** solves the problem and is consistent with the constraints from the gravitational anomaly.

3.5 Detector Development

3.5.1 Development of Semiconductor Detectors

Since about two decades, silicon detectors form the core of the large detector experiments at particle colliders. Driven by increasing luminosity and thereby increasing particle density and occupancy, the requirements for silicon detectors have become more stringent with every new system designed. The group of K. Jakobs has more than ten years experience in the development of silicon particle detectors and has contributed significantly to the current ATLAS silicon strip system.

In the past years, the group has focused on research and development (R&D) and prototyping in the area of silicon detectors for the ATLAS High-Luminosity LHC (HL-LHC) Upgrade. This effort has two main branches: (i) novel detector designs and materials are investigated with the aim of increasing the radiation hardness of the detectors, (ii) module designs and assembly procedures are prototyped for the complicated end-cap section of the future ATLAS strip tracker.

For the ATLAS tracker upgrade, we have prototyped the assembly of modules for the forward strip system. In addition, the front-end electronics hybrid for these modules is developed and procured by Freiburg in a related effort. Figure 3.15 shows the first wedge-shaped prototype forward module made here. The module is equipped with one of our hybrids.

In the research line for novel detectors, we

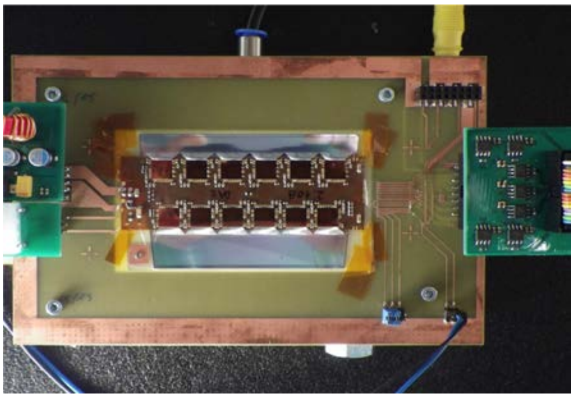


Figure 3.15: Prototype forward module for the ATLAS HL-LHC tracker upgrade. The module is shown in its testing frame with support cards for powering/biasing (left) and read-out (right).

are studying, among others, detectors in a 3D-configuration, where regularly spaced columnar electrodes penetrate deep into the silicon bulk. These electrodes aid both the depletion and the signal collection of the detectors after irradiation and provide a superior radiation hardness when compared to conventional planar detectors. In this 3D design, we also observed an effect of charge multiplication (or gain) for highly-irradiated detectors which previously was not observed in normal silicon particle detectors [jak9]. The charge multiplication effect is beneficial, as it is able to compensate for at least some of the charge lost due to radiation-induced damages in the detector. Current studies investigate to which extent the effect can be used on a larger scale in the silicon detector upgrade of ATLAS.

Another area of research constitutes semiconductor sensors made from high-Z materials such as Cadmium-Zinc-Telluride (CZT). These activities are carried out in collaboration with the Freiburg material research centre (*Freiburger Materialforschungszentrum* FMF). By contrast to the silicon detectors for charged particles described above, these CZT detectors are designed to convert and detect high energy photons, coming from, e.g. radioactive decays or medical X-Ray tubes. Our main ongoing activity in this field is the development of a real time radiation monitoring network as part of the EU-FP7 project REWARD[1]. This project is conducted together with two local partners (the FMF and the company XIE GmbH), and several other European partners coming from industry, academia and civil protection authorities.

[1]www.reward-project.eu

3.5.2 Development of Muon Detectors

In the second long-shutdown (LS2) of LHC in 2018, 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 $2-3 \times 10^{34}$ 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.

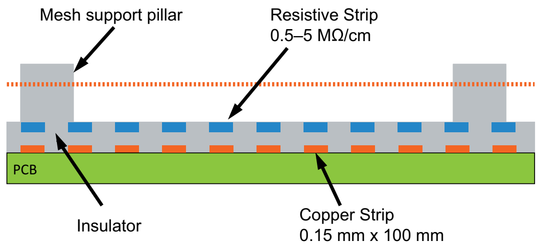


Figure 3.16: Schematic view of the micromegas detectors.

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 layout of the detector is illustrated in Fig. 3.16. 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 $100\ \mu$m has been achieved in test beams with large chambers. The present effort is fully concentrated on developing the final chamber design and on preparing the chamber production in Germany of the 32 MM chambers (chamber type SM2).

The availability in Freiburg of a large 3D coordinate measuring machine (CMM) has proven to be very valuable for the ATLAS experiment. The alignment bars, which provide the 3D reference system for the ATLAS end cap muon chambers, have been produced and measured here with the CMM. This has resulted in an alignment precision of 40 μm in the forward muon system of the present detector. With optical sensors mounted on the bars the position of each chamber with respect to the others is measured, providing a reference frame for all muon chambers.

The detector development activities regarding the muon chambers will concentrate on the NSW until 2018. In the following high luminosity run, the new chambers need to be commissioned and new reconstruction techniques need to be developed for the high rate environment. In parallel a R&D effort for the phase II muon chamber upgrade will start, which is focussed on replacing the chamber and trigger electronics to cope with the high event rate.

3.5.3 Developments in Front End Electronics

For the upcoming measurements of deeply virtual Compton scattering at the COMPASS-II experiment, the existing spectrometer was extended by an additional electromagnetic calorimeter, a new 2.5 m long liquid hydrogen target and by a new recoil proton detector based on scintillating counters surrounding the target. The high intensity beam muon flux produces knock-on electrons in quantity and together with the wide beam halo, these yield background rates of several MHz in the recoil detector counters. This demands a great deal on the front-end and digitization electronics as well as on any low latency trigger which is based upon the recoiled particle. We have developed a modular high speed (1GS/s) and high resolution (>10.5 effective bits) transient recorder system, which allows for trigger decisions based on digital comparisons of signal amplitudes, coincidence times and geometric conditions. Featuring digital pulse processing in real-time to bypass hardware discrimination, the developed firmware resolves pile-up pulses for double or triple signal overlays as soon as the leading edges of consecutive pulses are separated by at least one rise time.

The hit information obtained from the transient recorder system, named GANDALF, is buffered for the subsequent readout. In parallel a data volume reduced version of this hit information is provided as trigger primitives with a fixed latency for the proton trigger subsystem. The trigger primitives from up to 18 GANDALF modules contained in a single VME64x/VXS crate are transmitted via the backplane to the so called TIGER module. TIGER is a high-performance trigger processor that was developed in our group to fit in the GANDALF framework and extend its versatility. The synchronous transfer protocol was optimized for low latencies and offers a bandwidth of up to 8 Gbit/s per link. The centerpiece of the TIGER module is a Xilinx Virtex-6 SX315T FPGA, offering vast programmable logic, embedded memory and DSP resources. It is complemented by an additional dual-port double-data-rate memory, a computer-on-module with an Intel Atom processor and a mobile PCI Express graphics processor mezzanine card, respectively. Besides the VXS backplane ports, the board features two optical SFP+ transceivers, 32 LVDS inputs and 32 programmable LVDS outputs and a Gigabit Ethernet port for configuration and monitoring.

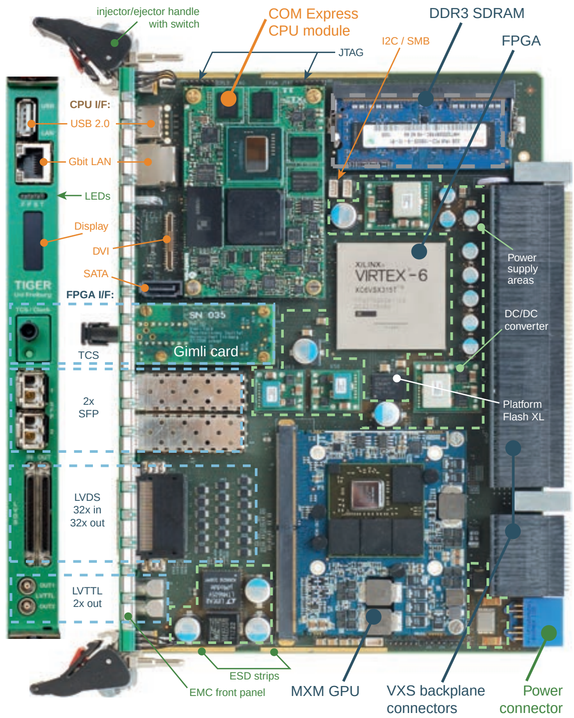


Figure 3.17: Photo of the TIGER module. The dual-port double-data-rate memory (DDR3) and the computer-on-module (COM Express CPU) are located in the upper part while the mobile PCI Express graphics processor unit (MXM GPU) is in the lower part of the module.

The GANDALF module by itself is a 6U-VME64x/VXS carrier board which can host two custom mezzanine cards. Although our initial focus was on the digitization of signals from the recoil detector, we tried to keep the module as general as possible. Exchangeable mezzanine cards allow for very different applications such as analog-to-digital (ADC) or time-to digital (TDC) conversion, coincidence matrix formation, fast pattern recognition or fast trigger generation.

Time-to-Digital Converters (TDC) perform precise time stamp measurements of discriminated signals in time-of-flight or drift-time measurements. In the COMPASS experiment, so far, all the time measurements have been based solely on the F1-TDC ASIC, developed by our group at the turn of the millennium. In the meantime increased input rates and longer trigger latencies for detectors situated next to the muon beam demand for a replacement of the existing digitizing electronics. Our research went towards the implementation of a shifted clock sampling algorithm with 160 ps time bin size realizing the TDC logic purely in FPGA firmware. This approach takes advantage over ASICs in significantly reduced development costs and higher flexibility with respect to the balance between resolution, the dynamic range and the number of channels. A 128 channel TDC firmware has successfully been realized in the main FPGA on the GANDALF module.

Today, the GANDALF framework with all its versatile components is not only used by the COMPASS collaboration but also by the NA62 Experiment at CERN and experiments at JPARC.

3.6 GRID Computing

The huge amount of data collected at the Large Hadron Coller, e.g. at the ATLAS experiment, imposes new challenges to distributed analysis and storage of the data volume. In order to meet these requirements a new information technology called Grid computing has been developed, mainly by particle physicists. The data are distributed and analysed in a hierarchical model which is organised in three levels called Tiers. The Tier-0 centre is located at CERN, ten Tier-1 centres are operated within ATLAS, one being GridKa at the KIT in Karlsruhe. The Tier-1 centres are surrounded by Tier-2 centers called the Tier-2 cloud, where the final data analyses are performed.

The ATLAS cloud around GridKa consists of 12 Tier-2 centres located in Austria (1), Czech Republic (1), Germany (7), Poland (2) and Switzerland (1). Freiburg hosts and operates one of these Tier2 centres (see Figure 3.18) within the ATLAS computing model as part of the World Wide LHC Computing Grid (WLCG). The computing nodes and storage disks provided by Freiburg to the worldwide ATLAS community are shown in the first row of Table 3.1. The pledged resources have increased by 40% over the last three years.

Figure 3.18: The Freiburg ATLAS Tier-2 centre

Besides operating the yearly increasing resources, the group of M. Schumacher has the responsibility for several ATLAS Grid specific tasks in the whole Tier-cloud around the GridKa Tier-1 centre. 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 summarising, reporting and analysing the results of these tests in weekly operation meetings. These tasks are extremely important for the very successful and efficient operation of the whole Tier-2 cloud. In addition, Freiburg is coordinating other specific tasks in the whole cloud and is responsible for the documentation of all services, the status of and developments in the cloud. Significant contributions are also made to the development and installation of the testing framework “HammerCloud“, which has to be adapted regularly to new services and changes in the ATLAS computing model. This tool is used by three major LHC experiments in the WLCG, by ATLAS, CMS and LHCb. In order to meet the increased requirements by the ATLAS experiment after the first long shutdown of the LHC in 2013/14 the resources need to be increased by 25% in 2015 and then by 15-20% for each following year.

The Tier-2 centre is integrated in the interdisciplinary Black Forest Grid (BFG), where 21 groups from five faculties, use the common infrastructure and computer cluster located at the computer centre of the university. The BFG is dominated by the AT-

LAS Tier-2 and other resources from particle physics (see Table 3.1). All participating groups, even if they have only contributed marginally, profit from the large ressources, as in principle all members can use up to 100% for a limited duration, given that the computing power is not required by the other parties.

	Cores		Storage (TB)	
ATLAS Tier-2	1324	43%	1920	86%
Particle Physics	864	29%	288	13%
Other Physics	384	13%	24	1 %
Other Faculties	456	15%	0	0%
Sum	3028		2232	

Table 3.1: Grid resources in the Freiburg Black Forest Grid (BFG).

In the common concept of the universities in Baden-Württemberg for the future of high performance computing in the next five years, a distributed computer cluster located at four university computer centres based on Grid technology is built up. With the research cluster "bwForCluster" each university computer centre will support the activities in a few main research areas in the federation. In Freiburg, the field of particle physics, with its requirement for intensive computing resources, and extensive experience in Grid computing, is one of three research fields.

3.7 Important Publications and Conference Talks

3.7.1 Publications

Group Dittmaier

[dit1] M. Billoni, S. Dittmaier, B. Jäger and C. Speckner, "Next-to-leading-order electroweak corrections to $pp \to WW \to 4$ leptons in double-pole approximation at the LHC," JHEP **1312** (2013) 043.

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3.7.2 Conference Talks

Group Dittmaier

1. C.Schwinn, Higher order threshold effects for top and squark pair production, “Workshop on Heavy Particles at the LHC”, Zurich, January 2011.

2. S. Dittmaier, Higgs search at LHC/Tevatron from a theoretical point of view, Workshop ”Beyond the Standard Model”, Bad Honnef, March 2011.

3. F.Siegert, Recent Developments in Sherpa, “Standard Model@LHC”, Durham, April 2011.

4. C.Schwinn,Higher order threshold effects for top-pair production at hadron colliders, “LoopFest X”, Northwestern University, Evanston (USA), May 2011.

5. S.Dittmaier, NLO QCD and electroweak corrections to Higgs strahlung off W/Z bosons at Tevatron and the LHC with HAWK, “XXIst International Europhysics Conference on High Energy Physics”, Grenoble, July 2011.

6. C.Schwinn, NNLL threshold resummation for the total top-pair production cross section, “Rencontres de Moriond, QCD and High Energy Interactions”, La Thuile, March 2012.

7. F.Siegert, Simulation of prompt photon production in Sherpa, Workshop on Photon Physics and Simulation at Hadron Colliders, Paris, March 2012.

8. S. Dittmaier, NLO QCD corrections to $pp/p\bar{p} \to WWbb$, “LoopFest XI”, Pittsburgh, May 2012.

9. S. Dittmaier, The Quest for the Higgs Boson as a Theory Perspective, 6th Annual Helmholtz Alliance Workshop on “Physics at the Terascale”, DESY Hamburg, Dec 2012.

10. S. Dittmaier, NLO QCD corrections to off-shell ttbar production at hadron colliders, “Loops and Legs In Quantum Field Theory”, Wernigerode, April 2013.

11. S. Dittmaier, Hauptvortrag “Präzisionsberechnungen für den LHC” bei DPG-Tagung, Dresden , March 2013.

12. S. Dittmaier, $O(\alpha\alpha_s)$ corrections to Drell-Yan processes in the resonance region, “RADCOR 2013 - 11th International Symposium on Radiative Corrections”, Lumley Castle, UK, Sep 2013.

13. C.Schwinn, Higher-order soft and Coulomb corrections to squark and gluino production at the LHC, “RADCOR 2013 - 11th International Symposium on Radiative Corrections”, Lumley Castle, UK, Sep 2013.

14. F.Siegert, Sherpa@NLO, “QCD@LHC 2013”, DESY Hamburg, Sep 2013.

15. F.Siegert, Recent MC developments for V+jets production, “6th International Workshop on Top Quark Physics (Top 2013)”, Durbach, Sep 2013.

16. C.Schwinn, Theory precision on the W mass with a WW threshold scan, “Sixth TLEP Worksh”, CERN, Oct 2013.

Group Herten

1. K. Temming, A Setup to Study Properties of Micro-Pattern Gasous Detectors with Laser-Photoelectrons, IEEE 2011 Nuclear Science Syposium and Medical Imaging Conference, Valencia, 2011.

2. J.-E. Sundermann, Search for SUSY in the jets + missing transverse energy channel with zero and one lepton in ATLAS, Phenomenology 2011, Madison, USA, May 2011.

3. M. Rammensee, Search for SUSY in jets plus missing transverse momentum final states with the ATLAS detector 2011, PLHC Conference, Perugia, Italy, June 2011.

4. R. Brunelière, ATLAS Overview of MET Searches, Implications of LHC results for TeV-scale physics, CERN, September 2011.

5. S. Zimmermann, Detector Control System for the ATLAS Muon Spectrometer and Operational Experience after the First Year of LHC Data Taking, ICALEPCS International Conference on Accelerator and Large Experimental Physics Control Systems, Grenoble, 2011.
6. S. Caron, SUSY searches at ATLAS, Rencontres de Moriond, Moriond, France, March 2011.
7. R. Brunelière, Searches for supersymmetry at ATLAS, Les Rencontres de Physique, La Thuile, Aosta, Italy, February 2012.
8. G. Herten, Plenary Talk, LHC Highlights, DPG Frühjahrstagung Göttingen, March 2012.
9. G. Herten, ATLAS Overview, SUSY 2012, Beijing, August 2012.
10. K. Temming, Studies of micromegas chambers using UV-laser-photoelectrons. Nuclear Science Symposium and Medical Imaging Conference (NSS/MIC), 2012 IEEE, 2012: 1768-1778, Anaheim, 2012.
11. V. Consorti, Inclusive searches for squarks and gluinos with the ATLAS detector, Workshop on Physics at the LHC, Kruger National Park, South Africa, December 2012.
12. R. Brunelière, ATLAS BSM Monte Carlo simulation system and strategy, MC4BSM 2013, DESY, Hamburg, April 2013.
13. V. Consorti, Search for squarks and gluinos with the ATLAS detector using final states with jets and missing transverse momentum in 20 fb-1 of sqrt(s)=8 TeV pp collisions, EPSHEP 2013, Stockholm, July 2013.
14. S. Amoroso, Inclusive searches for squarks and gluinos with the ATLAS detector , High Energy Physics in the LHC era, Valparaiso, Chile, December 2013.

Group Ita

1. Ita, H., Latest results for V-boson+jets production at the LHC with BlackHat, Loops and Legs in Quantum Field Theory, Wernigerode, Germany, April 2012.
2. Ita, H., NLO QCD Predictions for Vector-Boson Production, Zürich Phenomenology Workshop, Zürich, Switzerland, January 2013.
3. Ita, H., New methods for perturbative QCD and theories of quantum gravity (invited talk), DPG-Frühjahrstagung 2013, Dresden, Germany, March 2013.

Group Jakobs

1. Hartert, J., W, Z and Diboson production at the LHC with ATLAS, Lake Louise Winter Institute, Canada, February 2011.
2. Köhler, M., Comparative Measurements of Irradiated 3D Silicon Strip Detectors with p- and n-Side Readout, 6th Trento Workshop on Advanced Silicon Radiation Detectors, Trento, Italy, March 2011.
3. Kühn, S., Tau physics in ATLAS, 23rd Rencontres de Blois on “Particle Physics and Cosmology”, Blois, France, June 2011.
4. Parzefall, U., Silicon for High-Luminosity Tracking Detectors, Technology and Instrumentation in Particle Physics (TIPP 2011), Chicago, USA, June 2011.
5. Vivarelli, I., Searches for supersymmetry in jets plus missing transverse momentum final states with the ATLAS detector European Physical Society High Energy Physics Conference, Grenoble, France, July 2011.
6. Venturi, M., Boson and diboson production at ATLAS, 15th Lomonosov Conference on Elementary Particle Physics, Moscow, Russia, August 2011.
7. Fehling-Kaschek, M., SUSY searches in ATLAS, LHC on the March, Protvino, Russia, November 2011.
8. Jakobs, K., Higgs boson searches in the ATLAS experiment - Recent results-, The Zurich phenomenology workshop “Higgs search confronts theory”, Zurich, January 2012.

9. Lohwasser, K., Neues vom Standardmodell - Elektroschwache Präzisionsmessungen an LHC und Tevatron (Hauptvortrag), DPG-Frühjahrstagung Göttingen, March 2012.

10. Bernhard, R., Searches for Standard Model Higgs Boson at ATLAS, XLVIIth Rencontres de Moriond QCD, La Thuile, Val d'Aosta, Italy, March 2012.

11. Betancourt, C., The Punch-through effect in silicon strip detectors 7th Trento Workshop on Advanced Silicon Radiation Detectors, Ljubljana, Slowenien, March 2012.

12. Schmidt, E., Search for the SM Higgs Boson in $H \to WW \to \ell\nu\ell\nu$ with ATLAS, SPRING 2012 - Second MCTP Spring Symposium on Higgs Boson Physics, Ann Arbor (MI), USA, April 2012.

13. Glatzer, J., Higgs decay to fermions in ATLAS, $H \to \tau\tau, bb, \mu\mu$, SM@LHC Conference, Copenhagen (Denmark), April 2012.

14. Ruthmann, N., Physics with Tau Lepton Final States in ATLAS, The XIth International Conference on Heavy Quarks and Leptons, Prague, Czech Republic, June 2012.

15. Jakobs, K., Experimental Conference summary talk, VII. Conference on Physics at the LHC, Vancouver, Kanada, June 2012.

16. Thoma, S., Search for the neutral MSSM Higgs bosons in the $H \to \mu^+\mu^-$ and $H \to \tau^+\tau^-$ decay modes with the ATLAS detector at the LHC, 36th International Conference on High Energy Physics, Melbourne Australia, July 2012.

17. Aad, G., ATLAS measurements of jets and heavy flavour produced in association with W and Z bosons, SUSY 2012, 20th International Conference on Supersymmetry and Unification of Fundamental Interactions, Beijing, China, August 2012.

18. Lohwasser, K., W and Z production and constraints on proton structure from ATLAS, SUSY 2012, 20th International Conference on Supersymmetry and Unification of Fundamental Interactions, Beijing, China, August 2012.

19. Winkelmann, S., Searches for third generation squarks via gluino mediation with the ATLAS detector, SUSY 2012, 20th International Conference on Supersymmetry and Unification of Fundamental Interactions, Beijing, China, August 2012.

20. Barber, T., Upgrading the ATLAS Silicon Tracking for the HL-LHC, 9th International Conference on Radiation Effects on Semiconductor Materials Detectors and Devices, Florence (Italy), October 2012.

21. Betancourt, C., A Charge Collection Study with Dedicated RD50 Charge Multiplication Sensors 9th International Conference on Radiation Effects on Semiconductor Materials Detectors and Devices, Florence (Italy), October 2012.

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25. Parzefall, U., ATLAS Upgrades Towards the High Luminosity LHC: extending the discovery potential, IEEE Nuclear Science Symposium and Medical Imaging Conference, Anaheim (Californien) USA, November 2012.

26. Jakobs, K., Die Entdeckung eines Higgs-artigen Teilchens am LHC (Plenary Talk), DPG-Frühjahrstagung Dresden, March 2013.

27. Weiser, C., $H \to bb$ in ATLAS, “Higgs - Quo Vadis”, Aspen (USA), March 2013.

28. Giuliani, C., Searches for direct pair production of third generation squarks with the ATLAS detector, LHCP 2013, Barcelona, May 2013.

29. Jakobs, K., Higgs boson physics at ATLAS (Plenary Talk), Lepton-Photon Symposium, San Francisco (USA), June 2013.

30. Kühn, S., ATLAS Phase-2 Strip Tracker Upgrade, Vertex 2013, Lake Starnberg, Germany, September 2013.

31. Madar, R., Search for Fermionic Higgs Boson Decays in pp Collisions at the ATLAS and CMS Experiments, The XXXIII international symposium on Physics in Collision (PIC2013), Beijing, China, September 2013.

32. Venturi, M., Probing the spin and parity of the Higgs boson with the ATLAS detector, WIN 2013, Natal, Brazil, September 2013.

33. Balbuena, J.P. et al., Monte Carlo and TCAD Simulation Tools in the Development of Spectroscopy and Pixel Detector Systems based on CdTe/CZT, 2013 IEEE Nuclear Science Symposium & Medical Imaging Conference & Workshop on Room-Temperature Semiconductor X-Ray and Gamma-Ray Detectors, Seoul, South Korea, October 2013.

34. Betancourt, C., Charge Collection Measurements on Dedicated Charge Multiplication SSDs, 2013 IEEE Nuclear Science Symposium & Medical Imaging Conference, Seoul, South Korea, October 2013.

35. Kühn, S., The REWARD Project: Real Time Wide ARea Radiation Surveillance with Semiconductor Detectors, 2013 IEEE Nuclear Science Symposium, Seoul, South Korea, October 2013.

Group Königsmann

1. Schill, C., Azimuthal Asymmetries from Unpolarized Data at COMPASS, Int. Workshop on Deep Inelastic Scattering, Newport News, April 2011.

2. Schill, C., Single Spin Asymmetries at COMPASS with Transverse Target Polarization, Int. Workshop on Deep Inelastic Scattering, Newport News, April 2011.

3. Nerling, F., Spin-exotic Search in the $\rho\pi$ Decay Channel: New Results on $\pi^-\pi^0\pi^0$ (Diffractively Produced on the Proton), Int. Conf. on Hadron Spectroscopy, Munich, June 2011.

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11. Büchele, M., A 128-channel Time-to-Digital Converter (TDC) inside a Virtex-5 FPGA on the GANDALF Module, Topical Workshop on Electronics for Particle Physics TWEPP, Oxford, September 2012.

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14. Herrmann, F., First Measurements Towards GPDs with the COMPASS-II Experiment at CERN, Int. Conference on the Structure of Baryons, Glasgow, June 2013.
15. Nowak, W.D., Transverse Target Spin Asymmetries in Exclusive ρ^0 Muoproduction, Int. Conf. Meson-Nucleon Physics and Structure of the Nucleon, Rome, October 2013.
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4. Lai S., Tracker and Calorimeter Performance for the Identification of Hadronic Tau Lepton Decays in ATLAS, International Conference on High Energy Physics EPSHEP 2011, Grenoble (France), Juli 2011.
5. Warsinsky, M., Search for BSM Higgs Bosons at ATLAS, 26. Rencontres de Physique de La Vallee d'Aoste, La Thuile (Italy) March 2012.
6. Schumacher, M., Searches for Higgs Bosons Beyond the Standard Model at LHC in Comparison to TEVATRON, DESY Theory Workshop 2012, Hamburg (Germany), September 2012.
7. Lai S., Search for MSSM Higgs Search at ATLAS and CMS, Hadron Collider Physics Symposium, HCP-2012, Kyoto (Japan), November 2012.
8. Lai S., Suche nach dem Higgs-Boson des Standard-Modells im Zerfall $H \to \tau\tau$ mit ATLAS (Eingeladener Vortrag), DPG-Frühjahrstagung, Dresden (Germany), March 2013.
9. Boehler M., Searches for BSM Higgs Bosons at the LHC, Rencontres de Moriond QCD and High Energy Interactions, La Thuile (Italy), March 2013.
10. Flechl M., BSM Higgs - experimental results, Large Hadron Collider Physics Conference LHCP 2013, Barcelona (Spain), May 2013.
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3.8 PhD, Diploma and Master Theses

3.8.1 PhD-Theses

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3. Stefan Horner, Searches for Supersymmetry in single-lepton final states with the ATLAS detector and improved background model for the searches for new physics, 2011.

4. Song Xie, A Gas Monitoring Chamber for ATLAS MDTs, 2011.

5. Kathrin Störig, QCD background estimation for Supersymmetry searches with jets and missing transverse momentum with the ATLAS experiment at the Large Hadron Collider, 2012.

6. Michael Rammensee, Search for supersymmetric particles in final states with jets and missing transverse momentum with the ATLAS detector, 2013.

Group Jakobs

1. Jochen Hartert, Measurement of the $W \to e\nu$ and $Z/\gamma^* \to ee$ Production Cross-Sections in Proton-Proton Collisions at $\sqrt{s}$ = 7 TeV with the ATLAS Experiment, 2011. `http://www.freidok.uni-freiburg.de/volltexte/8411/pdf/Dissertation_JochenHartert.pdf`

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3. Inga Ludwig, Electrical tests of silicon detector modules for the ATLAS experiment and a study of the discovery potential of the $t\bar{t}H, H \to W^+W^-$ process, 2011. `http://cdsweb.cern.ch/record/1399602`

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6. Julian Glatzer, Search for Neutral MSSM Higgs Bosons Decaying to $\tau_{had}\tau_{had}$ in $\sqrt{s}$ = 7 TeV Proton-Proton Collisions with the ATLAS Detector, 2013. `http://www.freidok.uni-freiburg.de/volltexte/9204/`

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9. Sascha Thoma, Search for the neutral Higgs Bosons of the Minimal Supersymmetric Standard Model in the $\tau_{lep}\tau_{had}$ decay mode with the ATLAS experiment, 2013. `http://www.freidok.uni-freiburg.de/volltexte/8935/pdf/Thesis_SaschaThoma_2013_01.pdf`

Group Königsmann

1. Florian Herrmann, Development and Verification of a High Performance Electronic Readout Framework for High Energy Physics, 2011.

Group Schumacher

1. Martin Schmitz, Higgs production in Vector Boson Fusion in the $H \to \tau\tau \to \ell\ell + 4\nu$ final state with ATLAS: a sensitivity study, Bonn 2011, Erstgutachter M. Schumacher, Zweitgutachter N. Wermes.

2. Nicolas Möser, A Sensitivity Study for Higgs Boson Production in Vector Boson Fusion in the $H \to \tau\tau \to \ell h + 3\nu$ Final State with ATLAS, Bonn 2011, Erstgutachter M. Schumacher, Zweitgutachter N. Wermes.

Group van der Bij

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2. Valerio Bertone, Higher Order and Heavy Quark Mass Effects in the Determination of Parton Distribution Functions, 2013.

3.8.2 Diploma/Master Theses

Group Dittmaier

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2. M. Hecht, “Predicting $W+\gamma$ Production At The LHC In Next-To-Leading Order QCD Accuracy”, Feb 2012.
3. L. Altenkamp, “QCD Corrections to HZ Production via Gluon Fusion at the LHC”, May 2012.
4. L. Salfelder, “Predictions for 4 Lepton + 2 Jet Production at the LHC”, Juli 2013.
5. L. Forner, “QED Corrections to Dijet Production at the LHC”, Aug 2013.

Group Herten

1. Yusuf Erdogan, Kinematische Rekonstruktion des $t\bar{t}$-Untergrunds in supersymmetrischen 1-Lepton-Endzuständen am ATLAS Experiment, 2011.
2. Roman Karimi, Suche nach Großen Extra-Dimensionen im Monojet-Kanal mit dem ATLAS-Experiment, 2011.
3. Stefan Weber, Aufbau einer Messkammer zur Bestimmung der Eigenschaften von Micro-Pattern Gas Detectors (MPGDs), 2011.
4. Antonia Strübig, Study of phenomenological MSSM models with ATLAS experiment, 2012.
5. Sabrina Bernhard, Gasüberwachung in Gasdetektoren mit Hilfe der Messung von Driftgeschwindigkeiten bei unterschiedlichen elektrischen Feldstärken, 2013.
6. Fabio Cardillo, A general search for new phenomena with the ATLAS detector in pp collisions at $\sqrt{s}=8$ TeV, 2013.

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2. Adrian Driewer, Messungen an planaren, bestrahlten Silizium-Streifendetektoren für den HL-LHC, 2011.
3. Luzie Weithofer, Measurement of the W charge asymmetry in the associated W+jet production, 2011.
4. Hannah Arnold, Messung des Wirkungsquerschnitts der assoziierten Produktion eines W-Bosons mit einem charm-Jet am ATLAS Experiment, 2012.
5. Daniel Büscher, Search for the Higgs Boson in the Channel $WH \to e\nu bb$ using Boosted Decision Trees in Proton-Proton Collisions at $\sqrt{s}$ = 7 TeV with the ATLAS Experiment, 2012.
6. Paul Günther, Studien zur Bestimmung der WW- und $\tau\bar{\tau}$-Untergründe in der Suche nach dem Higgs-Boson im Prozess $H \to WW^* \to \ell\nu\ell\nu$ im ATLAS Experiment, 2012.
7. Philip Sommer, A Measurement of the Electron Identification Efficiency using $W \to e\nu$ Decays in the ATLAS Experiment, 2012.
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10. Helge Haß, Search for the Standard Model Higgs boson in the $H \to \tau\tau \to \ell\nu_{\ell}\nu_{\tau}h\nu_{\tau}$ decay mode in proton-proton collisions at $\sqrt{s}$ = 7 TeV with the ATLAS experiment, 2013.

11. Marc Hauser, Bau und Messung der Funktionalität von Siliziumstreifendetektormodulen für den Ausbau der Endkappen des inneren Detektors am ATLAS-Experiment, 2013.

12. Johanna Nagel, Studies on the $H \to \tau_l \tau_h$ decay mode exploiting the tau_h substructure with data from the ATLAS experiment at the LHC, 2013.

13. Carsten Burgard, Study of Higgs boson production via Vector Boson Fusion in the $H \to WW \to \ell\nu\ell\nu$ decay mode with the ATLAS detector, 2013.

Group Königsmann

1. Maximilian Büchele, Entwicklung eines FPGA-basierten 128-Kanal Time-to-Digital Converter für Teilchenphysik-Experimente, 2012.

2. Tobias Kunz, Entwicklung einer Simulationsumgebung für das COMPASS-II-Experiment mit Geant 4, 2012.

3. Tobias Szameitat, Entwicklung einer Monte-Carlo-Simulation für das COMPASS-II-Experiment, 2012.

4. Tobias Baumann, Entwicklung einer Schnittstelle zur Übertragung von Pulsinformationen eines Rückstoßdetektors an ein digitales Triggersystem, 2013.

5. Steffen Bauer, Analyse der exklusiven tief-virtuellen Compton-Streung am COMPASS Experiment, 2013.

6. Philipp Jörg, Untersuchung von Algorithmen zur Charakterisierung von Photomultiplierpulsen in Echtzeit, 2013.

7. Christoph Michalski, Entwicklung eines Echtzeit-Strahlprofil-Monitoring-Systems für das COMPASS-II Experiment, 2013.

8. Matthias Gorzellik, Entwicklung eines digitalen Triggersystems ür Rückstoßproton-Detektoren, 2013.

9. Michael Kunz, Analyse der virtuellen Photon-Asymmetrie A_2 und der Spin-Strukturfunktion g_2 des Protons, 2013.

10. Robert Schäfer, Charakterisierung eines Detektors zum Nachweis von Rückstoßprotonen am COMPASS Experiment, 2013.

Group Schumacher

1. Vera Stalter, Studien zur kollinearen Näherung für den Prozess $H \to \tau\tau \to ll + 4\nu$ und Messung des Wirkungsquerschnitts für den Prozess $Z \to \tau\tau \to \mu\mu + 4\nu$, 2011.

2. Florian Kiss, Messung des Transversalimpulsspektrums des Z-Bosons im myonischen Endzustand mit dem ATLAS-Detektor, 2011.

3. Anna Kopp, Search for Charged Higgs Bosons in the Topology $tt \to bH^+bW^- \to b\tau\nu bqq$ based on Data taken by the ATLAS Detector in 2010, 2011.

4. Nicole Utecht, Untersuchung der Z-Bosonproduktion mit Zerfall $Z \to \tau\tau \to e\mu + 4\nu$ mit dem ATLAS-Experiment am LHC, 2011.

5. Christian Schillo, Suche nach neutralen Higgs-Bosonen des MSSM im Endzustand $h/A/H \to \tau\tau \to e\mu + 4\nu$ mit dem ATLAS-Detektor, 2011.

6. Julian Maluck, Studien zur Optimierung und Massenrekonstruktion in der Suche nach dem Higgs-Boson des Standardmodells im Zerfall $H \to \tau\tau \to ll + 4\nu$ mit dem ATLAS-Experiment, 2013.

7. Dirk Sammel, Suche nach dem Higgs-Boson des Standardmodells im Zerfallskanal $H \to \tau\tau \to ll + 4\nu$ mit Schwerpunkt in der Higgs-Strahlung mit dem ATLAS-Detektor, 2013.

Part III

Teaching

Chapter caption: BSc students attending the lecture in Experimental Physics 1 held by G. Herten with the assistance of H. Wentsch.

1.1 Overview

The education of prospective physicists and physics teachers in general and specialised subjects is performed by lecturers from the Institute of Physics and the associated institutes according to Humboldt's educational ideal. A broad course programme is offered, which covers topics from fundamental basic principles to practical applications with early exposure to contemporary modern research. Basic knowledge in physics is also needed in many other disciplines. The Institute of Physics offers dedicated lectures and laboratory classes to course programmes in various other faculties.

Currently three modular degree programmes specialising in physics are offered.

- *Bachelor of Science in Physics (BSc)*
  The BSc programme started in winter semester 2008/09. It encompasses six semesters with a total workload of 180 credit points (CP). The degree programme is currently in the process of accreditation.

- *Master of Science in Physics (MSc)*
  The MSc programme started in winter semester 2011/12. It encompasses four semesters with a total workload of 120 CP. This degree programme is also currently in the process of accreditation. The MSc courses are taught in English.

- *Erstes Staatsexamen (first state examination) in teacher-training for secondary schools*
  The programme for prospective secondary school teachers encompasses ten semesters and currently finishes with the *Erstes Staatsexamen* (first state examination) before the prospective teachers start a two-year long internship at a secondary school. Since winter semester 2010/11 new examination regulations apply, and the programme is also modularised with a total work load of 300 CP.

In all degree programmes the lectures are accompanied by several tutorial classes with less than twenty participants each. Enrolment to the diploma degree programme, which encompasses five years, stopped in summer 2008. This degree programme will officially discontinue by summer 2014.

The development of the number of new enrolments in each course programme is summarised in Fig. 1.1 and is commented below. In addition, the PhD degree "Dr. rer. nat." from the joint Faculty for Mathematics and Physics can be awarded. For obtaining a PhD degree no enrolment and no structured course programme is mandatory. Two Research Training Groups, funded by the *Deutsche Forschungsgemeinschaft DFG* (German Science Foundation), are currently hosted and co-hosted at the Institute of Physics: the Research Training Group 1102 "Physics at Hadron Colliders" and the International Research Training Group 1642 "Soft Matter Science: Concepts for the Design of Functional Materials", respectively. The education programme of the participating PhD students includes specialised lectures, seminars, topical workshops and annual conventions. In total approximately 160 PhD students are currently performing the research for their dissertation in physics, about one third at the associated research institutes and in the groups of the co-opted members of the institute.

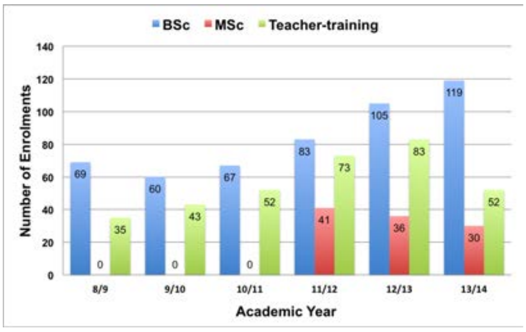


Figure 1.1: Number of new enrolments in the three currently offered degree programmes during the last six academic years.

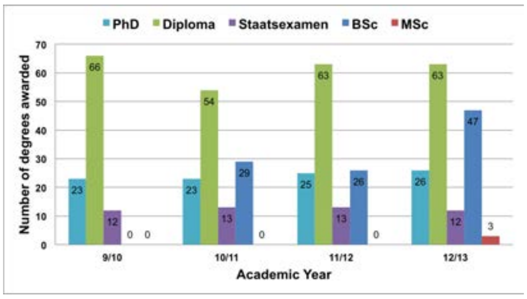


Figure 1.2: Number of degrees awarded during the last four academic years.

The number of awarded Diploma, *Erste Staatsexamen* and PhD degrees has been constant over the last years (see Fig. 1.2). The increase in the number of BSc degrees in the last year is to a large extent due to students, who either changed their place of study to Freiburg during the BSc programme, or who need more than six semesters to finish the course programme, mainly because of their participation in an international exchange programme.

	Mathematics		Theo. Physics	Exp. Physics	Laboratory Courses	Oral Examination	Elective Subjects
1	Analysis 9 CP	LA 1 9 CP		Exp 1 7 CP	Scien. Programming 5 CP		
2		LA 2 9 CP	Theo 1 8 CP	Exp 2 7 CP	Basic Course 1 6 CP		
3			Theo 2 8 CP	Exp 3 7 CP	Basic Course 2 6 CP	Exp 1+2 2 CP	Non-Physics 8 CP
4	Adv. Math. 9 CP		Theo 3 8 CP	Exp 4 7 CP	Exp. Methods 5 CP	Theo 1+2 2CP	
5			Theo 4 8 CP	Exp 5 7 CP	Advanced Course 7 CP		Seminar 4 CP Soft Skills 4 CP
6	BSc Thesis and Colloquium 10+2 CP						Physics 12 CP Soft skills 4 CP

Figure 1.3: Overview of the six semester BSc course programme together with the allocated credit points (CP). (LA - Linear Algebra, Adv. Math. - Advanced Mathematics, Theo - Theoretical Physics, Exp - Experimental Physics, Scien. Programming - Scientific Programming, Exp. Methods - Experimental Methods.)

1.2 Degree Programmes

1.2.1 BSc Programme

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 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 preference of the students. This allows the students to specialise already during the BSc programme and to get a first insight into modern 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. 1.3. The BSc studies are completed by the BSc 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 the work and scientific results in a thesis and a public presentation of the results.

Figure 1.4: Students during the lecture in Experimental Physics 1 in the major lecture hall.

The number of enrolments in the BSc programme has increased significantly over the last years (see Fig. 1.1). At the same time the duration of the edu-

<table>
<tr><th></th><th colspan="2">Compulsory</th><th>Advanced Physics</th><th>Elective Subject</th><th>Term Paper</th></tr>
<tr><td>1</td><td>Advanced QM
10 CP</td><td>Master Laboratory
8 CP</td><td rowspan="2">3 Lectures
in Main
Research Areas
3 x 9 CP</td><td rowspan="2">Physics or from MSc/
MA Programmes of
other Disciplines
9 CP</td><td rowspan="2">Presentation and
Written Handout

6 CP</td></tr>
<tr><td>2</td><td colspan="2"></td></tr>
<tr><td>3</td><td colspan="4">Research Traineeship 30 CP</td><td></td></tr>
<tr><td>4</td><td colspan="2">MSc Thesis 28 CP</td><td colspan="2">MSc Colloquium 2 CP</td><td></td></tr>
</table>

Figure 1.5: Overview of the four semester MSc course programme together with the allocated credit points (CP). (QM - Quantum Mechanics, MA - Master of Arts.)

cation at secondary schools has been changed from nine to eight years, and the abolition of the compulsory military service has taken place. In general, high-school graduates have shown a larger interest in physics during recent years. As there are no specific admission requirements, the drop-out rate is at the level of 40% to 50%. Most of these students leave the challenging course programme already during the first year. This rate is approximately constant since decades and all over 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. The obtained academic records in the BSc physics programme are usually accredited as course achievements in the new discipline.

1.2.2 MSc Programme

The MSc programme is taught in English in order 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 is undertaken by a MSc Admission Committee. The MSc programme 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 one of the current projects of one of the research groups at the Institue 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 semester among various "Term Papers", where they learn to give oral presentations in English on a topic of modern research, accompanied by a written summary in English. Three courses have to be choosen from state-of-the-art topics in the main research areas of the department. 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, or from advanced English classes and classes in scientific writing. During the second year, the students carry out their Research Traineeship project and MSc thesis project. The study programme completes with the submission of the MSc thesis and a public presentation of the results. An overview of the MSc course programme is given in Fig. 1.5.

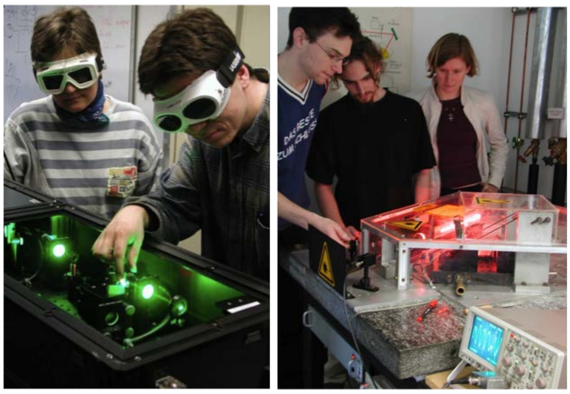


Figure 1.6: Students in the laboratory classes.

We are confident that the number of enrolments in the MSc programme (see Fig. 1.1) will grow in the future. Advertisement of the programme has increased over the last year, e.g. on the web pages of the *Deutscher Akademischer Austauschdienst DAAD* (German Academic Exchange Service). The drop-out rate is at the level of a few percent only.

1.2.3 Teacher-training Programme

Students in the teacher-training programme usually choose two major subjects. The programme comprises classes in the scientific discipline and subject didactics in each of the two major subjects, classes in general educational sciences, ethical-philosophical basic classes, a four-months long internship at a secondary school, and courses in so-called "Personal

			Subject Didactics	Other Courses
4	Adv. Theory 7 CP	Adv. Experiment 7 CP	Basic Course 2 CP	General Educational Science 18 CP Ethical-Philosophical Courses 12 CP Module Personal Competences 6 CP
5	Internship at School 16 CP		Advanced Course 3 CP	
6	Elective Subject 10 CP	Adv. Laboratory 6 CP		
7	Elective Subject 8 CP		Demonstration Laboratory Course 4 CP Oral Exam 1CP	
8	Thesis work in one subject and Final Oral Exam in both subjects 40 CP			
9				
10				

Figure 1.7: Overview of the teacher-training programme from fourth to tenth semester together with the allocated credit points (CP). (Adv. - Advanced)

Competences" at the "Centre for Key Competences". A half-year long thesis project can be performed either in physics or the second major subject. This project, together with the final oral examinations in both major subjects, completes the study programme at the university. An overview of the teacher-training course programme is given in Fig. 1.7. The number of credit points devoted to the scientific discipline in the major subjects is significantly larger compared to the other federal states in Germany. We are convinced, that this constitutes a strength of our current teacher education and should not be compromised in future reformations of the degree programme.

Students with mathematics as second major subject attend the same mandatory lectures in the first three terms as their fellow BSc students. If the second major subject is not mathematics, the mathematics lectures for engineers are attended. In the fourth term the programme branches away from the BSc programme. Special lectures in advanced theoretical and experimental physics are offered and the education in subject didactics starts, before entering the internship at a secondary school. During the internship, they first assist experienced teachers, and then teach on their own for the first time. Since one year, the basic and advanced courses in the subject didactics are imported from the *Pädagogische Hochschule* (University for Education).

The number of enrolments in the teachers programme has also increased over the last years with the exception of the most recent one (see Fig. 1.1). The decrease in the last year, which is also observed in other disciplines and also in other universities in Baden-Württemberg, might be related to the announcement by the state government to change the study programme for prospective teachers without providing a detailed outline of the changes. It was only recently clarified that a transition to a BSc and Master of Education (MEd) programme, in strong cooperation with the *Pädagogische Hochschule* in Freiburg during the MEd programme is envisaged. The new course programme is expected to start in winter semester 2015/16. The current drop-out rate is at the same level as in the BSc programme. Most of the students here as well, who drop out, do not leave the university, but enrol in a different discipline, where the achieved academic records are usually accredited.

1.2.4 Teaching Export

The Institute of Physics supplies the largest teaching support 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, state examination Dentistry, BSc Embedded Systems, BSc Environmental Sciences, BSc Geography, BSc and MSc Geology, BSc and MSc Computer Science, Bsc and MSc Mathematics, state examination Medicine, BSc Microsystem Engineering, and state examination Pharmacy. In addition to participation in the basic experimental physics lectures of the BSc physics programme, as done by students from engineering sciences, computer science and mathematics, two dedicated lectures and laboratory classes are offered for students from other natural sciences, and from medicine and pharmacy. Several hundreds of students participate in these dedicated lectures and laboratory courses each term.

1.3 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. It offers eleven consultation-hours per week for students to ask questions and get advice concerning examination procedures. The counsellor office is the second important corner stone. Two study counsellors, one for BSc/MSc programmes and one for the teacher programme, offer individual advice with respect to the study plan and general aspects of the study programme during ten consultation-hours per week. They also coordinate the course programmes. The 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. Students have various opportunities to get help and advice at each level of their study progress in individual face-to-face consultations on short time scales.

1.4 Quality Management

All basic courses including tutorial classes and a significant fraction of the specialised courses are evaluated with a questionnaire each term. The survey is organised by the student representatives in cooperation with the Dean of Studies. 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. This body is responsible for the budgeting and allocation of specific funds to promote the quality of teaching. Currently the largest fraction of the money is spent on hiring additional teaching tutors to allow for an additional support of the students in small groups in tutorial classes and laboratory courses. The remaining funds are used to support excursions and the participation of students in workshops and conferences, e.g. the annual meetings of the German Physical Society. Other specific funds for investments in the area of teaching are used to extend the number of available study rooms for students, upgrading their associated equipment (nine new rooms were equipped during 2012), and to update and upgrade the computer pools for students, facilities in the laboratory courses, and to set up new modern experiments, e.g. a Paul trap in the advanced laboratory course, and an experiment related to ultrasonic sound in the demonstration course of the teacher-training programme.

1.5 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, the “Garden of Physics” (see Fig. 1.8), and nine recently equipped discussion rooms encompassing 56 work places in the basement of the West Building. An extension of the computer pools and the discussion rooms for students is desirable. The department holds only three lecture halls with 340, 150, 60 seats, respectively, and five seminar rooms with up to 30 seats each. Due to the increase in the enrolments for the degree programmes in physics and for other disciplines, which import lectures, a video transmission of the lecture in Experimental Physics 1 to a second lecture hall had to be provided, as the capacity of the major lecture hall was not sufficient to host all students. A larger lecture hall, additional seminar and work rooms, and larger computer pools for students can only be provided by a new building at the physics campus.

1.6 Support for Students

1.6.1 New Students

The body of student representatives offers various forms of assistence to students, particularly to new students. They provide practical help in organising the students’ life and in planning individual time tables. Before the beginning of the winter term, a one-

Figure 1.8: Students discussing in the "Garden of Physics".

week long "Welcome and Kick-Off event" is organised, which helps students in a viable transition from school to university.

Welcome and introduction seminars are organised by the Dean of Studies and the general study counsellors during the first week of each teaching period. The presentations give an overview of the study programme, the examination procedures and rules, the structure of the Office for Studies and the various options to obtain advice and support. General help is also provided by the central *Service Center Studium* (Service Centre for Studies SCS).

1.6.2 Female Students

The fraction of female students in the course programmes is currently at the level of 25%, 20% and 35% in the BSc, MSc and teacher-training programmes, respectively. In order to increase the number of female students and to help women in organising their studies and career planning, specific programmes have been developed.

Each year a special open day for female secondary school students is organised. The female pupils are informed about the study programmes and the research activities. They also have the possibility to participate in small practical workshops organised by the research groups, providing their first contact to modern research.

A specific mentoring programme MeMPhys (mentoring in mathematics and physics) has been developed and set up already a decade ago. Each interested female student is mentored by a more experienced female 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.

The Annual Women's Meeting of the German Physical Society took place in Freiburg in 2012. The conference was organised to a large extent by female students, PhD students and postdocs from the Institute of Physics. The programme comprised scientific lectures on new research results, given by well-known, successful female scientists, which may serve as role models for young students, and talks and panel discussions elaborating and critically reviewing the compatibility of scientific career, and family planning and the current status of female physicists in the society.

1.6.3 Foreign Students

Dedicated support is provided to students from foreign countries, who enrol in the MSc programme or spend several months to two semesters 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 Insti-

Figure 1.9: Horst Fischer presents the Christmas Lecture for the general public.

tute of Physics also has its own ERASMUS counsellor. 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). Since half a year the Institute of Physics offers additional mentoring by a MSc student in the second year.

1.7 Promotion for Physics

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 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 an university to perform an internship for several weeks. Each year on average ten pupils choose to join a research group at the Institute of Physics for this project. A significant fraction of the pupils enrol in a physics course programme past internship.

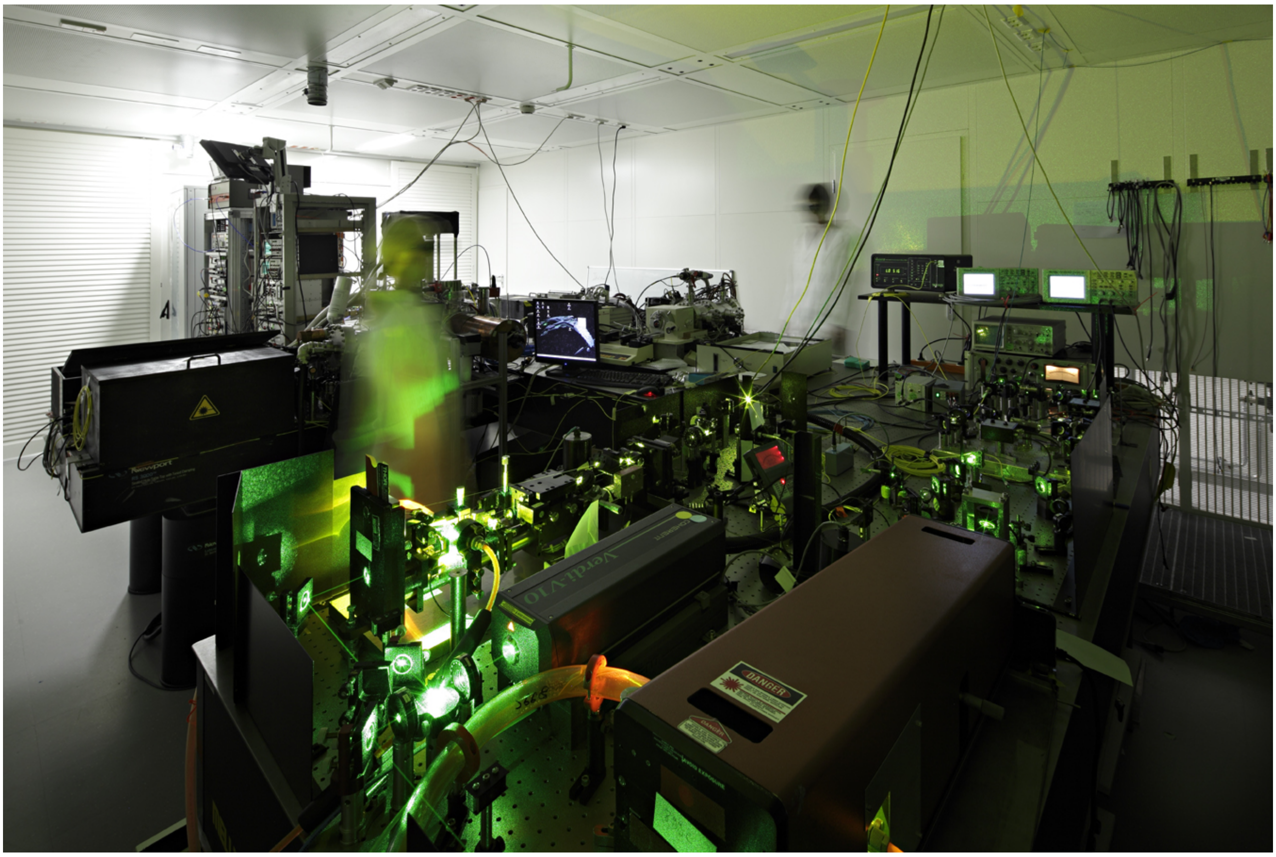
The Institute of Physics participates every year in a science fair called "Science Days", held at the theme park in Rust. During three days pupils from secondary schools can interactively perform small experiments, and are informed about the opportunities to study physics in Freiburg.

The particle physics groups participate in the international Master Classes "Hands on Particles Physics", organised simultaneously at 160 institutes in 37 countries worldwide every year in March. Secondary school pupils have the opportunity to attend lectures on particles physics and to perform measurements on real 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 seven such visits take place every year.

Other activities for the general public include the participation in the biannual two-day long Science Market organised by the University of Freiburg in the centre of the city and the well attended public Christmas Lectures in physics every year (see Fig. 1.9).

Part IV

Infrastructure



Chapter caption: Experimental lab in the Gustav-Mie building for measuring ultra-cold atom gases.

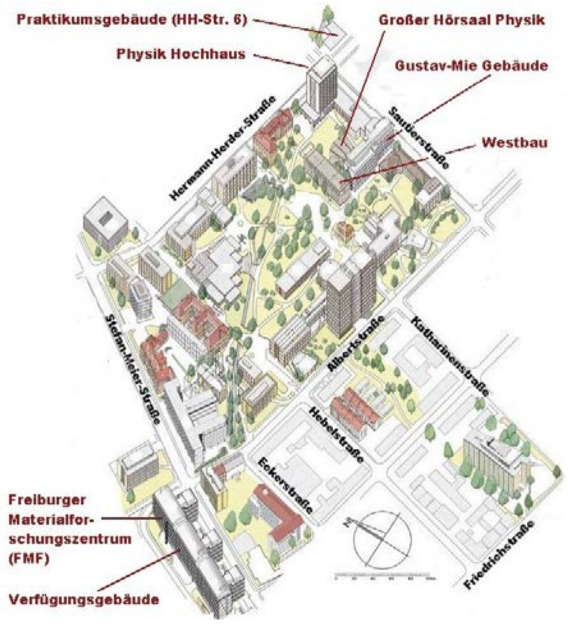


Figure 1.1: Map of the Physics Campus.

1.1 Buildings

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).

The Physics high-rise (Physik Hochhaus) provides office spaces for theoretical and experimental research groups, as well as two major lecture halls and some tutoring rooms 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. A recently equipped lab is shown in the figure on the previous page. Besides the physics labs the building also hosts several chemical labs in the basement, and two clean rooms. Finally, the experimental setups of the advanced laboratory courses, which occupy the second floor, the Computer Pool for students, and the Institute of Physics' second social room are found there.

The low-rise building, which connects the Physics high-rise and the Gustav-Mie building, provides the space for the mechanical and electrical workshops, and the electronic design and development lab. In addition, the experimental labs of three research groups are temporarily located here.

The West building (West Gebäude) houses the administration office spaces, the library of the Institute of Physics, the offices for some experimental groups, several discussion rooms and work space for students and teaching in the basement, and the rooms of the *Fachschaft Physik* (body of student representatives).

The main lecture hall (Großer Hörsaal Physik) is located in a dedicated building, with additional rooms for the teaching experiments. The buildings described so far enclose the *Garden of Physics*, as a central social focus point.

The Laboratory building (Praktikumsgebäude) just across the road is occupied by experiments of the introductory laboratory courses. Finally, the labs and offices of two experimental research groups are accommodated by the Verfügungsgebäude near the Freiburger Material Forschungszentrum (FMF) outside of the Physics Campus, and one theory group is temporarily located in Rheinstraße 10 (not shown in Fig. 1.1).

1.2 Administration

The administration of the Institute of Physics is organized as a 'Department System', which provides a central management of the human and financial resources.

An essential element of this system is that, in addition to their individual resources, all chairs equally participate in a pool system, which in particular provides central infrastructure such as the mechanical and electronics workshops, the electronic design and development lab, the IT support group, technical staff, central liquid nitrogen support and further resources. A similar pool system also exists for scientific personnel from which scientific staff can be assigned based on demand, as well as for a general fund which apart from financing the common infrastructure is also available to support short term demands of individual chairs.

The administration and the research groups are supported by eleven dedicated secretaries, most of which are on half-time positions.

1.3 Workshops and Technical Support Groups

The Institute of Physics has outstanding workshops with highly qualified personnel, which are organized in the three units: Mechanical Workshop (MW), Electronic Workshop (EW), and Electronic Design and Development Lab (see Fig.1.2). They offer unique services and are essential resources for the experimental physics groups; they are a cornerstone of the physics research in Freiburg. Each unit is run by a dedicated head with additional support by commis-

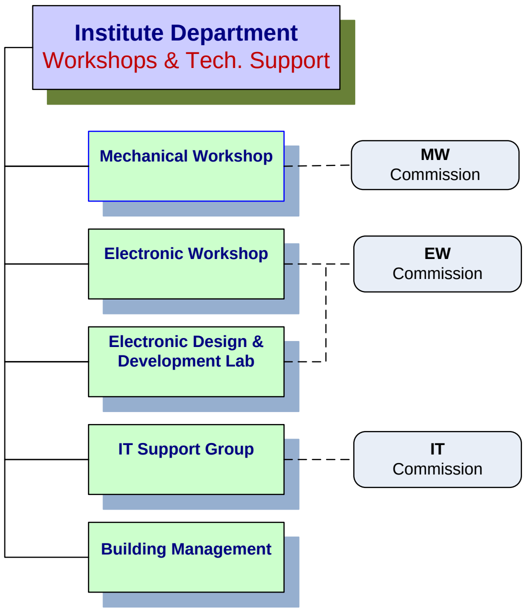


Figure 1.2: Organisation chart of the workshops and technical support groups.

sions, which consist of representatives of the workshops and of the professors. The mechanical workshop has 19 highly qualified employees, the electronic workshop is run by six well trained electronic technicians, and the electronic design and development lab by five skilled electronics development engineers. At present eight young persons are trained to *Feinwerkmechanikern/innen* (precision mechanics) in the mechanical workshop, and the electronic workshop is host to four apprentices trained to electricians.

1.3.1 Mechanical Workshop

The mechanical workshop is equipped to manufacture all sorts of high-precision parts (see Fig.1.3). The available manufacturing tools allow them to meet essentially any demand, which is possible with today's mechanical manufacturing technology. Besides the usual lathe and milling tools the mechanical workshop currently owns also

- four CNC milling machines;
- two milling centers with four- and five-axis control;
- one CNC rotation centre;
- two CNC rotation machines with driven tools;
- welding equipment of stainless steels, 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 per clamping, which enhances the manufacturing efficiency and quality. Figure 1.3 provides a view on the mechanical workshop. It also shows one of the 50 special huge light guides, which were produced in the workshop for the COMPASS experiment at CERN.

1.3.2 Electronic Workshop

The well trained six electronics technicians of the electronics workshop offers a wide choice of services. Here a short overview:

- counseling in all electronics related questions;
- development and production of instruments and measurement systems;
- CAD aided print board layout routing and in-house production of two-layer print boards;
- sourcing of multilayer print boards and SMD parts;
- management and provision of electronic parts;
- repair and maintenance.

1.3.3 Electronic Design and Development Lab

This group of dedicated engineers provides service in electronic design and development to support the research activities of mainly the experimental groups of the Institute of Physics. It assists in designing innovative electronic assemblies in the framework of their research. The built systems are optimized solutions for specific experimental problems.

Both analog, e.g. low-voltage and power electronics, and digital, e.g. FPGA and microcontroller based, designs are offered. A wide spectrum of high-end equipments, hardware and software tools are deployed in the design and development work, including circuit simulations and tests. The group also undertakes the operation of a clean room for semiconductor sensors. Highlights of designed and/or developed electronic circuits in recent years include:

- high voltage switch and trigger generator/controller to drive pockels cells;
- fast (<100ns) high voltage (40kV) switch driving capacitive loads (field electrodes);

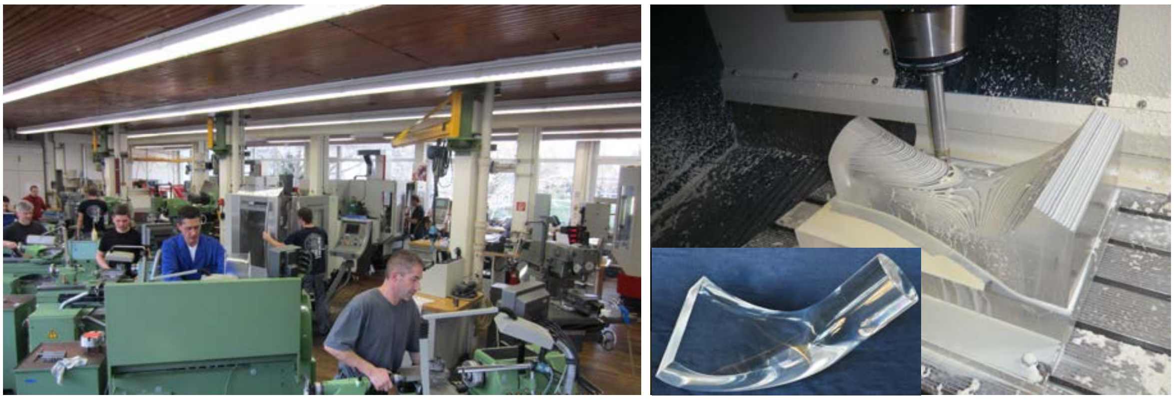


Figure 1.3: Left: View of the Mechanical Workshop. Right: 'Huge' light guide manufactured for the COMPASS experiment at CERN.

- multilayer, flexible PCBs (so called hybrids) for the readout electronics of the silicon-strip tracking detector for the planned upgrade of the ATLAS experiment at CERN;
- several low noise, low drift, gain-programmable amplifiers, e.g. for mV range applications.

Work done over the past few years has resulted in many cases in designs that can be adapted to meet new and/or common requirements of the experimentators. This is one advantage of in-house designed, built and tested equipment.

1.3.4 Clean Room Facilities

The Gustav-Mie building houses an industrial style class 10000 clean room of approximately 65 m^2, with about 15 m^2 under laminar flow boxes qualified as class 100. The clean room depicted in Fig. 1.4 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 fully equipped, including a Delvotec ultrasonic wire bonder shown also in Fig. 1.4, a wire pull tester, an automatic probe station, a semi-automatic metrology microscope and a dispensing robot. The clean room facilities will be significantly extended in 2014 by converting the two adjoining labs into clean room space, resulting in a total clean room area of about 100 m^2, divided into three sections.

1.3.5 IT Support Group

The institute is currently establishing an IT support group of three persons financed from institute resources, in order to expand the IT support, which was available so far to the theory groups, into an IT service which handles the needs of the whole institute, including the experimental groups and the administration. The tasks of the group include:

- maintenance, configuration and troubleshooting of computers and other IT infrastructure;
- operation of complex IT infrastructures;
- administration of UNIX and Windows based servers;
- hardware and software installations for personnel computers;
- sourcing of IT components.

1.4 Building Management

The building management for the maintenance and servicing of building installations and infrastructure such as heating, ventilation, air-conditioning, postal delivery services and further tasks are handled by a janitor, and two desk officers located 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 from the university.

1.5 Teaching and Student Facilities

The Office for Studies is located in the West building and is comprised of the examination office, the

Figure 1.4: Left: View of the clean room in the Gustav-Mie building. Right: The Delvotec 6400 series ultrasonic wire bonder housed in the clean room.

student counselor office and the programme coordination office (for details see Part III, Section **1.3**).

Three main lecture theatres are available to the Institute of Physics; the main lecture hall (340 persons), and lecture halls I (150 persons) and II (60 persons) in the first floor of the Physics high-rise building. A total of five seminar rooms with a capacity of 15 to 40 persons are found in the Physics high-rise, the Gustav-Mie and the West buildings.

The basic laboratory courses for physicists and lab courses for medical students, students of pharmacy and natural sciences are all held in the Laboratory building (Fig. 1.1), where the lab experiments occupy four floors. These experiments are maintained by a lab course technician. The 25 experiments for the advanced laboratory classes are located in the Gustav-Mie building, and maintained by a further technician.

Two Computer Pools for students are available in the Gustav-Mie building (see also Part III, Section **1.5**), and the *Fachschaft Physik* has separate rooms in the West building.

The Institute of Physics provides several spaces for both learning and leisure. A large Common Room (Fig. 1.5) in 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 social room in the Gustav-Mie building is equipped with a large black board and desks, as well as kitchen utensil (cooker, dishwasher, etc.). It is used by student gatherings and often is also booked for tutorial classes.

Figure 1.5: Impression of the common room found in the top floor of the Physics high-rise.

1.6 Library

The Physics Library occupies the first floor in the West building. It is organized as a *Präsenzbibliothek* (reference library), and is open to researchers 24 hours a day, seven days a week and to students during the week. It also offers plenty of silent work space.

1.7 Computational Infrastructure

Major computational hardware of the Institute of Physics is located in two server rooms in the basement of the high-rise building and the Gustav-Mie building. The computer rooms for students have 34 PC workstations. There are also storage-, file-, web- and mail-servers available. Two student assistants are in charge of the student computer pools and organize software updates and the account assignments.

Several physics groups are main users and key stakeholders of the *Black Forest Grid* (BFG), which is an interdisciplinary research cluster of several faculties and centres, run by the computing centre of the university and the particle physics groups (see Part II, Section 3.6 for details on grid computing).

Part V

Activities of the Institute

Chapter caption: Examples of conference/workshop posters of recent conferences (co-)organized by the Institute of Physics, and conference photo of the “Standard Model at the LHC” conference.

During the past years, the Institute of Physics has organized various International Conferences, workshops, and symposia. Several workshops were co-organized with FRIAS. 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 all scientists and students. It takes place every Monday afternoon during term times and also provides an ideal forum for presentations and discussions of topics not directly addressed in the Freiburg research areas.

Physicists from our institute were very active in promoting physics at schools and in presenting results on research in public lectures, as part of our outreach strategy. Presentations at schools were given to attract the best pupils to enrol in the fascinating subjects of Physics or other Natural Sciences. Special training programmes were also addressed to school teachers to make them familiar with the current front lines of research. As part of the outreach programme, several events are repeated on a yearly basis.

The various activities are summarized in the following subsections. For the conferences and workshops only the major ones, with large international participation, are listed.

1.1 Conferences

- **DPG Meeting for female physicists** (16. Deutsche Physikerinnentagung), University of Freiburg, 25.-26.10.2012; Local organizers: E. von Hauff, S. Kühnhold, M. Bujak, L. Sommerlade, H. Arnold, K. Reininger, B. Grüner, R. von Waldenfels, N. Leonhard, M. Astruc Hoffmann, V. Blattmann, L. Schätzle, K. Schleicher, K. Ortstein, S. Fernandez-Robledo; `http://www.physikerinnentagung.de/dpt12/`

- **"SM@LHC" ("Standard Model at the LHC")**, University of Freiburg, 9.-12.4.2013; Organizing Committee: J. Alcaraz, J. Andersen, M. Campanelli, V. Ciulli, S. Dittmaier, K. Jakobs, F. Krauss, E. Laenen; Local Organizing Committee: H. Ita, K. Lohwasser, M. Schumacher, C. Schwinn, F. Siegert, C. Weiser; `http://www.smatlhc2013.uni-freiburg.de/`

- **"Higgs Couplings 2013"**, University of Freiburg, 14.-16.10.2013; Organizers: S. Dittmaier, K. Jakobs, M. Schumacher; `http://hc2013.uni-freiburg.de/`

- **Clustertreffen 2013** (Conference of the German-speaking community of cluster physics), Herzogenhorn near Freiburg, 6.-11.10.2013; Organizers: B. v. Issendorff, F. Stienkemeier, M. Mudrich; `http://www.clustertreffen.uni-freiburg.de/`

1.2 Workshops, Symposia and Schools

- **IRTG "Soft Matter Science" Workshops**, University of Freiburg, 15.4.2011 and 8.-9.11.2012; Organizer: G. Reiter

- **Helmholtz Alliance School "LHC Precision Predictions for Pedestrians 2011"**, University of Freiburg, 10.-14.10.2011, Organizers: S. Dittmaier, M. Schumacher

- **Workshop on Quantum Coherence in Energy Conversion**, University of Freiburg, 24.-28.10.2011; Coordinators: A. Hammack (Berkeley), C. Smyth (Toronto), J. Zimmermann (Freiburg)

- **Workshop on "Quantum Dynamics on Complex Networks - Entanglement, Recurrence, and Trapping"**, University of Freiburg, 15.03.2012; Organizer: O. Mülken

- **Andrejewski-Day at the Faculty for Mathematics and Physics, "The mathematics of quantum transport"**, University of Freiburg; 18.05.2012; Organizers: A. Buchleitner, K. Wendland

- **542. WE-Heraeus Seminar on "Classical and Quantum Transport in Complex Networks"**, Bad Honnef, 29.07.-01.08.2013; Organizers: O. Mülken, A. Blumen

- **"Innovative Concepts in Photovoltaics"**, sponsored by the German Physical Society (DPG), 22.-27.09.2013, Coordinator: E. von Hauff

1.3 Workshops co-organized by FRIAS

- **Mini-Workshop Quantum Efficiency**, University of Freiburg and FRIAS, 25.-28.07.2011; Organizers: H.P. Breuer, A. Buchleitner, T. Wellens, J. Zimmermann

- **Graphene Nano-Workshop**, University of Freiburg and FRIAS, 08.11.2011; Organizers: D. Bercioux, H. Grabert

- **Black Forest Focus 7: Multidimensional Optical Spectroscopy and Imaging: Temporal and spatial resolution at the cutting edge**, University of Freiburg and FRIAS, 14.-18.03.2012; Organising Committee: K. Buse, H. Grabert, J. Korvink, S. Mukamel

- **International Workshop on "Topological States of Matter"**, University of Freiburg and FRIAS, 18.-22.03.2012; Organizers: D. Bercioux, D. Urban

- **Black Forest Focus 8: Electronic and Excitonic Transport in Soft Matter**, University of Freiburg and FRIAS, 10.-14.10.2012; Organising Committee: A. Blumen, H. Grabert, A. Mateo-Alonso, G. Reiter

- **3. Interdisziplinäres Symposium des Freiburg Institute for Advanced Studies: "Der Wert des Körpers"**, University of Freiburg and FRIAS, 13.-14.06.2013; Organizers: J. Timmer, W. Eßbach

- **Black Forest Focus 9: Protein Dynamics: From Water Hydration to Crowding Effects**, University of Freiburg and FRIAS, 25.-29.09.2013; Organising Committee: H. Grabert, F. Rao, G. Stock

- **Workshop for Quantum Simulations of Open Quantum Systems**; A FRIAS Junior Researcher Conference, University of Freiburg and FRIAS; 13.-15.11.2013; Organising Committee: F. Mintert, U. Warring

1.4 Colloquia and Seminars

- **Colloquium of the Physics Institute**: Every term, weekly, University of Freiburg, 2011-2013; Organizers: Professors of the Institute of Physics, `http://www.mathphys.uni-freiburg.de/physik/kolloquium.php`

- **Quantum Efficiency Lecture and Colloquium**: Every term, University of Freiburg, 2011-2013; Organizers: A. Buchleitner, H.-P. Breuer, E. v. Hauff, `https://portal.uni-freiburg.de/qe/QE_SS%202013/QE_SS%202013`

- **Astrophysical Colloquium of the KIS**: weekly around the year, Kiepenheuer-Institut für Sonnenphysik (KIS), 2011-2013; Organizers: O. von der Lühe, S. Berdyugina, `http://www.kis.uni-freiburg.de/index.php?id=556&L=1`

- **Seminar "Fundamentale Wechselwirkungen" (Fundamental Interactions)**, Every term, University of Freiburg, 2011-2013; Organizers: S. Dittmaier, H. Ita, J. van der Bij, `http://portal.uni-freiburg.de/ag-dittmaier/seminars/fundi`

- **Seminar "Physics at Hadron Colliders"** organized within the Research Training Group (Graduiertenkolleg), every term, University of Freiburg, 2011-2013; Organizers: S. Dittmaier, G. Herten, H. Ita, K. Jakobs, K. Königsmann, M. Schumacher, J. van der Bij, `http://wwwhep.physik.uni-freiburg.de/graduiertenkolleg/home.html#seminar`

- **Mathematics-Physics Colloquium**, Every term, University of Freiburg, 2011-2013; Organizers: A. Buchleitner, K. Zimmermann, D. Gross, K. Wendland, `http://www.mp.uni-freiburg.de/`

- **IRTG-Seminar "Soft Matter Science"**, Every term, weekly, University of Freiburg, 2011-2013; Organizer: G. Reiter, `http://www.softmattergraduate.uni-freiburg.de/h/allevents/seminars/`

1.5 Public Lectures

- **"Reise zum Urknall mit dem Large Hadron Collider im CERN"**, Lions Club Freiburg, 08.02.2011; Lecturer: G. Herten
- **"Die Dunklen Mächte des Universums - Über Dunkle Energie, Dunkle Materie und deren Verbindung zur Teilchenphysik"** , Planetarium Freiburg, 10.11.2011; Organizer: Volkshochschule Freiburg; Lecturer: H. Fischer
- **"Aufbruch in die Terra Incognita der Teilchenphysik - der Large Hadron Collider: erste Ergebnisse und Perspektiven"**, Freiburg, 23.11.2011, "Tag der Weltmaschine"; Lecturer: M. Schumacher `http://www.weltmaschine.de/service__material/tag_der_weltmaschine/freiburg/`
- **"Über den Ursprung der Masse - Die Suche nach dem Higgs-Teilchen am Large Hadron Collider"** at the MNU-Bundeskongress (Deutscher Verein zur Förderung des mathematischen und naturwissenschaftlichen Unterrichts e.V.), Freiburg, 04.04.2012; Lecturer: M. Schumacher
- **"Über den Ursprung der Trägheit - Die Suche nach dem Higgs-Teilchen am Large Hadron Collider"** at the Freiburg Colloquium of the Studienstiftung, June 2012; Lecturer: M. Schumacher
- **"Ist das Higgs-Teilchen entdeckt"**, University of Freiburg, 28.09.2012; Lecturer: K. Jakobs; `http://www.pr.uni-freiburg.de/pm/2012/pm.2012-09-19.247`
- **"The ATLAS Roadmap for the Higgs Boson and Beyond"**, 1.2.2013 Karlsruhe, KSETA Inauguration Symposium, KIT Karlsruhe, Lecturer: P. Jenni
- **"Der lange Weg zum Higgs-Boson und mehr am LHC"**, 19.4.2013 München, Symposium der Bayerischen Akademie der Wissenschaften - Grossgeräte der Physik, Lecturer: P. Jenni
- **"Chaos, Quanten, Unbestimmtheit"**, Studium Generale, Mainz, June 2013; Lecturer: A. Buchleitner
- **"Die Entdeckung des Higgs-Teilchens und das Management von Großprojekten in der Wissenschaft**, Fa. Siemens und Universität Erlangen, 24.07.2013, Lecturer: K. Jakobs
- **"Dem Higgs-Teilchen auf der Spur"**, 21.9.2013 Wuppertal, Highlights der Physik 2013 BMBF - Vom Urknall zum Weltall, Lecturer: P. Jenni
- **"Das Higgs-Boson und der lange Weg zum Nobel-Preis"**, University of Freiburg, 16.10.2013; Lecturer: S. Dittmaier; `http://www.pr.uni-freiburg.de/pm/2013/pm.2013-10-09.263`
- **"Reise zum Urknall - Raum, Zeit, Energie und Materie"**, Volkshochschule Donaueschingen, 16.10.2013; Lecturer: G. Herten
- **"Dem Higgs-Teilchen auf der Spur"**, 12.12.2013 Hannover, VolkswagenStiftung, Forum Herrenhaeuser Nobelpreistage: Physik, Lecturer: P. Jenni
- **"Weihnachtsvorlesung"**, every year, December 2011, 2012, 2013; Lecturer: H. Fischer

1.6 Lectures at Physics and Interdisciplinary Schools

- **Setting up of an undergraduate laboratory and regular lecture series**, every February/March since 2006, Royal University of Phnom Penh, Cambodia, Lecturer: H. Helm
- **Quantum Measures for non-Markovianity**, New Trends in Quantum Dynamics and Entanglement, 14.-25. Februar 2011, Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Lecturer: H.-P. Breuer
- **Many-particle dynamics, simulations, and decoherence**, Summer School Quantum Information meets Statistical Mechanics, San Lorenzo de El Escorial, Spain, July 2011, Lecturer: A. Buchleitner

- **Physics at the LHC - from the Standard Model to searches for new physics -**, Euro Summer Campus, Strasbourg, France, July 2011, Lecturer: K. Jakobs
- **Searches for Physics Beyond the Standard Model at the LHC**, Int. School of Physics, Les Houches, France, August 2011, Lecturer: K. Jakobs
- **Physics at the LHC - from the Standard Model to searches for new physics -**, CERN School of Physics 2011, Cheile Gradistei, Romania, September 2011, Lecturer: K. Jakobs
- **Particle Detection and first Physics Results from the LHC**, School on High Energy Physics, Quin Nhon, Vietnam, December 2011, Lecturer: K. Jakobs
- **Transport in complex quantum systems**, 23rd Chris Engelbrecht Summer School, Salt Rock, South Africa, January 2012, Lecturer: A. Buchleitner
- **Searches for Higgs Bosons at the LHC**, YETI UK HEP Young Experimentalists and Theorists Institute, Durham, January 2012, Lecturer: M. Schumacher
- **Searches for the Higgs Boson of the Standard Model at the LHC**, Heidelberg Graduate School, Neckarzimmern, February 2012, Lecturer: M. Schumacher
- **Fundamental processes in organic photovoltaics**, Europhotonics Spring School, March 25-31, 2012, Barcelona, Spain, Lecturer: E. von Hauff
- **Transport and disorder**, XXVIII Heidelberg Physics Graduate Days, April 10-13, 2012, Lecturer: T. Wellens
- **Physics at the LHC -from the Standard Model to searches for new physics-**, CERN School of Physics 2012, Cargese/Corsica, France, 2012, Lecturer: K. Jakobs
- **Higgs Boson Physics at the LHC**, HGF Terascale Alliance School “Prejudice meets Reality”, Bonn, August 2012, Lecturer: M. Schumacher,
- **Zufall und Komplexität in der Physik**, Sommerakademie der Studienstiftung des deutschen Volkes, Olang, September 2012.Lecturer: A. Buchleitner
- **Basics of impedance spectroscopy for organic & dye sensitised solar cells**, International Krutyn Summer School, September 30-October 6, 2012, Krytun, Poland, Lecturer: E. von Hauff
- **Higgs Boson Physics at the LHC**, BND School - Belgium-Dutch-German Graduate School in Particle Physics, Bonn, October 2012, Lecturer: M. Schumacher
- **Discovery of a new boson at the LHC - or evidence for the Higgs boson?-**, WE-Heraeus Physics School, Bad Honnef, December 2012, Lecturer: K. Jakobs
- **Advanced theory of open quantum systems**, Lectures held at Imperial College, 18.-19. March 2013, London, GB, Lecturer: H.-P. Breuer
- **The quantum-classical transition in complex quantum systems**, Rome School on Open Quantum Systems and the Quantum-Classical Boundary, Rome, April 2013, Lecturer: A. Buchleitner
- **Coherence in excitonic systems - quantum design principles for optimal transport**, WE-Heraeus Physics School, Bad Honnef, May 2013, Lecturer: A. Buchleitner
- **Nonlocal Young experiments**, WE-Heraeus Physics School, Bad Honnef, May 2013, Lecturer: C. Gneiting
- **Quantum dynamics of many-particle systems: spectral structure, decay, and relaxation**, 38th Nathiagali Summer School, Islamabad, Pakistan, June 2013, Lecturer: A. Buchleitner
- **Higgs analyses at the LHC**, CERN-Fermilab HCP Summer School, CERN/Geneva, Switzerland, August/September 2013, Lecturer: K. Jakobs
- **“Methods and paradigms of physics and philosophy - (in-)compatible?”**, Sommerakademie der Studienstiftung des deutschen Volkes, Krakau, September 2013, Lecturer: A. Buchleitner

1.7 Presentations of the Institute of Physics to the Public

- **Presentation at the "Science Days"** at the Europa-Park Rust near Freiburg, October 2011, 2012, 2013; Organizers: H. Krämer, M. Walther, H. Dummin http://www.science-days.de/science-days/sponsoren-partner/partner/
- **Presentation at the "Freiburger Wissenschaftsmarkt"** in the city centre of Freiburg: "Das ATLAS-Experiment am LHC", 8./9. July 2011;
"Das Higgs-Teilchen und die Dunkle Materie", 12./13.07.2013; Organizers: M. Schumacher, G. Herten, K. Jakobs http://www.uni-freiburg.de/forschung/wissenschaftsmarkt
- **Presentation meeting with Dr. Jeanne Rubner, Süddeutsche Zeitung, "Universität und Medien - ein schwieriges Verhältnis?"**, Nachbetrachtungen zum Fall Guttenberg, Universtity of Freiburg, 16.11.2011; Organizer: A. Buchleitner; http://portal.uni-freiburg.de/qe/events

1.8 Lectures, Presentations for High-school Teachers and Students

- **Open house presentations ("Tag der offenen Tür")**, University of Freiburg, November 2011-2013; Organizers / Lecturer: M. Schumacher, H. Krämer, H. Fischer, T. Filk, S. Dittmaier;
- **Master Classes for High-school students at the Particle Physics Department of the Institute of Physics**, University of Freiburg, March 2011-2013; Organizers: M. Böhler, F. Bührer, U. Parzefall, http://portal.uni-freiburg.de/jakobs/Schulprojekte
- **Schnupperstudium** (one-day internship in groups at the Institute of Physics) for female high-school students, University of Freiburg, April 2011-2013; Organizers: E. von Hauff, S. Zimmermann, http://www.studium.uni-freiburg.de/service_und_beratungsstellen/zsb/schnupperstudium
- **Higgs- oder nicht Higgs-Boson? Über die Entdeckung eines neuen Teilchens am Large Hadron Collider (LHC)**, DPG-Lehrerfortbildung Teilchenphysik, Bad Honnef (Germany), October 2012, Lecturer: M. Schumacher
- **Presentation in the course of "Advanced education for teachers"** on the topic "LHC und ATLAS - Die Weltmaschine und ihre Möglichkeiten", University of Freiburg, March 2011; Lecturers: G. Herten, K. Jakobs, T. Rave
- **Aufbrüche - Chancen für eine neue Lernkultur**, Tagung 'Abitur - was dann?', Ev. Akademie Tutzing, 2011, 2012, 2013, Lecturer: A. Buchleitner
- **Presentations on detectors in Particle Physics to the 'Freiburger Seminar'**, a group uniting final year high-school students with a strong interest in natural sciences, guided by dedicated teachers, Lecturers: U. Parzefall, T. Rave
- **Several lectures at high-schools in the Freiburg area** (about five per year from 2011-2013), Lecturers: T. Filk, U. Parzefall

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