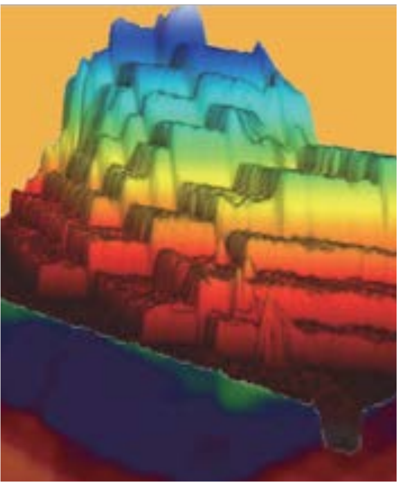
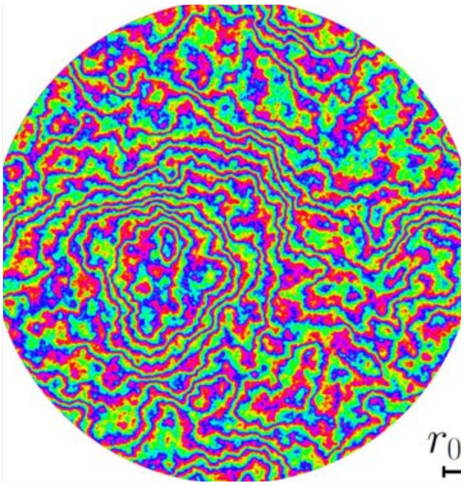
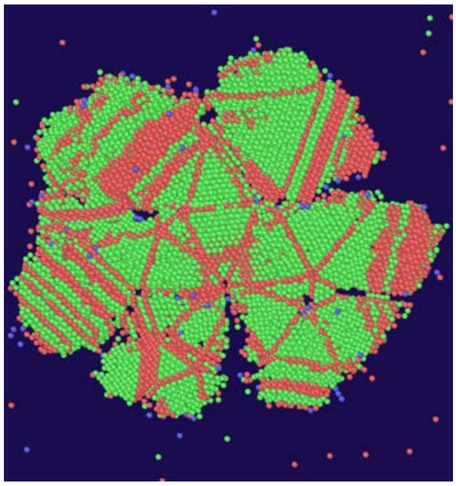
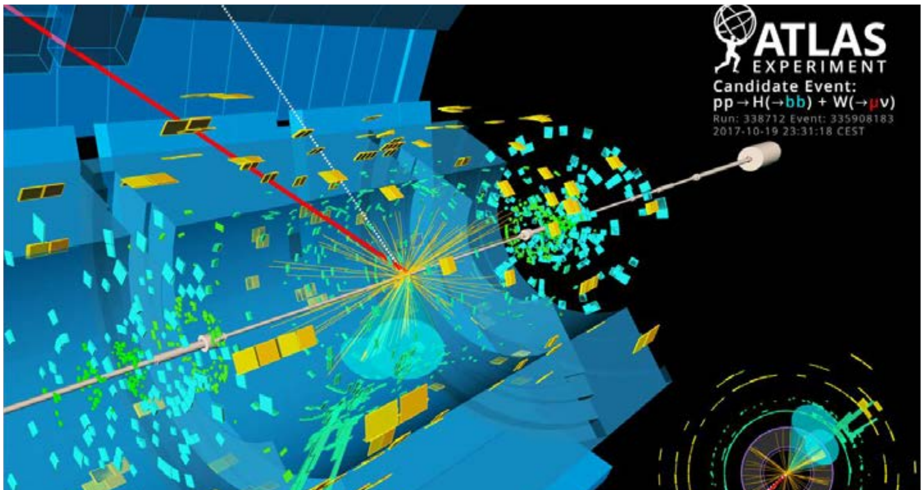
Freiburg Institute of Physics

Activity Report 2018-2021









Albert-Ludwigs-Universität Freiburg

INSTITUTE OF PHYSICS
UNIVERSITY OF FREIBURG

ACTIVITY REPORT 2018 - 2021

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

Front cover (top to bottom):
(i) Artistic view of an individual ion interacting with several atoms simultaneously via their wave-like characters (image: Ella Marushchenko). (ii) 3D AFM height image showing the crystal morphology of "3D single crystals" of iPS. (iii) Color-coded phase shifts of light propagating in a turbulent atmosphere. (iv) Cross section of a hard sphere crystal cluster, color codes different crystal structures. (v) View inside the field cage of the Time Projection Chamber of the XENONnT detector. (vi) View of a candidate event for the production of a Higgs boson decaying to pair of b-quarks in association with a W boson decaying to a muon and the corresponding neutrino.

IMPRESSUM

Published
March 2022 by the
Freiburg Institute of Physics (IoP)

Printed by
University of Freiburg

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.

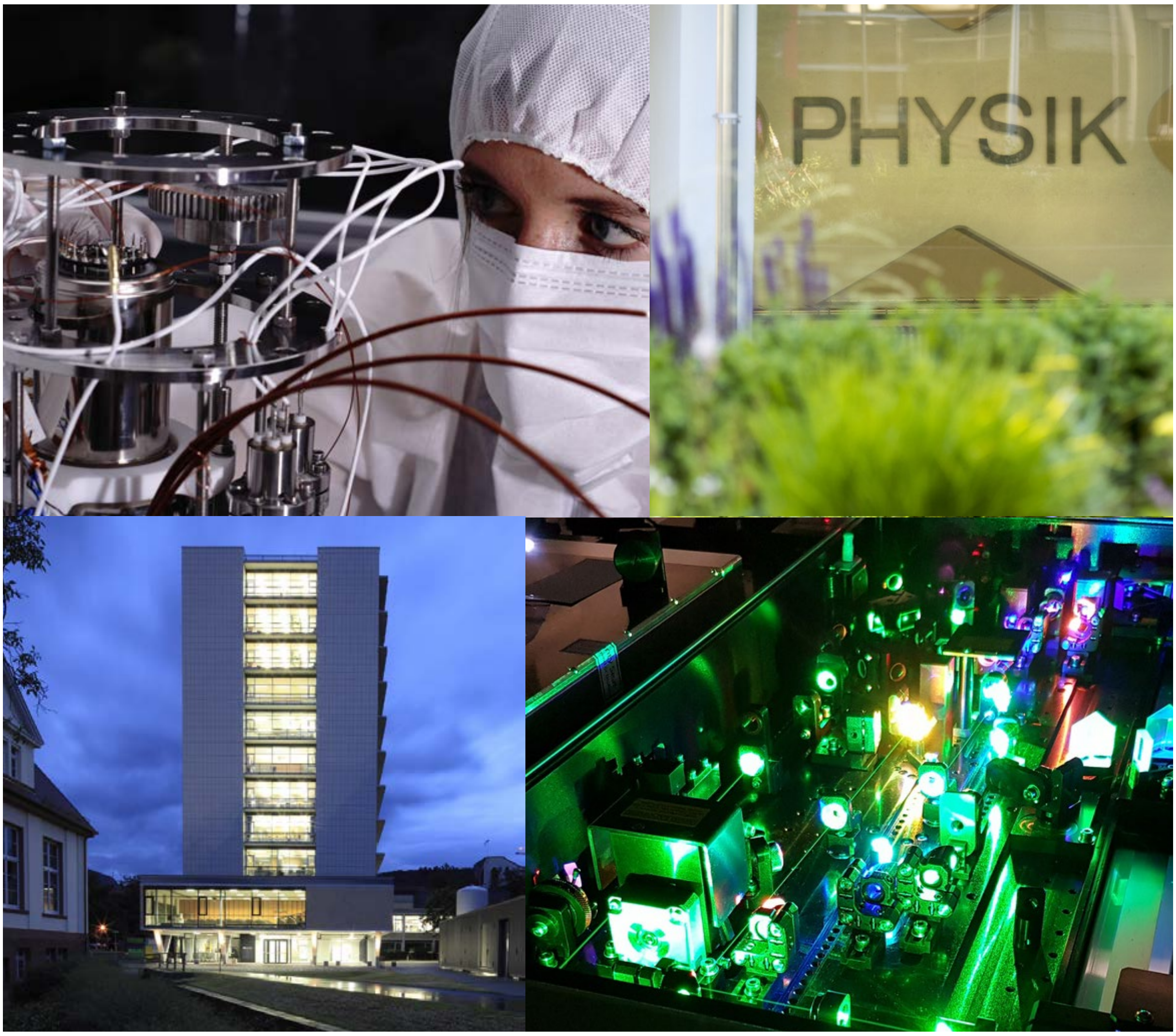
The present activity report provides a concise description of the scientific activities of the research groups during the years 2018 to 2021, of the teaching and outreach program, and of the available infrastructure. The part of the scientific activities is divided into three main chapters dedicated to the three main research areas of the institute. The variable structure of these chapters reflects the diverse and lively scientific cultures of the research areas at this institute.

Following the inaugural meeting of the Scientific Advisory Board on July 17./18., 2014, and its 2nd meeting on April 12./13., 2018, the 3rd meeting is scheduled for April 4./5., 2022.

Contents

Part I

The Institute of Physics



Chapter caption: Collection of photos providing an impression of the Institute of Physics in Freiburg (image credits: R. Glade-Beucke, M. Herrmann, Group Stienkemeier).

1.1 Overview

The Institute of Physics (IoP) is one of the two sections in the Faculty of Mathematics and Physics of the Albert-Ludwigs-University of Freiburg. Its members conduct research in a wide range of areas, covering particle physics and field theory, physics at atomic and molecular scales, as well as solid state physics and very complex systems such as polymers. With currently (February 2022) 22 full professors, five permanent lecturers (apl. Professor), one junior professor and three co-opted members, the department is of moderate size compared to others in Germany, however, it offers its students a broad range of topics covering all major aspects of physics in lectures, seminars and laboratories.

The institute is embedded in the interdisciplinary research landscape defined through the University of Freiburg and other institutions in the larger Freiburg area. This includes Freiburg's five Fraunhofer Institutes, the Leibniz Institute for Solar Physics (KIS), the EUCOR partners (KIT and the Universities of Basel, Strassbourg and Mulhouse) but also extends to several international laboratories (CERN, DESY, LNGS, FERMI FEL etc.). This environment and the broad research diversity offered make the institute attractive for national and international researchers and students.

At the end of the year 2021, 566 students were enrolled in Bachelor of Science, Master of Science or Teacher-training studies ("Lehramt"). A total of 126 young researchers work towards their PhD degree, and 87 institute members are at the PostDoc stage of their career. Together with faculty and the administrative and technical staff, our team comprises 295 individuals who are committed to foster and deliver high-quality academic research and training.

1.1.1 Location and Buildings

The Institute of Physics is organized as a department composed of 14 experimental and 11 theoretical research groups. Ideally, all research activities should be concentrated at the central site of the Institute at Hermann-Herder-Straße 3 and 6 (see Fig. 1.1), however, due to substantial lack of (modern) laboratory space at the central site, all experimental groups suffer from severe space constraints and have to cope with non-ideal working conditions. Two experimental groups (Sansone, von Issendorff) even have to be accommodated outside of the physics campus in the "Verfügungsgebäude"; other groups are facing problems (e.g., access, ventilation, floor load) in the old workshop/laboratory building between the Physics High-Rise and the Gustav-Mie Building as well as in the former accelerator building. The long standing plan to improve the situation and to provide a modern, competitive environment is to build a new building right next to the main physics campus (see Fig. 1.1, blue circle). Unfortunately, again no decision towards the construction of this building has been taken within this reporting period and there is currently no concrete schedule. The general lack of laboratory space also seriously impacts the ability of the institute to host prestigious externally funded junior research groups (e.g., ERC starting grantees, Emmy-Noether-groups).

Fortunately, all teaching activities can be carried out at the central site. Also the library of the institute as well as a large number of student work places and the examination office ("Prüfungsamt") are located here. This allows for regular direct contacts between lecturers, the local research staff and students.

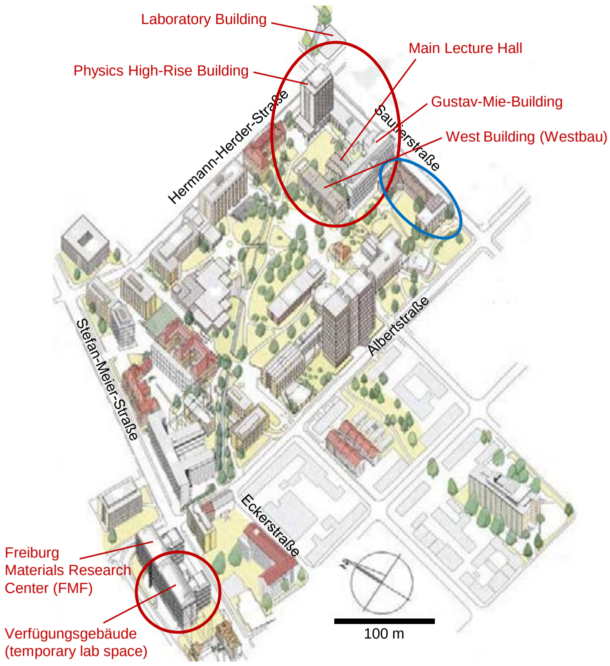


Figure 1.1: Map of the Natural Sciences Campus highlighting the buildings currently employed by the Institute of Physics (red) and the site of the projected new physics building (blue).

1.1.2 Organization

The organization structure of the Institute of Physics is shown in Fig. 1.2: the institute is led by the Managing Director, assisted by the senior manager as head of the central administration and the deputy senior manager/head of technical services. The teach-

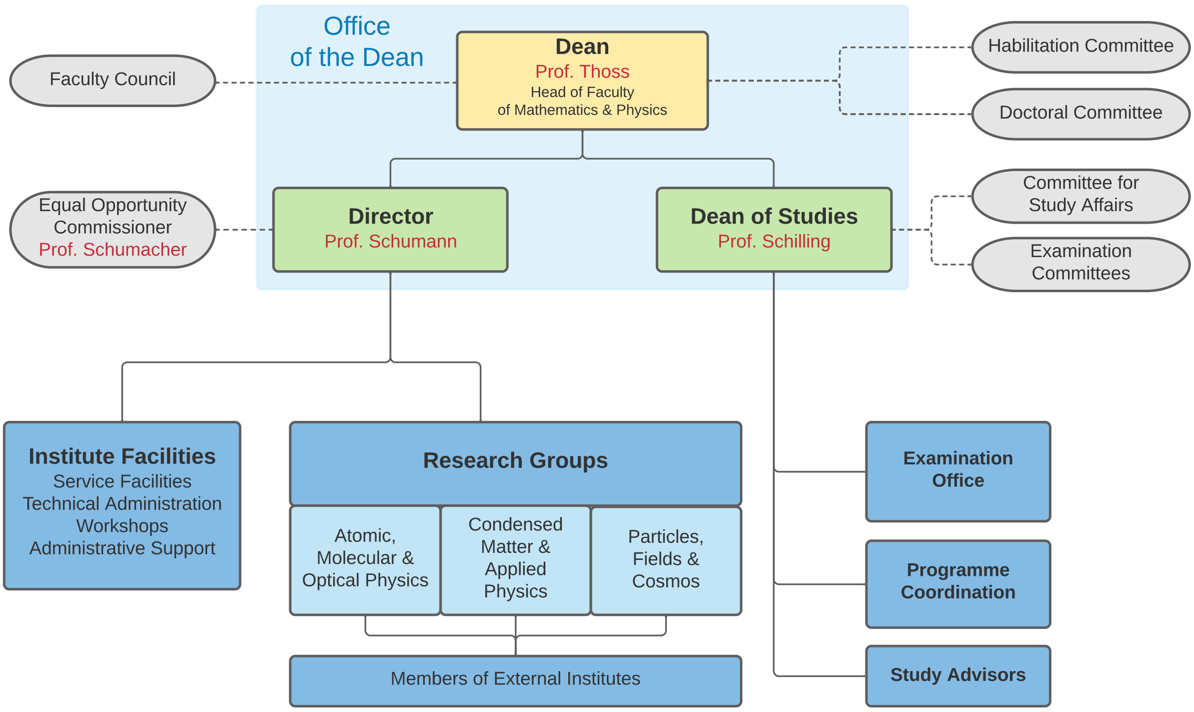


Figure 1.2: Organization chart of the Institute of Physics. Together with the Institute of Mathematics, the Institute of Physics constitutes the Faculty of Mathematics and Physics.

ing administration is led by the Dean of Studies, assisted by the program coordinator, the study advisers and the examination office. The offices of the Managing Director (at present Prof. M. Schumann) and the Dean of Studies (Prof. T. Schilling) are executed by full professors of the institute for a period of typically two years. The Institute of Physics is one of the two entities within the Faculty of Mathematics and Physics. The faculty's executive body is the Faculty Board, with the Managing Director of the Institute of Physics and the Dean of Studies (Physics) as official members. The faculty's official decision taking body, including professors, permanent staff, PhD/PostDoc representatives and students, is the faculty council (Fakultätsrat). The Offices of Dean of the faculty (at present, Prof. Thoss, Institute of Physics) and first Vice-Dean (Prof. Kebekus, Managing Director of the Institute of Mathematics) alternate between the Institutes of Mathematics and Physics, in intervals of typically two years. The position of the second vice-Dean (at present Prof. Schumann) is usually taken by the institute director of the unit which provides the Dean. The two institutes, of Physics and Mathematics, work closely together at the faculty level, and regarding strategic decisions for the faculty, but operate largely independently in terms of administration, finances and teaching given their rather different requirements.

The institute's central administration takes care of general management duties, ranging from maintaining the infrastructure, management of personpower and staff to organization of the financial budgets provided by the university as well as third-party funding. The head of the central administration is Dr. Holzer. It is also responsible for the organization of the teaching program of the institute. These efforts are led by the Dean of Studies. This also includes dealing with compatibility issues between the curricula of various study programs, also at other faculties, as the institute offers physics courses for many other faculties (e.g., medicine, biology, chemistry, earth sciences).

Support for the research groups at the institute is provided by a technical support department comprising technical experts: the support units "Mechanics" and "Electronics" as well as the IT Group represent the backbone of the research infrastructure.

More detailed information on the infrastructure, facilities and support units of the Institute is provided in Chapter IV.

1.1.3 Research

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

Research Groups at the Institute of Physics

Atomic, Molecular and Optical Physics

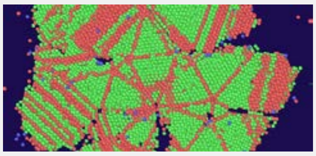
Experimental Physics

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

Theoretical Physics

- **Quantum Optics and Statistics**
  Prof. A. Buchleitner
  apl. Prof. H.-P. Breuer

Condensed Matter and Applied Physics



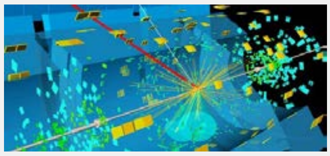
Experimental Physics

- **Experimental Polymer Physics**
  Prof. G. Reiter
- **Nanophysics and Molecular Nanomagnets**
  Prof. O. Waldmann
- **Solar Energy – Materials and Technology**
  Prof. A. Bett (IoP and ISE)

Theoretical Physics

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

Particles, Fields and Cosmos



Experimental Physics

- **Experimental Particle Physics**
  Prof. B. Heinemann (IoP and DESY)
- **Experimental Particle Physics**
  Prof. G. Herten,
  apl. Prof. U. Landgraf
- **Experimental Particle Physics**
  Prof. K. Jakobs
  Hon.-Prof. P. Jenni
  Emmy-Noether Group
  S. Argyropoulos
- **Experimental Particle Physics**
  Prof. M. Schumacher
- **Experimental Astroparticle Physics**
  Prof. M. Schumann
  apl. Prof. H. Fischer

Theoretical Physics

- **Theoretical Astroparticle Physics**
  JProf. S. Vogl
- **Theory of Particle Physics and Quantum Field Theory**
  Prof. S. Dittmaier
- **Theoretical Particle Physics and Phenomenology**
  NN

Members of external Faculties & Institutes

Leibniz Institute for Solar Physics (KIS)

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

University of Freiburg

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

Fraunhofer Institutes

- **Solar Energy Systems (Fraunhofer ISE)**
  Prof. A. Bett
- **Theoretical Materials Physics (Fraunhofer IWM)**
  apl. Prof. C. Elsässer
  Prof. M. Moseler
- **Spectroscopy of Optical Materials (Fraunhofer IPM)**
  PD F. Kühnemann

* co-opted members of the Institute of Physics

Figure 1.3: Research groups at the Institute of Physics and at external institutes - status as of January 2022. (IoP = Institute of Physics, KIS = Leibniz Institute for Solar Physics, IMTEK = Department of Microsystems Engineering, IWM = Fraunhofer Institute for Mechanics of Materials, IAF = Fraunhofer Institute for Applied Solid State Physics, IPM = Fraunhofer Institute for Physical Measurement Techniques, ISE = Fraunhofer Institute for Solar Energy Systems. Institutes outside of Freiburg: HZB = Helmholtz-Zentrum Berlin, DESY = Deutsches Elektronen Synchrotron Hamburg)

Atomic, Molecular and Optical Sciences: The atomic and molecular physics group has a broad expertise ranging from quantum optics, ion trapping, femtosecond spectroscopy of macro-molecular structures, cluster physics, the use of strong-field and XUV-/X-ray radiation to attosecond physics The groups share expertise and interest in controlling systems at the level of individual quanta to permit the detailed analysis from few atoms up to complex structures and transport processes on very diverse scales. The activities of the Leibniz Institute for Solar Physics (KIS) which also heavily rely on optics are also part of this group (see Part I, Sec. 1.2).

Condensed Matter and Applied Physics: The broad context of the condensed matter and applied physics research area is the investigation of classical and quantum theories of complex systems, with a strong computational component, in combination with topics of applied experimental research on polymers, nano-magnetism, biology and photovoltaics.

Particles, Fields, Cosmos: The institute accommodates several internationally very visible experimental and theoretical particle physics groups. The experimental program is mainly focused on experiments at the European Centre for particle physics, CERN, in Geneva/Switzerland and at the Italian underground laboratory LNGS. Physicists from the institute have contributed significantly to the precise investigation of the Higgs boson and the search for phenomena from "new physics" via their strong involvement in the ATLAS experiment. The astroparticle physics group concentrates on the direct search for dark matter and other very rare processes. The activities in theoretical particle physics range from precision studies of the strong and electroweak interactions and aspects of quantum field theory to theoretical astroparticle and neutrino physics.

During this reporting period, the researchers of the Institute of Physics published several hundred articles in international, peer-reviewed journals providing the optimal reach and environment for the respective subjects; examples from every group can be found in Part II. Competitive funding from national (mainly DFG and BMBF) and international sources (EU etc.) was attracted, significantly exceeding the direct funding provided by the University. Four research groups carried out research activities funded by ERC grants during this reporting period: CoG "NANOREACTOR" (PI Dzubiella, 2015-2020), CoG "TIAMO" (PI Schaetz, 2015-2021), AdG "COCONIS" (PI Stienkemeier, 2016-2022), CoG "ULTIMATE" (PI Schumann, 2017-2022).

A new DFG Research Unit (Forschergruppe) FOR 5099 "Reducing complexity in non-equilibrium systems" was established for four years (spokespersons Stock and Thoss). A new permanent researcher position was created for S. Wolf, a PI of this Research Unit. The institute's programs for young researchers, such as research training groups (RTGs), are listed in Sect. 1.1.5

1.1.4 Activities, Events, Positions

In this section we summarize some of the most important activities and events that took place in Freiburg, organized by members of the institute, during the reporting period. We also list important changes in the institute's personnel and some highlights regarding awards and mandates.

Activities

With more than 900 participants, one of the highlights during the reporting period was the *1st DPG Fall Meeting*, dedicated by the German Physical Society (DPG)'s three sections to the topic "Quantum Science and Information Technologies", in Freiburg on September 23-27, 2019 (chair: Buchleitner), see Fig. 1.4. This pilot event of a new, cross-disciplinary, topical DPG conference format brought together physicists from atomic and molecular, condensed matter, high energy, fundamental, applied and industry physics, all with a joint interest in various aspects of information science and quantum technologies. Given the very positive feedback from participants and across the DPG community, the DPG decided to establish topical Fall Meetings as a regular element of its conference portfolio.

Two international conferences were hosted at the Institute of Physics during the reporting period: *High Precision for Hard Processes* (HP2 2018) in Octo-

Figure 1.4: Participants of the German Physical Society's 1st Fall Meeting, dedicated to "Quantum Science and Information Technologies", in September 2019, in Albert-Ludwigs-University's Kollegiengebäude II. The meeting took place in the very city centre, around the Platz der Alten Synagoge (image credits: DPG/Patrick Seeger).

ber 2018 (Dittmaier, Ita et al.) and *Axion-WIMP* (PATRAS 2019) in June 2019 (Schumann, Fischer). In addition, two PhD schools were held in Freiburg: the *DFT Spring School 2019* in March 2019 (Härtel) and the *Freiburg-Nagoya-Strasbourg International Summerschool 2019* on ”Sustainability, Ethics and Transformation” (Buchleitner).

While the world-wide Covid-19 pandemic severely affected everybody’s daily life and also the scientific community, it is worth noting that the Institute of Physics remained largely operational and always open for its members.

Prizes, Awards and Mandates

Prof. Jakobs served as *spokesperson* of the international ATLAS collaboration ($\sim$3000 members) at CERN from 2017-2021. During his leave of absence his research group in Freiburg was led by interim professor Weiser.

Apl. Prof. Fischer received the *Teaching Award 2019* of the University of Freiburg for his experiment-based teaching, especially in the introductory lecture for students of medicine, and for his annual Christmas Lectures.

Prof. Sansone received the *Innovation Award Synchrotron Radiation 2020* for developing innovative investigation methods exploiting the radiation emitted by seeded free electron lasers even on the attosecond scale.

Apl. Prof. Filk, together with Andreas Woitzik und Clara Fuchs received the *Teaching Award 2021* of the University of Freiburg for their innovative lecture ”Compact Advanced Physics” which is targeting future teachers. Prof. Filk was also awarded a *WE-Heraeus-Senior Professorship* for innovative teaching concepts in physics.

Prof. Heinemann, W3-professor for experimental particle physics jointly appointed together with DESY Hamburg, was appointed *research director* for the area ”high-energy physics” at DESY in December 2019. She is the first woman in the DESY directorate since its foundation in 1959. Prof. Heinemann has an active research group at the Institute of Physics and and will continue to research and teach in Freiburg.

Dr. L. Bruder (group Stienkemeier) and Dr. V. Lang (group Schumacher) have received elite PostDoc fellowships from the BW foundation in 2020 and 2021, respectively. This program funded by the state Baden-Württemberg allows promising PostDocs to conduct an independent research project.

Dr. K. Dulitz (group Stienkemeier) has received the Liebig Fellowship (Fonds der Chemischen Industrie) which has allowed her to establish her own junior research group at the Institute of Physics.

Positions and Developments

During this reporting period, the institute has seen several important developments which will shape its future:

- Prof. Dzubiella (Helmholtz-Zentrum Berlin, HU Berlin) was newly appointed as W3-Professor of ”Applied Physics - Computational Physics” to strengthen the Master of Applied Physics.

- With a total of five institutes, Freiburg is the largest site of the Fraunhofer Gesellschaft for applied research in Germany. To further strengthen the cooperation with the local Fraunhofer Institutes, Prof. Bett (Fraunhofer ISE) was appointed on a joint W3-professorship for ”Solar Energy – Materials and Technology”. In addition, PD Kühnemann (Fraunhofer IPM) was appointed lecturer (Privatdozent) at the institute.

- Prof. van der Bij (Theoretical Particle Physics) retired end of 2021. His succession was already fixed in 2016 with the successful evaluation of the tenure track program of JProf. Ita and his promotion to full professor (W3).

- JProf. Vogl (MPP Munich) was appointed to succeed JProf. Ita on a (non-tenure track) W1-junior professorship. He started in 2020 and is working on Theoretical Astroparticle Physics – a new scientific topic in Freiburg.

- Prof. Ita left the Institute in fall 2021 for personal reasons and moved to the Paul Scherrer Institute (PSI, Switzerland). The process to appoint a new Professor for Theoretical Particle Physics was already started; the new colleague’s research profile is expected to complement the existing groups.

- Prof. Hennig (University Hospital Freiburg), co-opted at the Institute of Physics, retired in 2021. His research is continued by Prof. Bock (University Hospital) who is also co-opted.

- Prof. von der Lühe, who holds a joint W3-professorship with the Leibniz Institute for Solar Physics (KIS), will retire in 2022. The process to appoint a new professor for Experimental Solar Physics jointly with KIS was already started; four candidates presented themselves in March 2022.

- Prof. Herten (Experimental Particle Physics) extended his contract for two years and will now retire in 2023. The process to appoint his successor was already started. To complement and broaden the institute's particle physics profile, the new colleague should work on experimental flavor physics of heavy quarks and/or leptons including neutrinos.

1.1.5 Education and Qualification of Young Researchers

Within the boundary conditions imposed by the university and the state, the institute strives to optimally train its young scientists to prepare them for a successful career inside and outside of science.

Several externally funded research training groups (RTGs) were active at the institute in the reporting period. These RTGs offer funding to excellent doctoral researchers but – equally important – also establish environments for research and fruitful collaboration and provide advanced academic and non-academic training.

- The Research Training Group (RTG) *Mass and Symmetries after the Discovery of the Higgs Particle at the LHC* (RTG 2044, funding period 2015–2019) received funding for a 2nd period (2019-2024).
- The International Research Training Group (IRTG) *Cold Controlled Ensembles in Physics and Chemistry* (IRTG 2079), together with partners at the University of British Columbia (Vancouver, Canada) was funded in the period 2015–2020 and received extension funding 2020–2022.
- The new RTG *DynCAM – Dynamics of Controlled Atomic and Molecular Systems* was approved in 2021 and will start its first period in 2022 (RTG 2717).
- The International Research Training Group (IRTG) *Soft Matter Science: Concepts for the Design of Functional Materials* (IRTG 1642), together with the Faculty of Chemistry and Pharmacy of the University of Freiburg, and partner groups at Strasbourg and Mulhouse, ended in 2019 after its second funding period.
- The EU-funded international graduate school *QUSTEC – Quantum Science and Technologies at the European Campus* was established in collaboration with the Universities of Basel and Strasbourg, KIT Karlsruhe, as well as the research division of IBM Zurich (funding period 2019-2024).

Support for excellent postdoctoral researchers is provided by the *Georg H. Endress Postdoc Cluster on Quantum Science and Quantum Computation*. It was established in 2018 in collaboration with the University of Basel and is expected to run for 10 years.

In addition to the already existing Emmy-Noether-Group of S. Buhmann, three new junior research groups were established at the Institute of Physics during the reporting period: S. Vogl (theoretical astroparticle physics) was appointed as junior professor (W1), S. Argyropoulos (experimental particle physics) started an Emmy-Noether-Group and K. Dulitz (molecular physics) started her group funded by a Liebig Fellowship. Reports from these groups can be found in Part II of this report.

Ten advanced junior researchers from the institute received permanent academic positions:

- Stefan Buhmann (Emmy-Noether-fellow in group Buchleitner) accepted a full professorship at the University of Kassel,
- Robert Bennett (PostDoc in group Buhmann) received a lecturer position at the University of Glasgow,
- Alberto Rodriguez (Akad. Rat in group Buchleitner) received a faculty position (Profesor titular de Universidad) at the University of Salamanca,
- Lei Zhang (PostDoc in group Jakobs) became professor at Nanjing University,
- Fernando Febres Cordero (visiting professor in groups Ita/Dittmaier as recipient of the Sofja Kovalevskaja Award) accepted an associate professorship at Florida State University Tallahassee,
- Samuel Abreu (PostDoc in group Ita) obtained a staff position at CERN and a lecturer position at Edinburgh University,
- Kathrin Becker (PostDoc in group Schumacher) was appointed as lecturer/assistant professor at the University of Warwick,
- Shigeki Hirose (PostDoc in group Jakobs) joined the University of Tsukuba as assistant professor,
- Clemens Kreutz (PostDoc in group Timmer) became permanent group leader the Institute of Medical Biometry and Statistics (IMBI) at Freiburg University Hospital, and
- Rajagopal Seelam (PostDoc in group Thoss) was appointed assistant professor at the Central University of Rajasthan.

1.1.6 Equal Opportunity Measures

The Institute of Physics strives to establish an environment which provides equal working conditions and career opportunities for all employees at all career stages including students, regardless of gender, ethnicity, etc. The faculty for Mathematics and Physics employs an equal opportunity officer and a deputy, one from each institute. At present, Prof. Huber-Klawitter (Mathematics) is equal opportunity officer and Prof. Schumacher (Physics) her deputy. Expenses for equal opportunity measures were directly covered by the general institute budget so far, however, efforts are ongoing to establish a dedicated equal opportunity budget at faculty level.

The mentoring program for female doctoral researchers and PostDocs *kite* (`www.kite-mentoring.uni-freiburg.de`) consists of the three pillars mentoring, training and networking. While the program was initially only available for researchers of the research training groups, it is now open for all female members of the Faculty of Mathematics and Physics.

To support parents in increasing the compatibility of studying/working and raising children a "kids-parents room" was created in the "Westbau" and is almost ready to be used. (The completion was somewhat delayed by Covid-induced shortage of material and construction companies.) It provides space for children and their parents, is equipped with toys and can be accessed with strollers.

In order to foster the exchange between parents about challenges and possible solutions regarding the compatibility between studying/working while raising children, a dedicated e-mail-list is in place since many years and bi-monthly meetings are held which are open for all parents at the faculty. Bi-monthly meetings also take place for female researchers at the faculty (doctoral students, PostDocs, faculty members and guest scientists) to discuss topics of research, family planning and career opportunities.

The faculty strives to increase the fraction of female researchers in particular at professorship level and intensively uses the instrument of "proactive search" in the appointment procedure to identify qualified female researchers and to encourage them to apply.

Additional measures for students are discussed in Part III, Section 1.8.2,

1.2 Associated Institutes and co-opted Members

In various research fields, the institute has long-term institutional partnerships with other faculties within the University of Freiburg, as well as with external research institutions (see Fig. 1.3). The program of the Master of Applied Physics was established together with several of these institutions and they actively contribute to its curriculum.

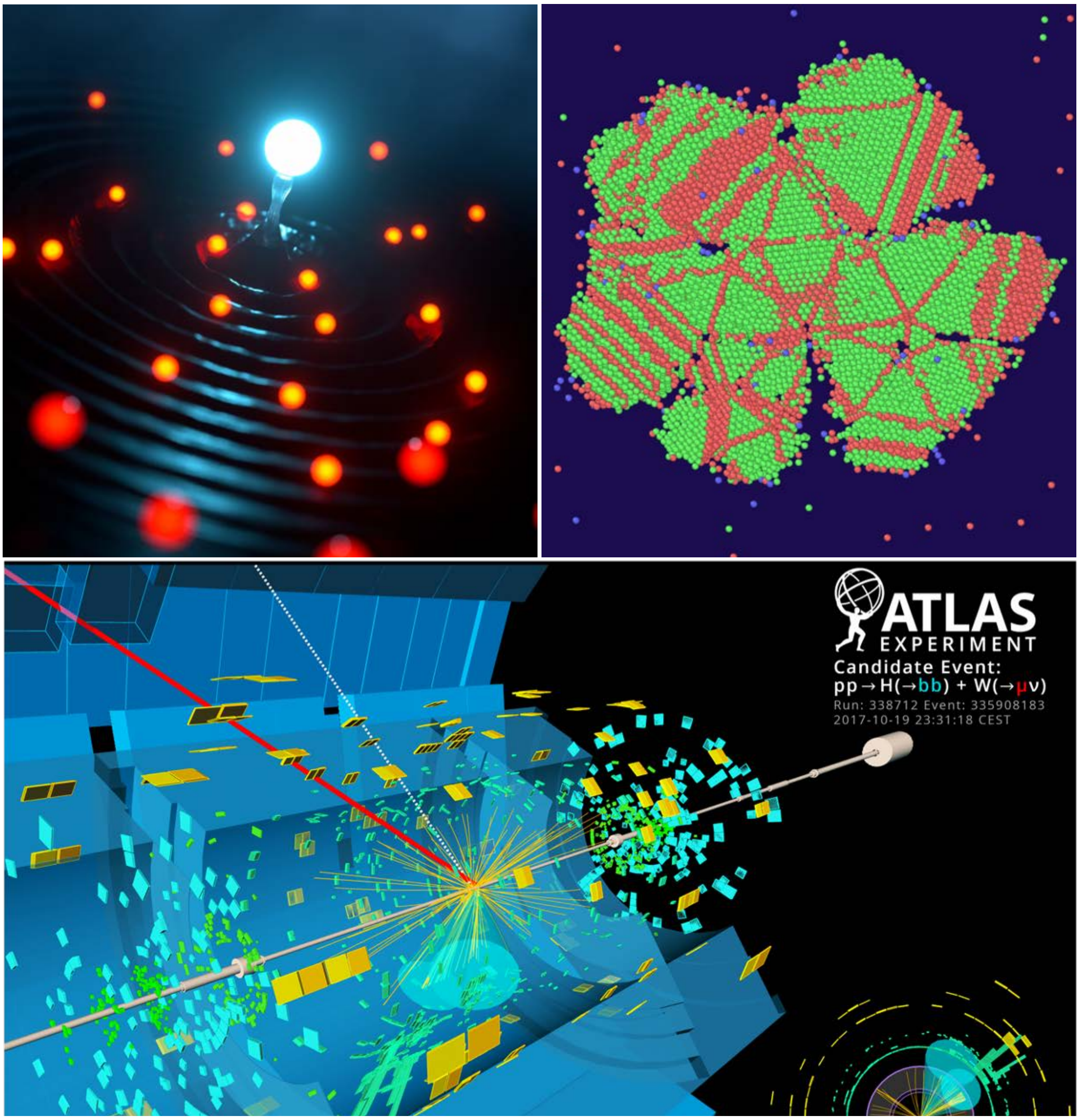
As of today, six professors of the Institute of Physics hold joint appointments with external institutes. These are Prof. von der Lühe and Prof. Berdyugina (Leibniz-Institut für Sonnenphysik (KIS) of the Leibniz-Gemeinschaft), Prof. Moseler (Fraunhofer Institute for Material Mechanics, IWM), Prof. Bett (Fraunhofer Institute for Solar Energy Systems, ISE), Prof. Lau (Helmholtz Zentrum Berlin, HZB of the Helmholtz-Gemeinschaft), and Prof. Heinemann (DESY Hamburg of the Helmholtz-Gemeinschaft).

Three colleagues from other faculties, Prof. Rotter (Faculty of Biology), Prof. Bock (Faculty of Medicine) and Prof. Rohrbach (Faculty of Engineering) are co-opted members of the Institute which means that they can supervise PhD theses in physics. Prof. Hennig (Faculty of Medicine), who retired at the end of 2021, was also co-opted. Several members of external institutes such as Fraunhofer IWM, Fraunhofer IPM, Fraunhofer IAF, Leibniz Institute für Sonnenphysik (KIS), Helmholtz Zentrum Rossendorf teach at the Institute of Physics and supervise theses.

On the other hand, some members of the institute actively conduct research programs at the Research Centres of the University, such as the *Freiburg Materials Research Centre (FMF)*, the *Freiburg Centre for Data Analysis and Modelling (FDM)*, and the *Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien (FIT)*.

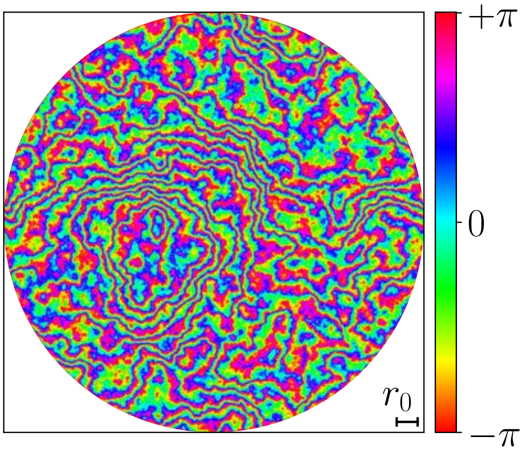
Part II

Scientific Activities 2018 - 2021



Chapter 1

Atomic, Molecular and Optical Sciences



- **Quantum Optics and Statistics**
  A. Buchleitner
  H.-P. Breuer
  S.Y. Buhmann (Univ. of Kassel)
  A. Rodríguez (Univ. of Salamanca)
  T. Wellens (Fraunhofer IAF, Freiburg)
- **Experimental Attosecond and Laser Physics**
  G. Sansone
- **Experimental Atomic, Molecular and Optical Physics**
  T. Schätz
- **Molecular and Nanophysics**
  F. Stienkemeier
  K. Dulitz
- **Clusterphysics**
  B. von Issendorff
- **Cluster and Synchrotron Spectroscopy**
  T. Lau (IoP and HZB)
- **Solar Physics**
  S. Berdyugina (IoP and KIS)
  M. Roth (IoP and KIS)
  O. von der Lühe (IoP and KIS)

Chapter caption, left: Color-coded phase shifts of light propagating in a turbulent atmosphere. The turbulence strength is characterized by the transverse correlation length r_0. Right: Artistic view of an individual ion interacting with several atoms simultaneously via their wave-like characters (image: Ella Marushchenko).

1.1 Overview

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

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

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

The extension of the study of atomic quantum objects to complex molecular systems is a central research topic in the group of **F. Stienkemeier**. Low temperature conditions allowing for well defined initial states are established in cold beams as well as helium droplets. Intense electromagnetic fields including XUV free-electron lasers broaden the range of experimental tools to form and study extreme states of matter. The junior research group of **K. Dulitz** is extending this research theme to detailed investigations of the mechanisms that govern reactive collisions under cold and controlled conditions. The group of **B. von Issendorff** has pioneered the structural and thermodynamic study of clusters of atoms, exploring the transition region between the nanoscopic and the microscopic regime, where fundamental properties of matter strongly change as function of size and temperature. The group of **G. Sansone** focuses on the generation of trains and isolated attosecond pulses by high-order harmonic generation in gases and using seeded free-electron lasers. The pulses are applied for the time-resolved investigation of nuclear and electronic dynamics in molecules and clusters, with particular attention to coincidence techniques that enable the characterization of molecular dynamics in the molecular frame. Since January 2018 **T. Lau** holds the new professorship established together with Helmholtz-Zentrum Berlin. He works in the field of synchrotron spectroscopy of size-selected free clusters, molecules, and complexes with a focus on understanding and controlling their electronic states and magnetic moments.

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

These topics of AMO Sciences at the Institute of Physics are covering a wide spectrum while remaining closely interlinked. In addition, they are getting strengthened by local, national and international collaborations. In the following we briefly describe ongoing, new and planned collaborative research and training initiatives.

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

The *Georg H. Endress Postdoc cluster* at the *Centre for Quantum Science and Quantum Computing (QSQC)*, mainly funded by the Georg H. Endress foundation and embedded within EUCOR – the European campus, is a cross-border collaboration between the University of Basel (Switzerland) and the Albert Ludwigs University of Freiburg. It represents a dedicated ten-year initiative to foster and educate outstanding young scientists to provide the academic talent and technology skills for the rapidly developing field of QSQC. The Center seeks to attract outstanding and highly motivated early-career scientists in QSQC to engage in cutting-edge projects involving the existing quantum science research groups in Basel and Freiburg. Since 2018 the Center has already appointed 18 Fellows for maximally three years each, and has recently opened a new call aiming to appoint up to six new Fellows. The main research areas of the Center involve quantum computation and quantum simulation, sensing and metrology, quantum technologies, complex quantum systems, quantum materials, and other emerging topics in quantum science.

QUSTEC - Quantum Science and Technologies at the European Campus (funding period 2019 – 2025)
QUSTEC is a doctoral training programme which has been established by the European Grouping of Territorial Cooperation (EGTC) and EUCOR – The European Campus. The doctoral school consists of 37 PhD students which benefit from an outstanding training and research programme in the field of Quantum Science and Technology. The PhD research projects are carried out at the Institute of Physics, Albert Ludwigs University of Freiburg, and the other QUSTEC partner institutions:

- University of Basel, Switzerland
- Karlsruhe Institute of Technology, Germany
- University of Strasbourg, France
- IBM Research – Zurich, Switzerland
- Walther-Meißner-Institute for Low Temperature Research, Germany

These institutions offer a wide spectrum of highly topical and innovative research themes. The QUSTEC programme has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie actions (MSCA) COFUND scheme for a five-year period with a total amount of 9.1 million euros. In addition to 4.2 million euros from the European Union, there is co-financing from the participating partner organisations as well as from *Santander Universities.*

DFG-funded IRTG 2079 "Cold Controlled Ensembles in Physics and Chemistry" (funding period 2015 – 2019, extension funding 2019 – 2022)

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

The IRTG provides a structured doctoral program including seminars, summer schools, meetings, and guest programs. The research is of interdisciplinary character and connects to diverse fields of atomic and molecular physics, quantum optics, condensed-matter physics, and physical chemistry. The involved groups efficiently foster synergy effects in technological developments, scientific achievements as well as for creating a unique training environment for young scientists. All doctoral projects are embedded into binational collaborations between the IoP and UBC and include long-term stays at both locations. Doctoral projects are co-supervised, having one German and one Canadian supervisor. The extended working periods in Freiburg and Vancouver offer a tremendous advantage for the qualification of the doctoral students, both for a future career in academia as well as in industry, due to the added interdisciplinary and intercultural experiences. In addition, the collaborative research is enhancing the educational program of the Institute of Physics, from the Bachelor to the PhD level, by dedicated seminars, summer schools, meetings, and guest lectures. The graduate school includes more than 35 doctoral researchers and several Postdoctoral fellows in Freiburg and at UBC.

From 2015 to 2021, the doctoral and postdoctoral researchers of the IRTG 2079 published more than 100 scientific papers including many joint publications by UBC and the University of Freiburg. During this period, 28 doctorates were completed. The successful and productive cooperation has resulted in numerous joint projects that will be continued in the next years. In addition, the scientific exchange with the Mercator Fellows has further broadened international collaborations. The RTG 2079 expires in 2022.

DFG funded RTG 2717 "Dynamics of Cold Atomic and Molecular Systems" (funding period 2022 – 2026)

DYNCAM RESEARCH TRAINING GROUP DYNAMICS OF CONTROLLED ATOMIC AND MOLECULAR SYSTEMS

Building on the experience and activities of the IRTG 2079, a new DFG-funded Research Training Group (RTG 2717) was proposed, and was approved with a start in January 2022. The RTG 2717 "Dynamics of Cold Atomic and Molecular Systems" (DynCAM) focuses on the investigation and control of the electron and nuclear dynamics of systems in well-defined quantum states. Related experimental activities include modern techniques for producing controlled atomic, molecular and cluster arrangements, as well as new techniques in the generation and characterization of ultra-short light pulses. In a series of complementary experimental and theoretical projects, the involved researchers aim at studying interactions and dynamics at low temperatures and on ultra-short time scales.

In total, around 35 doctoral researchers and several postdoctoral researchers are expected to contribute at the IoP in Freiburg. Although the RTG formally is not an International Research Training Group, it will continue the close collaborations and exchange program with groups from the UBC in Vancouver, Canada.

Future plans

Together with colleagues from Condensed Matter and Applied Physics (see p. 67 below) and from the Institute of Mathematics, we seeded an initiative for an Excellence Cluster proposal in the next round of the German Federal Excellence Strategy for universities. The proposal – currently in preparation for a university-wide pre-selection process – merges complementary expertise on the characterization and control of complex systems, across diverse scales and disciplines. If retained by the university leadership, a pre-proposal will be submitted in 2023.

1.2 Research Groups

1.2.1 Quantum Optics and Statistics – Group Buchleitner

The **Department for Quantum Optics and Statistics is coached by Andreas Buchleitner, together with Deputy Coaches Heinz-Peter Breuer and, until 2019, Alberto Rodríguez González and Thomas Wellens**, and has been fortunate enough to host **Stefan Buhmann's Emmy Noether group, from 2014 to 2020**. Our research covers a broad spectrum reaching from quantum optics over atomic physics to statistical physics and quantum information science. We address mathematical and foundational aspects, concrete experimental scenarios, and potential technological applications. Much of our recent work derived inspiration from modern experimental approaches in atomic and molecular physics, quantum optics and optical communication, as well as from first the experimental platforms for quantum computation. During the reporting period, three **members of the team received faculty positions in Salamanca (Rodriguez), Glasgow (Bennett), and Kassel (Buhmann), or were hired (Wellens, Ketterer)** by the *Competence Center Quantum Computing Baden-Württemberg* at the Fraunhofer Institute for Applied Solid State Physics IAF in Freiburg. We co-initiated and ran, with the support of IoP's management and staff, the **1st Fall Meeting of the German Physical Society, in September 2019 in Freiburg**, dedicated to *Quantum Science and Information Technologies*. In 2021, we embarked on research projects under the roof of the *Competence Network Quantum Technology in BW*, as well as of the *Competence Center Quantum Computing Baden-Württemberg*.

Macroscopic Quantum Electrodynamics – Stefan Y. Buhmann

This former Emmy Noether group uses macroscopic quantum electrodynamics (QED) to describe the interaction of photons with atoms or molecules on the one hand and macroscopic media and bodies on the other. In this way, the impact of environments on fundamental quantum effects can be accounted for in the spirit of a generalised Purcell effect.

Starting from a focus on Casimir–Polder dispersion forces and their impact in a variety of areas, our activities have widened to include QED-based descriptions of excitation decay and transfer channels in photonic Bose–Einstein condensation, coming to a full circle with the recent direct detection of the quantum vacuum.

Applied dispersion forces

Solving a long-standing controversy, we have shown that the Abraham stress tensor leads to the correct description of dispersion forces in media [syb1], as later confirmed by our survey of experimental data. We have used this description to analyse the dynamics of ice formation, the escape of greenhouse gases from melting ice and the stability of gas hydrates on Enceladus and Pluto.

Quantum friction

Motivated by their impact on quantum friction, we have compared two paradigms of open quantum systems dynamics, namely the Markov approximation and linear response theory. The respective disjoint regimes of validity as marked by distinct asymptotic time scales can be bridged by a comprehensive description [syb10].

Poisson spot

Continuing our collaboration with the experimental group of Thomas Reisinger at the Karlsruhe Institute for Technology, we have analysed the Poisson-spot matter-wave signal of cold indium atoms to find clear evidence for the predicted impact of Casimir–Polder interacions [syb7].

Excitation decay and transfer

Building on our successful QED-description of interatomic Coulombic decay (ICD) [syb2], we have shown that the recently postulated super-ICD—an enhancement of the effect via mediator atoms—can be geometrically understood in terms of our analytical framework [syb4]. We have extended the perspective to include other energy decay channels such as Auger decay where renormalisation methods have to be applied.

Photonic Bose–Einstein condensation

At sufficient intensities, photons trapped in a cavity and equilibrating via dye molecules can form a Bose–Einstein condensate. We have used an open systems approach to establish a first-principles description of the responsible photon–dye dynamics. As a first application, we have shown that the photonic Bose–Einstein condensate can be used as a novel quantum sensor for chiral molecules; the scheme has been submitted to the European Patent Office.

Quantum-vacuum detection

In close collaboration with experimental group of Jérôme Faist at ETH Zurich, we have explored a new method for the direct detection of the vacuum fluctuations of the electromagnetic field: one or several ultrashort laser pulses traverse a nonlinear medium whose refractive index depends on the applied electric field. In the absence of such fields, the observed signal must therefore depend on the fluctuating vacuum field. We have established a description of the setup based on nonlinear quantum optics in striking agreement with experimental findings [syb9].

Future Plans

Following the appointment of Stefan Buhmann as full professor (W2) in November 2020, the group moved to the University of Kassel. Continuing joint activities with the Institute of Physics at the University of Freiburg include the following:

Discriminatory resonance energy transfer

Intialised within the framework of *IRTG Cold Controlled Ensembles in Physics and Chemistry*, we are currently studying to what extent resonance energy transfer depends on the handedness of donor, acceptor, and mediator.

Platforms for photonic Bose–Einstein condensation

As supported within the QUSTEC framework, we will exploit our general framework for photonic Bose–Einstein condensation to explore different geometries in close collaboration with experimentalists.

Polaritonic systems

In an ongoing collaboration with the Quantum Optics and Statistics group, we will explore weakly and strongly coupled polaritonic light–molecule states.

Quantum Theory of Open Systems – Heinz-Peter Breuer

An open quantum system is a quantum system which is coupled to some other quantum system, typically a complex environment, reservoir or heat bath, leading to large a variety of physical phenomena such as dissipation, decoherence, relaxation, irreversibility and the emergence of equilibrium and nonequilibrium stationary states. Central research topics are, in particular, Markovian and non-Markovian quantum processes [breuer9], detection of quantum correlations and entanglement [breuer4, breuer7, breuer8], quantum probing of complex systems [breuer6] and, more recently, the foundations of nonequilibrium processes in quantum thermodynamics [breuer1].

Quite recently we have performed a systematic study of non-Markovianity in quantum Brownian motion for a wide range of model parameters, including weak and strong dissipation [breuer5] (see Fig. 1.1). We have also carried out an analytical and numerical investigation of the driven Caldeira-Leggett model in order to examine classical and quantum system-environment and intra-environment correlations, and to compare different expressions for quantum entropy production [breuer2]. Quantum memory effects in the spin-boson model have been studied in collaboration with the group of Michael Thoss, employing numerically exact simulation techniques in the challenging regime of zero temperature [breuer3]. Fundamental features of quantum and classical non-Markovianity in many-body systems are examined within a project of the DFG research unit *Reducing Complexity of Nonequilibrium Systems.* Finally, questions on the experimental measurement of quantum non-Markovianity and on the influence of noise induced by quantum measurements have been investigated in a trapped-ion system in collaboration with the group of Tobias Schaetz [breuer10].

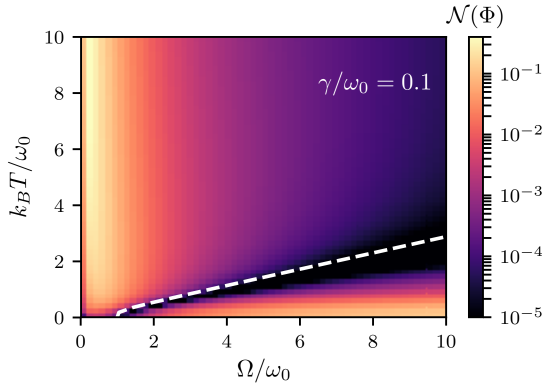


Figure 1.1: Degree of non-Markovianity $\mathcal{N}(\Phi)$ of quantum Brownian motion as a function of temperature and cutoff frequency [breuer5].

Nonequilibrium quantum thermodynamics

Quantum thermodynamics is concerned with the basic laws of equilibrium and nonequilibrium thermodynamics in the quantum regime. One of the topical fundamental problems in this field is a unique and consistent definition of work, heat and entropy production for nonequilibrium processes in open quantum systems coupled to thermal reservoirs [breuer2]. Despite numerous proposals, a satisfactory and generally accepted definition of these quantities has not yet been achieved, in particular in the regime of strong system-reservoir interactions, and the topic remains highly controversial. Presently, we are developing a general theory describing the thermodynamical behavior of open quantum systems coupled to thermal baths beyond perturbation theory [breuer1]. Our approach is based on the exact time-local quantum master equation for the reduced open system states, and on a novel principle of minimal dissipation illustrated in Fig. 1.2. This principle leads to a unique prescription for the decomposition of the master equation into a Hamiltonian part representing coherent motion and a dissipator describing decoherence. Employing this decomposition, we show how to define work, heat and entropy production, how to formulate the first and second law of thermodynamics, and establish the connection between violations of the second law and quantum non-Markovianity.

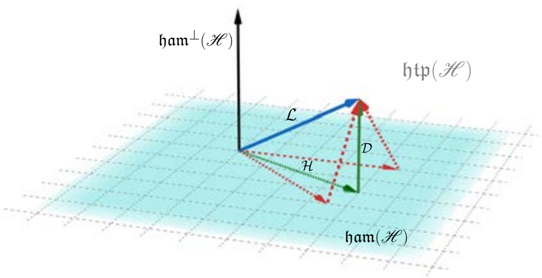


Figure 1.2: Illustration of the principle of minimal dissipation, which leads to a unique decomposition of the generator $\mathscr{L}$ of the master equation into a Hamiltonian part $\mathscr{H}$ and a dissipator $\mathscr{D}$ by requiring the dissipator to be minimal with respect to a suitable norm [breuer1].

Quantum Optics and Statistics (QOS) - Andreas Buchleitner

From 2018 to 2021, the Quantum Optics and Statistics group made a dedicated effort to analyse the potential of adaptive optics for free space quantum communication, elucidated the impact and potential of subtle quantum optical coherence phenomena in complex settings of light-matter interaction, made considerable progress in the description of spectral, dynamical and coherence properties of few to many-body quantum systems, and had a critical look at state of the art platforms for quantum computation.

Adaptive optics for free space quantum channels

In continuation of our earlier work on the decay of OAM (orbital angular momentum) entanglement of photons in turbulent atmosphere and across apertures (B.Sc. Unmüßig), we pushed our simulations to strong turbulence, where distortions of the photon's phase structure are amended by intensity fluctuations and optical vortices (PhD Sorelli).

In cooperation with the Fraunhofer Institute of Applied Optics and Precision Engineering (Jena), we investigated the potential of Adaptive Optics (AO) to reduce the detrimental effects of atmospheric turbulence. In particular, we could show that AO allows to realize a level of transmission fidelity which is required for secure quantum key distribution with higher dimensional entangled states, at moderate to strong turbulence strengths [abu1].

A radically different strategy to achieve robust state transfer explores localised eigenmodes as transfer channels (B.Sc. Schuler, M.Sc. Eichhorn, PhD Bachmann). The challenge consists in probing the medium's instantaneous transmission matrix on time scales short enough to beat random averaging by turbulent flow. After developing a computational tool box to accumulate simulation data, we currently obtain first, promising results. Our predictions on AO enhanced transmission as well as on eigenmodes of light in turbulence stimulated intense exchanges with groups in Ettlingen, Glasgow (PhD Bachmann), Johannesburg (M.Sc. Schneider, PhD Bachmann), Paris, and at Leibniz Instute for Solar Physics (KIS) in Freiburg, in view of possible experimental implementations.

Nonlinear multiple scattering of light on cold atoms

In an entirely different regime of light propagation across a disordered medium, we considered multiple scattering of intense, resonant laser light off a (dilute) cloud of cold atoms. The theoretical challenge lies in efficiently integrating the nonlinear inelastic response of the atomic scatterers to the incoming, intense radiation into a framework which describes the radiation transport within the medium. After a long-term effort, we finally succeeded to develop a general, scalable and readily implementable, yet numerically demanding solution to a problem hitherto deemed unsolvable (due to the exponential growth of the atomic Hilbert space with the number of atomic scatterers) [abu2]: A single atomic scatterer's response to the primary injected radiation as well as to the multiply scattered, polychromatic secondary field impinging on it, is exactly described by a single atom, quantum optical master equation. The secondary field at the location of the atomic scatterers is self-consistently generated by diagrammatic multiple scattering theory, including a disorder average which allows to reduce the number of diagrams that need to be retained for a proper description of the propagation in the medium.

Multiple quantum coherence in thermal atomic gases

A hitherto open debate on the origin of multiple quantum coherence signals collected from the fluorescence of dilute thermal atomic gases (in the group of F. Stienkemeier) inspired us to formulate a theoretical approach (M.Sc. Ames) which goes beyond the wide-spread treatment of the inter-atomic dipole interactions by its standard electrostatic form (mediated by *virtual* photons). Our analysis, which builds on central elements of our above theory of nonlinear multiple scattering, describes the essential physics in terms of double scattering of *real* photons on pairs of atoms. The reproduction of all the salient features of the experimental observations by our model demonstrates the relevance of the vectorial character of the incoming radiation as well as of the atomic dipoles, and of the disorder average induced by the atomic scatterers' thermal motion. This settles the debate.

Experimental verification of QOS' C-data protocol – and its range of applicability

Our statistical analysis of (non-interacting) many-particle interferences across random multi-mode scatterers triggered a collaboration with F. Sciarrino's group in Rome, where our *C-data protocol* – building on the (scalable) experimental probing and subsequent statistical analysis of all two-point correlators – was implemented in the lab [abu3]. We could demonstrate that the protocol not only distills distinctive features of many-particle interference upon transmission, but also distinctive features of the random scattering potential.

Yet, since the C-data set only probes a small subset of all information inscribed into the transmitted many-particle state, it is clear that some information remains unresolved (M.Sc. Brunner). To elucidate the detailed structure thereof and to identify the minimal experimental effort for its extraction is a current topic of our research (PhD Brunner).

Eigenvector and spectral statistics of interacting bosons

Complementary to our studies of many-particle quantum dynamics with respect to (in-) distinguishability, interaction strength [abu4], substructure (B.Sc. Dohse, Hoger, PhD Njoya), and spectral densities (M.Sc. Mielke, Schäfer, PhD Brugger), we explored the localisation properties of many-particle eigenstates of the Bose-Hubbard Hamiltonian (BHH) across its entire spectrum.

Numerical analysis of the ground state's generalised fractal dimensions (GFD) [abu5] established its many-body multi-fractality in Fock space, throughout the Mott and the superfluid phase, and an unambiguous signature of the transition. An extension of this study across the entire excitation spectrum of the Bose-Hubbard Hamiltonian (B.Sc. Schneider, PhD Pausch) identified the (energy resolved) eigenstates' GFD fluctuations as a particularly sensitive probe of the BHH's chaotic phase (where the eigenvectors approach ergodicity in the thermodynamic limit) [abu6]. Remarkable agreement of the lowest order moments of the GFD distribution with random matrix theory (RMT) goes hand in hand with ever more distinct features of the full GFD statistics. The latter provide robust tools for the certification of distinctive features of complex quantum systems.

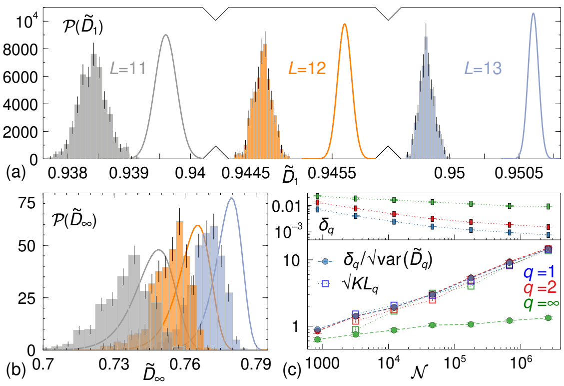


Figure 1.3: Probability distributions (coloured histograms) of the fractal dimensions $\tilde{D}_1$ (a) and $\tilde{D}_\infty$ (b) of the eigenvectors of the Bose-Hubbard Hamiltonian (BHH) vs. random matix (RMT) predictions (continuous lines), for increasing lattice size L. BHH and RMT distributions get more distinct with increasing Hilbert space dimension $\mathcal{N}$ (controlled by L), as illustrated in (c) by the distance δ_q of the distributions' mean values over the $\tilde{D}_q$'s variances, and by the square root of their Kullback-Leibler divergence KL_q [abu6].

Symmetry in many-particle interference

Many particle interferences can be certified by statistical features (see above), as well as by multiple interference-induced strict suppression laws for certain many-particle transmission events. The latter observation had led us to the formulation of zero-transmission laws for specific multi-mode scattering devices with particular symmetry properties. Yet the fundamental principle underlying distinct incidents of totally destructive many particle-interfences remained obscure.

Analysis of the symmetry properties of arbitrary many-particle states fed into a multi-mode scatterer [abu7] exposes the algebraic structure of unitaries which induce strict suppression of output configurations by destructive interference of all involved many-particle paths. These general symmetry considerations establish the hitherto missing link between the above special incidents of zero-transmission laws. Furthermore, they indicate how to reconstruct an input state's density operator from the counting statistics on output (B.Sc. Minke).

Many-body wave-particle complementarity

Since the occurrence of many-particle interferences sensibly hinges on the coherent superposition of many-particle transition amplitudes, the contrast of interference contributions to many particle counting statistics relies on the unavailability of *which-way information* on the many-particle level. The transition from fully indistinguishable to fully distinguishable many-particle paths unfolds through a hierarchy, because a given set of particles can be divided into subsets in multiple ways. This makes the quantum-classical transition on the many-particle level much more intricate than on that of a single particle. We quantified (interacting) many particle which way information through a many-particle state's entanglement between the interfering and the distinguishing degrees of freedom, and derived an inequality between the visibility of many-particle interference contributions and the level of available which way information [abu8]. This may pave the way for a systematic many particle decoherence theory (B.Sc. Grether, Neubrand, Wharam, M.Sc. Haen).

Benchmarking quantum computation platforms

In a collaboration with IBM Rüschlikon and Volkswagen Data:Lab we simulated and analysed the performance of Variational Quantum Eigensolvers (VQE) in finding the ground state of simple fermionic Hamiltonians, for different gate sets (ZuLa Welz) run within the VQE's quantum unit, and under variable levels of noise (ZuLa Woitzik) [abu9]. Through IBM, we could test the performance of this type of algorithms on actual hardware (IBM Q 5 Tenerife and Q 20 Tokyo) and found considerable drifts and inconclusive convergence behaviour garnished by strong fluctuations. We further observed (B.Sc. Fuchs, Strnad) that the optimal unitaries generated by the VQE exhibit the characteristic features of unitaries for optimal quantum state transfer – which we also encountered in the context of excitation transfer (B.Sc. Hess) in cold Rydberg ensembles.

With Volkswagen, we modelled the output of the D-Wave 2000Q quantum annealing hardware, with a minimal statistical model (M.Sc. Brugger). Our analysis of the real hardware's output infers a single qubit disorder strength in agreement with published data, and reveals the predicted scaling of the cumulated disorder strength with the register size (ranging from 10 to 2048 qubits). This suggests that static disorder is the dominant source of the statistical scatter of D-Wave output.

1.2.2 Experimental Attosecond and Laser Physics – Group Sansone

The **Attosecond and Ultrafast Science Group of Giuseppe Sansone** aims at investigating electronic and nuclear dynamics on ultrashort timescales (from few femtoseconds down to the few tens of attoseconds), by using few-cycle pulses in the near-infrared and visible spectral range, in combination with trains and isolated attosecond pulses generated by high-order harmonic generation (HHG) in gases. During the last four years, the group has developed two attosecond sources operating at 1 kHz and 50 kHz repetition rates, and delivering isolated and trains of attosecond pulses in the spectral region between 15 and 50 eV. The laboratories are equipped with advanced detection techniques, including extreme ultraviolet (XUV) spectrometers and a coincidence photoelectron-photoion spectrometer. The group is also active at large scale facilities delivering XUV pulses using table-top sources (ELI-ALPS, Szeged Hungary) and free-electron lasers (FELs) (FERMI and EuXFEL). The group takes advantage of the unique characteristics of the XUV radiation offered by these facilities, to design and perform experiments, which require specific, unprecedented properties of the radiation, such as the combination of high intensities and high-photon energy, and high-photon flux with shaping capabilities.

Research Report

Attosecond metrology and nonlinear spectroscopy at free-electron lasers

In 2020 the attosecond group demonstrated a novel approach for the temporal characterization of attosecond pulses based on the correlation analysis of the sidebands generated in a two-color photoionization process [sans1, sans4]. The development was motivated by the possibility to synthesize multiple coherent harmonics of a fundamental wavelength at the seeded FEL FERMI [sans2, sans3, sans8, sans10]. The technique allows one to overcome the lack of sub-optical cycle synchronization between the attosecond and infrared pulses, by using a correlation analysis of the single-shot photoelectron spectra. The correlation plot of the sidebands between the harmonics depend on their relative phase as shown in Fig. 1.4 and it can be used to completely reconstruct the temporal profile of an attosecond pulse train. Using this approach, the complete and independent shaping in amplitude and phase of an harmonic comb on the attosecond timescale was demonstrated [sans4].

The group has also reported the first example of

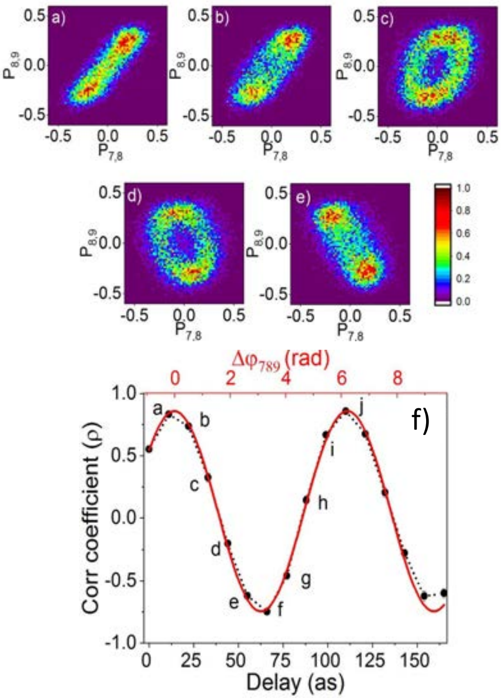


Figure 1.4: (a-e) Evolution of the correlation plots of the sidebands of the photoelectron spectra generated by a train of attosecond pulses at the FEL FERMI. (f) Calibration curve used for the reconstruction of the group-delay dispersion of a group of three harmonics.

complete characterization of the photoionization process in ions in the process of two-photon double-ionization of neon [sans9]. The experiment was also performed at FERMI, exploiting, in particular, the possibility to change the polarization of the intense XUV field from linear to circular.

Investigation of attosecond time delays in the recoil frame using a photoelectron-photoion coincidence spectrometer

The high repetition rate attosecond source developed in Freiburg is based on a commercial Yb laser system (Pharos-Light Conversion) delivering pulses with a duration of 290 fs. Using a home-made hollow-fiber compressor, the pulse duration is reduced to about 20 fs, which represents an optimal compromise between peak intensity and pulse duration for the generation of trains of attosecond pulses. These pulses have been used for the measurement of attosecond time delays in small molecular systems, including molecules characterized by tetrahedral symmetry, such as CF_4, CH_4, and CD_4. Thanks to the excellent stability of the delay-unit developed in the group [sans6], measurements of weak fragmentation channels and also angular- and time-resolved photoelectron spectra have been acquired. For the first molecule, a detailed analysis in the recoil frame of the photoelectron angular distribution gives access to the characterization of the attosecond time delay in this frame. The comparison of the experimental data with the predictions of theoretical models indicates that the molecular potential affects the dynamics of the photoelectron wave packet, depending on its emission direction in the recoil frame. The work has been performed in close collaboration with the group of Prof. Dr. Fernando Martin in Madrid and it is currently under review.
The preliminary data analysis of the measurements in CH_4 and CD_4 indicates the possibility to characterize the dependence of the attosecond time delays for different photoelectron emission directions in the laboratory frame.

Generation of isolated attosecond pulses and phase modulated spectroscopy

The group has achieved the generation of isolated attosecond pulses using a stretched hollow-core fiber for the temporal compression of a multi-mJ, carrier-envelope-phase stable laser source at 1 kHz repetition rate. Within the DFG Priority Program 1804 “Quantum Dynamics in Tailored Intense Fields”, the isolated attosecond pulses are currently used for the demonstration of a novel approach for the investigation of the ultrafast response of thin crystal samples and nanostructures. The work is performed in collaboration with Prof. Dr. Thomas Fennel (University of Rostock). The technique is based on the extreme sensitivity of the high-order harmonic generation process to an external perturbing field. A (weak) few-cycle pulse is sent onto a nanosample and is used to perturb the generation of an isolated attosecond pulse leading to a modulation of the phase and of the amplitude of the emitted XUV radiation. By monitoring the properties of the radiation using an XUV spectrometer, the electric field of the pulse can be reconstructed with a resolution of a few hundreds of attoseconds. The technique will be applied for the characterization of the ultrafast response of nanosystems exposed to different peak intensities of the few-cycle pulse.

The team has also started a collaboration with the groups of Prof. Dr. Frank Stienkemeier and Dr. Lukas Bruder for the application of phase-modulated techniques for the investigation of attosecond dynamics. In this collaboration, the expertise of the Stienkemeier/Bruder groups in coherent phase modulated spectroscopic techniques will be combined with an intense attosecond pulse train source for the investigation of small quantum systems.

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

The attosecond group is currently developing an end-station for the laser facility ELI-ALPS in Szeged, Hungary. The development is financed by a BMBF project (No. 05K19VF1, “Investigation of the correlated electronic dynamics using attosecond pulses”). The main scientific goal is the time-resolved investigation of two-photon double ionisation processes in atoms, such as neon and helium and small molecules (hydrogen), using the train or isolated attosecond pulses generated by the high-energy, attosecond beamlines available at ELI-ALPS. Towards this goal, the group has designed an end-station consisting of a split-and-delay unit, a focusing unit based on a short focal-length ellipsoidal mirror, a photoion-photoelectron spectrometer, an imaging unit, and an XUV spectrometer. Figure 1.5 presents a schematic view of the end-station. The project takes advantage

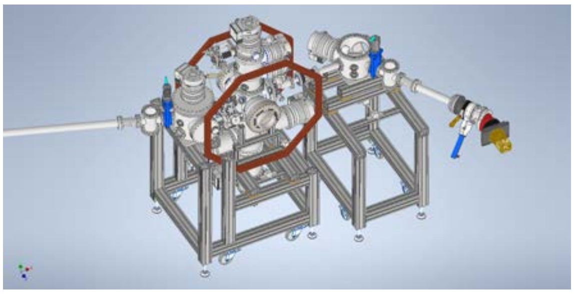


Figure 1.5: Schematic view of the end-station for nonlinear experiments to be installed on one of the SYLOS-driven attosecond beamlines available at ELI-ALPS.

of the complementary expertise of several research groups in nonlinear XUV spectroscopy (FORTH-Crete), design and development of XUV instrumentation (CNR-Padua), coincidence spectroscopy (Max-Planck-Institute for Nuclear Physics in Heidelberg), and of the close collaboration with the scientists at the ELI-ALPS facility.

Future Plans

Attosecond metrology for experiments at FELs

The group is planning to continue the successful activity at FERMI in the generation and application of attosecond pulses. We already participated to two beamtimes in September 2021 on the synthesis and application of attosecond pulses. The large amount of data acquired during those beamtimes is currently being analysed. In particular, the preliminary analysis indicates that the correlation technique introduced in ref. [sans4] can be used as an attosecond timing tool to retrieve the single-shot relative phase between the attosecond pulse train and the infrared field with resolution of a few tens of attoseconds. With this approach, it would be possible to implement experiments with attosecond temporal resolution even without sub-cycle synchronization between pump and probe pulses at seeded FELs.
At the same time, the group is planning to extend the approach demonstrated at FERMI also to other FELs operating in the soft X-ray and X-ray spectral range and using alternative seeding schemes (for example self-seeding schemes).
An additional beamtime at FERMI has already been awarded for the investigation of nonlinear photoionization of simple molecules using sculpted attosecond train pulses (Proposal No.20214098 “Coherent control of molecular fragmentation around an autoionizing state using shaped attosecond pulses”).

Characterization of attosecond dynamics using coincidence spectroscopy

We plan to further develop the application of coincidence spectroscopy using attosecond pulses. In particular, our medium-term goal is the generation of attosecond pulse trains and (close to) isolated attosecond pulses in the spectral region between 70 and 100 eV for the investigation of single-photon double ionization processes. Even though these processes present a small cross-section compared to that of single-photon single ionization, the excellent stability properties of the attosecond beamline developed in the group makes realistic the possibility to acquire data over extended time periods of a few days and even weeks without interruption. Towards this goal, we will develop in the upcoming years a multi-pass cell for the temporal compression of the Yb-laser systems available in the group with the goal to increase the energy of the pulses driving the HHG process.

Attosecond and nonlinear XUV spectroscopy at ELI-ALPS

We plan to finish the assembly and test of the end-station developed for the ELI-ALPS facility in 2022. Test data based on strong-field photoionization of gas targets will be acquired using the high-repetition rate laser sources available in Freiburg. After the testing phase, the end-station will be moved to ELI-ALPS and installed on the SYLOS-driven beamline for the investigation of multi-photon nonlinear photoionization processes.

1.2.3 Experimental Atomic, Molecular and Optical Physics – Group Schaetz

The endeavor to control increasingly large systems of particles at the quantum level might be one of the driving forces for physical sciences in the coming decades. **The experimental group of Tobias Schaetz** aims (i) to gain more profound 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. Our work builds on different trapping technologies. On the one hand, on conventional and novel radio-frequency (rf) traps, which we exploit to trap so-called Ion Coulomb Crystals (CCs). We further miniaturize the rf-traps to extend the ion ensembles in size and dimension, towards two-dimensional arrays of individual traps (see Figs.1.6), while preserving the unique controllability of individually trapped ions. On the other hand, we aim to explore trapping of ions and atoms by optical means, i.e., circumventing rf-driving fields and their related fundamental limitations for specific applications, while exploiting versatile optical trapping geometries.

Research Report

Analogue Experimental Quantum Simulations-QSim

A rich and powerful toolbox for individually trapped ions is available for quantum information processing, including quantum metrology and analogue experimental quantum simulation (AQS), demonstrating control with the highest fidelity for single and few ion CCs in 1D. In this context, we are further developing proposals and benchmarking their prospects via proof-of-principle realizations. Dependent on the requirements, we rely on different rf-architectures. Considering conventional rf-traps, we realized:

- Phonon Pair Creation via Controlled Two-mode Squeezing [schae5]: Quantum theory predicts intriguing dynamics during drastic changes of external conditions. We switch the trapping field of two ions sufficiently fast to create pairs of phonons and, thereby, squeeze the ions' motional state, accompanied by the formation of spatial entanglement (two-mode squeezed state). This process can also be interpreted as an analog to cosmological particle creation, a realization of our proposal of the year 2007.

- Measurement of Quantum Memory Effects and its Fundamental Limitations [schae8]: We reveal and experimentally demonstrate that the nature of projective measurements in quantum mechanics can lead to a nontrivial bias in non-Markovianity measures, quantifying the flow of information between a system and its environment. Here, we teamed up with one of the founders of the field, H.P. Breuer. We find that, in the current form, envisioned applications are fundamentally limited by quantum projection noise. In our trapped-ion system, we precisely quantify such bias and perform local quantum probing to demonstrate corresponding limitations. The combination of extended measures and our extendable experimental approach can become relevant for understanding more complex systems.

- Continuously Parametrized Quantum Simulation of Molecular Electron-Transfer Reactions [schae1]: Experimental studies of molecular systems in condensed-phase environments face difficulties in independently controlling the parameters that govern the molecular electron-transfer mechanism with high precision. In collaboration with the Buchleitner group, we propose that, instead, AQS allow to simulate and continuously connect vastly different regimes through precise tuning of, e.g., the phonon temperature, electron-phonon interaction, and electronic coupling. Such a setting does not only allow reproducing widely used transport models, such as Marcus theory. But it also provides access to transfer regimes that are unattainable for molecular experiments.

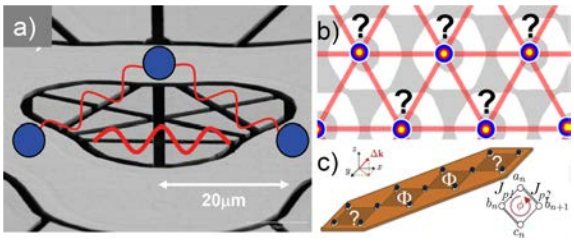


Figure 1.6: SEM image of our basic 2D array and prospects for scaling: a) additional subdivision of the electrodes permits tuning the individual trapping parameters in real time, such as, the trap depth, frequencies and orientation of the main axes (ions and individually controllable interactions animated). Three ions residing in three individual traps are suited to simulate basic anti-ferromagnetic interactions between three quantum spins, the onset of spin-frustration. b) In the envisioned, further scaled two-dimensional array, the whole quantum ensemble of spins evolves into an extended version of (a), an entangled and frustrated state. c) Layout for a "13-ion rhombic ladder". The ions, representing lattice sites, host and exchange phonons via tunneling, the latter simulating moving charged particles. Analogue to the Aharonov Bohm effect, these pick up geometric phases proportional to the area the loops enclose on the surface pierced by an external field. The dynamics can be controlled by Photo-Assisted-Tunneling [schae4].

Considering our novel 2D-architecture, QSim aims at setting up fully controlled and reconfigurable quantum lattices by individually trapped ions in multi-dimensional arrangements [schae10]. This includes identifying the prospect to address relevant problems that can be treated exploiting the platform in two dimensions, providing the required controllability and permitting means for benchmarking the reliability. We aim at identifying the features and limitations of the architecture and to study the crucial steps towards mid and long-term AQS applications. Selected experimental results are:

- Interference in a Prototype of a 2D Ion Trap Array Quantum Simulator [schae6]: We operate a basic triangular array of three individually trapped ions based on scalable microfabrication technology provided by Sandia National Laboratories (see Figs.1.6a). We demonstrate real-time tunability of coherent intersite coupling, sequential coupling, and interference between all three sites, via coherent states of motion - an essential building block for reconfigurable AQS with high connectivity.

- Floquet-Engineered Vibrational Dynamics in a 2D Array of individually Trapped Ions [schae4]: We show individual, real-time controlled Floquet engineering of the motion of ions located at microsites in the array. In contrast to previous approaches for AQS, where phonons are exploited as mediating bus, we attribute them an active role. In particular, the periodic drive enables tunneling of vibrational quanta between ions located in neighboring sites, mimicking charged particles. We control the flow of phonons on multiple pathways, their directionality and their interference. The tunneling phase can be interpreted as a geometric phase generated by synthetic gauge fields, following our proposal of 2012.

Trapping Ions Atoms and Molecules Optically (TIAMO and BaLiLaB)

Our current projects exploit optically trapping of $^{138}Ba^{+}$ ion(s), optionally submerged within a BEC of ^{87}Rb-atoms or a degenerate ensemble of spin-polarized ^{6}Li-atoms. They are dedicated to overcome fundamental limitations set by the rf-driven micromotion, e.g. limiting the extension to quantum effects in higher dimensional arrays of ions and the access of the quantum regime of atom-ion collisions due to rf-heating in state-of-the-art hybrid traps (combining an rf- for ion and an Optical Dipole Trap (ODT) for atom trapping). Our group had achieved optical trapping of an ion in an ODT, and within an 1D-optical lattice, as well as in a far-detuned ODT in the absence of rf-field featuring life- and coherence times comparable to atoms. We aim (i) to study and establish optically trapping of ions (and atoms) in general, (ii) to demonstrate substantial advantages of our approach in the context of interaction and reaction at ultra-low temperatures, and (iii) to explore further prospects by adapting methodology of quantum optics to gain control and state-sensitive detection on the level of individual quanta within the merged ion-atom system. Recently, we reported:

- Optical Trapping of CCs [schae7]: We demonstrate trapping of up to six $^{138}Ba^{+}$ in an ODT - without rf confinement, while the axial confinement was implemented via electrostatic fields. We realized spectroscopy of the axial motional modes of the CC in the classical regime within the ODT.

- Feshbach in BaLiLaB–still hybrid [schae2]: The field of ultra cold chemistry is well suited as a showcase, as well as an area of research struggling with the fundamental quest for quantum effects. We demonstrate Feshbach resonances between single $^{138}Ba^{+}$ and ^{6}Li, using magnetically tunable interactions. We control the experimental parameters to probe different interaction processes: (i) enhancing three-body reactions and the related losses to identify the resonances, and (ii) utilizing dominant two-body interactions to investigate and exploit the ion's sympathetic cooling in the ultracold atomic bath – still within the hybrid trap. We find inelastic processes to be suppressed by three to four orders of magnitude compared to elastic collisions, allowing to envision coherent dynamics. Instead of detecting the ion's state in the rf trap, we transfer it to an ODT, in complete absence of Li and detrimental rf-fields. Thus, we are now capable to exploit one of the key tools to tune and control atom-ion interactions in the quantum regime, which has propelled the field of degenerate quantum gases for more than two decades.

- Optical Traps for sympathetic Cooling of Ions with ultracold neutral Atoms [schae3]: We used a bichromatic ODT to trap and control $^{138}Ba^{+}$ immersed in a ^{87}Rb ensemble. We exploit state selective optical potentials to shape the individual ODTs, as well as using those for purifying CCs [schae9]. We observe highly efficient sympathetic cooling of single Doppler-cooled $^{138}Ba^{+}$ to sub-Doppler temperature/energy.

Future Plans

Plan for QSim

In our conventional rf-traps, we aim at: (i) transferring motional entanglement created by squeezing [schae5] into the robust electronic degree of freedom: our platform may allow to study the causal connections of squeezing, pair creation and entanglement, and might permit to cross-fertilize between

concepts in cosmology and applications of quantum information processing. (ii) We plan to realize our proposal on Molecular Electron-Transfer Reactions [schae1].
The main limitation within our basic 2D array is set by phononic decoherence via motional heating in vicinity of the rf-surface electrodes. We are currently implementing the established protocol of cleaning the surfaces by Ar-ion bombardment, which has been demonstrated in the community to permit reducing the heating rate by more than a factor of 100. This would potentially permit to study (i) the onset of spin frustration in triangular lattices. Accompanied with a moderate increase of lattice sites (9 to 13: see Figs.1.6), our platform might open a new route for future Floquet-based trapped ion AQS, e.g. targeting correlated topological phenomena and dynamical gauge fields, such as, studying Aharonov-Bohm cages, at bands, edge states and can be extended to investigate the Fractional Quantum Hall effect.

Plan for TIAMO and BaLiLaB

We aim at (i) - still in the hybrid trap - gaining further experimental data on selected Feshbach resonances to allow for improvements to the accuracy and detail of predictions from multichannel quantum scattering calculations. Providing the missing experimental data is predicted to allow for deeper insight into the molecular structure at short range, where additional interactions, such as second-order spin-orbit coupling shifts and splits resonances; (ii) coherently controlling the electronic degrees of freedom of $^{137,138}Ba^{+}$ including deterministic state-preparation and investigating ^{6}Li in its hyperfine ground state. Further optimizing the sympathetic cooling might enable an all-optical approach, in the absence of disturbing rf-fields and their detrimental heating mechanisms. This is predicted to permit (iii) studying chemistry in the pure s-wave regime, where molecular ions can be formed coherently by magneto- or rf-association, as well as stored and analysed after exothermic reactions, for example, via deep box-shaped rf-potentials; furthermore, (iv) exploiting Feshbach resonances in a (generic) atom–ion ensemble might find application in many-body systems, such as polaron and impurity physics as well as AQS.

Ultimately controlling pathways and recording quantum signatures, starting on the few-particle level, will allow for “scaling” Quantum by Quantum. Extending and exploiting the state-of-the-art tools within our platform(s) might become an advance for the deterministic control of complex quantum systems and magnified lattice structures, extendable in size and dimension.

1.2.4 Molecular and Nanophysics – Group Stienkemeier

A detailed understanding of the properties of atomic and molecular systems requires in many cases clean, unperturbed, and quantum state selected probes in order to isolate their quantum properties and, in particular, the quantum dynamics. In that respect the **Molecular and Nanophysics group of Frank Stienkemeier** has developed and is applying specific molecular beam techniques for the preparation of gas-phase targets isolated in vacuum, or molecules and molecular structures attached to larger clusters. Quantum state selectivity and related cold temperatures are provided by supersonic expansions or/and evaporative cooling of cluster ensembles, in particular also by the use of superfluid helium nanodroplets. For a comprehensive approach of studies, a wide variety of experimental techniques requiring distinct laser radiation sources are utilized. At the moment 5 molecular/cluster beam machines and related laboratories are operated in-house, making use of table-top laser sources spanning NIR to VUV wavelengths in high time or frequency resolution. The experiments are complemented by a mobile beam apparatus which is operated at other institutes or large-scale facilities, and experiments making use of dedicated endstations at large-scale facilities (FERMI, Trieste, EU-XFEL, Hamburg, SwissFEL, Villigen, ELI-Beamlines, Prague) extending available radiation sources to extremely high electromagnetic fields, high time-resolution and XUV/X-ray photon energies. Central techniques cover laser-induced fluorescence, photoion and photoelectron spectroscopy including angular resolution of particles and single-shot correlations. For a direct access to real-time dynamics, femtosecond time-resolved techniques are established, ranging all the way to multidimensional coherent techniques, maximizing the spectral-temporal information content.

Our research direction on collision experiments and cold chemistry has been continued by **Katrin Dulitz** as a **junior research group** leader.

Research Report

Excitation and energy transfer in molecules and organic nanostructures

Isolated organic dye molecules like acenes and perylenes, and their complexes and nanostructures are studied on rare-gas clusters and in helium nanodroplets using laser-spectroscopic techniques. The obtained information on the excited state electronic structure and dynamics is of utmost importance for an understanding of the properties that make these

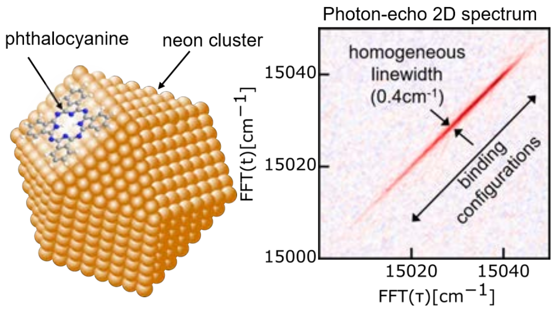


Figure 1.7: 2DES of a doped nano-cluster separates the homogeneous and inhomogeneous broadenings which provides unprecedented insight into the molecule-cluster binding configurations with high resolution.

systems exciting candidates for organic optoelectronics and photovoltaic applications (cf. singlet fission or triplet-triplet annihilation processes).

For example, the vibronic structure of the pentacene molecule isolated on neon cluster surfaces has been determined using laser induced fluorescence (LIF) spectroscopy, and interactions between acene molecules deposited on solid argon clusters have been studied. Furthermore, in a collaboration with Y. Xu and W. Jaeger (University of Alberta, Edmonton) dimers of perylene bisimide (PBI) isolated in helium nanodroplets have been studied by joint experimental and theoretical methods [sti2]. This study distinguished different unusual conformers of PBI dimers by their vibronic excitation energies, providing an impressive example of how sensitively the electronic properties of these systems depend on fine details of the intermolecular geometries. In an experimentally different approach, femtosecond laser pulses are employed to record the real-time dynamics. In an ongoing collaboration with the group of A. Baklanov (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk) with the focus on acene dimers, femtosecond time-dependent photoion and photoelectron spectra have been recorded.

Interferometric and multidimensional spectroscopy

Extending on the preliminary results from the previous reporting period, systematic 2D electronic spectroscopy (2DES) studies of molecular and cluster beam samples have been performed, marking the first 2DES experiments of isolated, cold targets in the gas phase so far reported [sti10]. As a next step, phthalocyanine (Pc) molecules in different cluster environments (He and Ne clusters) were studied leading to the highest spectral resolution in molecular 2DES so far reported, enabling the determination of the homogeneous linewidth in the Pc-Ne cluster system for the first time (Fig. 1.7).

Furthermore, the combination of 2DES with photoelectron spectroscopy (PES) was facilitated, introducing a highly differential probe to 2DES and a sensitivity improvement of two orders of magnitude [sti1].

In a cooperation with M. Gelin (Hangzhou Dianzi University) and W. Domcke (TU Munich) the influence of high laser intensities, pulse-phase distortions and temporal pulse overlap in 2DES was studied experimentally and theoretically.

In an approach related to 2DES, an extremely sensitive detection scheme for interparticle interactions was developed and dipole interactions were revealed in low-density atomic gases with mean inter-atomic distances of 27 μm [sti7]. Further investigations of these effects are currently conducted in collaboration with theorists from the group of A. Buchleitner (IoP, University of Freiburg).

Recently, wave packet interferometry (WPI), the basic interferometric principle underlying 2DES and related coherent nonlinear experimental techniques, was extended to the XUV spectral domain. This sets the basis for advanced coherent nonlinear and multidimensional spectroscopy schemes in the XUV and potentially in the X-ray domain. The harsh experimental challenges of extreme interferometer stabilization and high sensitivity were met with significant technical advancements. The XUV WPI experiments performed at the free electron laser (FEL) FERMI enabled to track the coherence decay of an electronic wave packet at a Fano resonance in Ar atoms [sti5] and the vibronic wave packet motion in highly excited states of the HeNe molecule. In a collaboration with M. Vrakking, O. Kornilov and coworkers (Max Born Institute, Berlin) the interferometric method was also implemented in high-order harmonic generation (HHG) with tabletop lasers for spectral characterizations with very high resolution (5 meV). Further interferometric experiments with HHG sources are currently developed in a DFG-funded collaboration with the group of G. Sansone (IoP, University of Freiburg).

Femtosecond dynamics of atoms, molecules and molecular structures

Results from femtosecond XUV-UV pump-probe experiments at the FERMI FEL on hydrogen-bonded clusters, detecting photoelectrons and photoions simultaneously (Fig. 1.8), revealed a combination of different processes triggered by multiple sequential single-photon ionization [sti8]. The recombination of quasi-free photoelectrons with cationic fragments to form excited neutral atomic species has been identified as a dominating process. In water clusters, hydrated electrons, i.e. electrons bound purely by

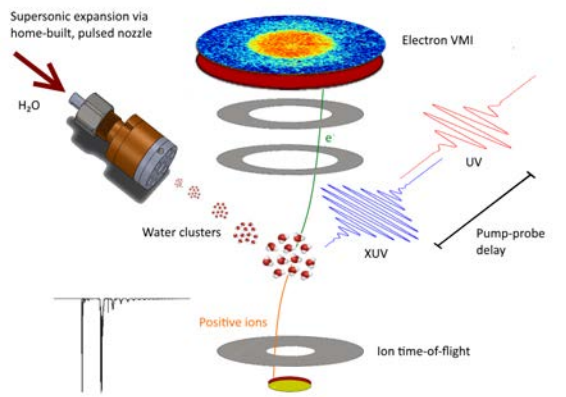


Figure 1.8: Schematic representation of the XUV-UV pump-probe experiments on hydrogen-bonded clusters at the low-density matter (LDM) beamline of the FEL FERMI. Clusters are produced by supersonic expansion using home-built pulsed valves. Photoelectrons are detected in an electron velocity map imaging (VMI) spectrometer, while photoions are simultaneously detected in a photoion time-of-flight (TOF) mass spectrometer.

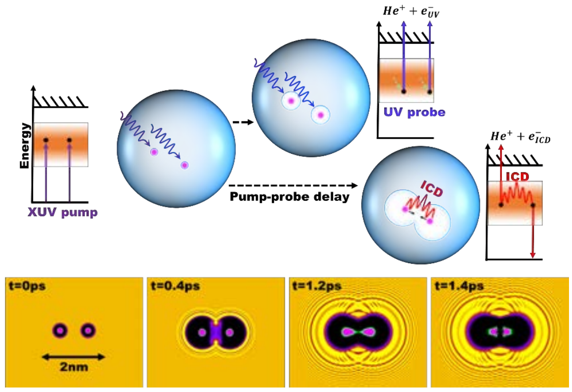


Figure 1.9: Schematic representation of the ICD process between two He atoms in a He nanodroplet (top), and simulations of two void bubbles forming around excited helium atoms leading to a significant acceleration of the ICD process.

the interaction with the aqueous solvent's dipole moment, are important in radiobiology and atmospheric chemistry and have been observed as a transient species, revealing their formation and decay times [sti8]. These studies have been extended to other hydrogen-bonded clusters (e.g. ethanol and ammonia), and also in collaboration with H.J. Wörner (ETH Zürich) using HHG XUV radiation .

The work on the dynamics of multiple excitations from FEL XUV radiation in confined systems has been extended to understand Interatomic Coulombic Decay (ICD) and Electron Transfer Mediated Decay (ETMD) processes [sti9]. As a prominent result, helium clusters revealed a fast autoionization mechanism strongly accelerated by cavity forces from the created void structures (Fig. 1.9) [sti4].

Funded by the DFG QUTIF priority program, a mobile cluster apparatus has been built to study the energy transfer dynamics of highly-charged dense systems. In neat and doped rare-gas clusters the generation of nanoplasmas is probed with femtosecond time resolution on a single-shot basis [sti3]. Extremely short and intense radiation pulses are used from different light sources: few-cycle NIR pulses in collaboration with R. Moshammer (MPI for Nuclear Physics, Heidelberg), intense MIR pulses (ELI-ALPS, Szeged), and XUV FEL pulses (FLASH, Hamburg). With accompanying molecular dynamics simulations the time-evolution of the dopant-induced Coulomb explosion has been studied by means of pump-probe ion- and electron-imaging spectroscopy.

Future Plans

The activities on excitation and energy transfer in molecules and organic nanostructures will continue with studies of well-controlled organic complexes in liquid helium nanodroplets and on rare-gas clusters. Since some of the most relevant excited electronic states of these complexes are potentially not detectable via fluorescence (e.g. charge transfer states and triplet states), additional and complementary detection schemes like e.g. VUV single-photon ionization have to be developed, including real-time pump-probe methodology.

To harvest the full potential of gas-phase 2DES, more efficient data acquisition schemes have to be implemented in order to further increase the attainable spectral resolution. The range of spectroscopic probes will be increased from isolated molecules and complexes in pure molecular beams to aggregates and molecular networks formed inside and on the surface of rare-gas clusters up to molecules dissolved in solution in the condensed phase. This will give access to molecular dynamics in different environments with the focus on non-adiabatic dynamics and cooperative conversion processes, e.g. singlet fission and exciton annihilation.

Interferometric experiments in the XUV domain will be progressed on HHG sources in collaboration with G. Sansone (IoP, University of Freiburg). Fundamental ultrafast molecular processes in prototypical molecules will be tackled with high spectro-temporal resolution. Focus will lie on super-excited molecular states not accessible with visible light and ultrafast dynamics elusive to femtosecond time resolution.

The activities on the photoionization-induced dynamics of small molecules and their weakly bound clusters at free-electron lasers will be continued in the direction of relaxation or fragmentation dynamics of molecules, contributing to an increasing comprehension of different processes of relevance for fields such as radiobiology, atmospheric chemistry and a fundamental understanding of condensed phase photo- and photoionization dynamics.

Probing multiple excitations and nanoplasma formation in rare-gas clusters, experimental methods and selectivity will be further refined. The broad size distributions on the cluster generation represents a challenge to overcome. A strong-field electric deflector to spatially separate clusters sizes for a more selective probing will be tested.

Cold and Controlled Chemistry – Katrin Dulitz

One research of this junior research group, funded by a Liebig Fellowship to K. Dulitz, is focused on the fundamental understanding of chemical reaction pathways and – using this knowledge – on the control of chemical reactions using quantum-state selection. The efficient suppression of chemical reactions is, for instance, required for the co-trapping of ultracold gases which is the starting point for the production of dense samples of heteronuclear molecules. Such molecules may feature long-range and anisotropic interactions which allow for new physics and chemistry studies in the quantum regime.

Research Report

To achieve these goals, the formation of ions through the reaction of ultracold lithium atoms (Li) with metastable atoms (He^*) and molecules (N_2^*, NO^*) was studied in a state-controlled manner at thermal energies (see Fig. 1.10) [du5, du6, du9]. The results provide important information about the underlying reaction mechanisms. For instance, using electronic state preparation of the reaction partners, it was found that both the total electron spin and Λ, i.e., the projection of the total molecular orbital angular momentum along the internuclear axis, are conserved in the collision process [du6]. To achieve the electronic state preparation of He^*, a novel state-selection scheme was developed [du8]. Recent results also indicate a violation of electron-spin conservation in the He^*-Li reaction. Further He-Li and He^*-Li collision studies have allowed for the quantification of the He^*:He excitation ratio in a supersonic beam and of the temperature of the ultracold Li atoms, respectively [du9].

As a new route for studying low-energy reactive collisions, two experimental approaches have been proposed by the group [du7]. These schemes only rely on the use of a single supersonic beam source.

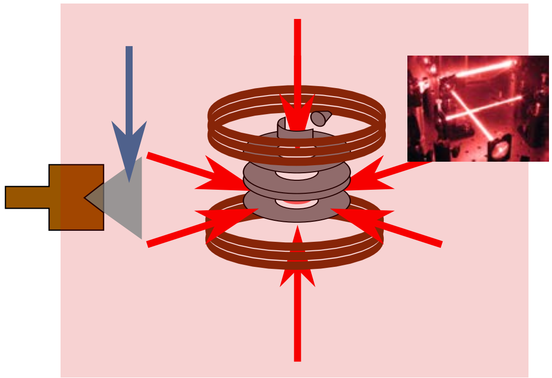


Figure 1.10: Schematic illustration of the experimental setup for reactive collision studies. Metastable atoms or molecules entrained in a supersonic beam are collided with ultracold lithium atoms confined in a magneto-optical trap. Laser-optical pumping is used to prepare the quantum states of one or both reaction partners prior to the collision process. The product ions are detected using an ion-time-of-flight spectrometer.

Close collaborations with the groups of S. Willitsch (University of Basel), T. Momose (UBC Vancouver) and B. Heazlewood (University of Liverpool) have allowed for the development of improved molecular beam sources [du2, du10] and quantum-state-selection schemes [du3], respectively.

In collaboration with the groups of F. Stienkemeier (see above) and M. Mudrich (University of Aarhus), this group is also involved in ultrafast reaction dynamics studies in supersonic beams and in doped helium nanodroplets [du1, du4] in Freiburg and at free-electron-laser facilities.

Future Plans

K. Dulitz (now K. Erath) has recently been awarded with an Attract grant by the Fraunhofer Society which will allow her to extend her research programme to the study of ultrafast dynamics in semiconductor materials, such as silicon carbide, in order to improve the laser processing of these materials in the frame of a group leadership at the Fraunhofer Institute for Solar Energy Systems (Fraunhofer ISE) in Freiburg.

1.2.5 Cluster Physics – Group von Issendorff

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. In fact, clusters can be seen as ideal model systems for the study of few to many-particle quantum dynamics.

The **experimental cluster physics group of Bernd von Issendorff** has been at the forefront of cluster science for many years. A range of crucial technologies for the study of clusters has been developed or improved by the group, from magnetron cluster sources over cryogenic ion traps to new generation magnetic bottle spectrometers. These experimental techniques, often in combination with advanced light sources, have allowed to study many different aspects of finite size effects, ranging from special geometric and electronic structures over phase transitions and ultrafast processes to magnetic properties.

The group currently operates three setups for photoelectron and photofragmentation spectroscopy on size-selected and temperature controlled clusters in-house. A mobile high intensity cluster source and a mobile high resolution cryogenic magnetic bottle spectrometer setup are available for experiments at free electron lasers. Together with the group of Tobias Lau (IP, HZB) it also operates the permanent endstation “ion trap” at the synchrotron BESSY II.

Research Report

Electronic and geometric structures

Photoelectron spectroscopy is one of the most powerful techniques for the study of matter, as (at least in principle) it directly reveals the electronic density of states of a system, which in turn yields important information about the geometric arrangement of the atoms. Systems studied range from metallic clusters over doped semiconductor clusters to molecular clusters. Examples of results are the determination of the geometric and electronic structure of silicon clusters [bvi7], of zinc clusters in the size range of the non-metal to metal transition [bvi8], or the determination of the binding motive and binding energy of the solvated electron in very large water clusters [bvi2]. Photoelectron spectroscopy at the FEL Flash on lead and silver clusters performed in collaboration with the group of Karl-Heinz Meiwes-Broer (Uni Rostock) for the first time revealed both the valence electron density of states as well as that of lower lying shallow core states.

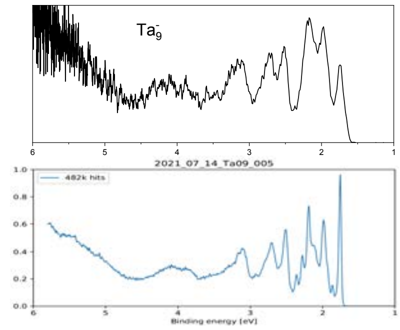


Figure 1.11: Comparison of photoelectron spectra of Ta_9^- clusters measured with a standard magnetic bottle spectrometer (top panel) and the new one (lower panel)

The recently developed new generation magnetic bottle spectrometer, which is currently the best spectrometer of this kind worldwide, is now employed for studies of a broad range of systems, yielding very promising results.

Electronic and nuclear dynamics

The dynamics of photoionization of simple metal (sodium and copper) clusters has been studied in detail by angle resolved photoelectron spectroscopy; here a surprisingly classical behaviour has been identified, with angular distributions resembling those of balls thrown off a rotating carousel. A comprehensive theoretical description has been developed, which demonstrates that it is decohering many-particle dynamics which leads to this semiclassical single particle behaviour [bvi1]. High resolution measurements of electron emission from acene

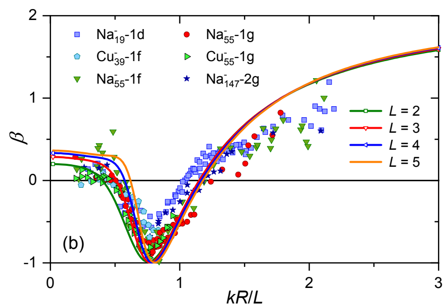


Figure 1.12: Photon energy dependence of angular distributions of photoelectron emitted from different angular momentum eigenstates of different copper and sodium cluster sizes. Scaled by cluster radius and angular momentum they converge to a universal function, which can be reproduced by a simple quantum model calculation assuming the clusters to be opaque for the photoelectron.

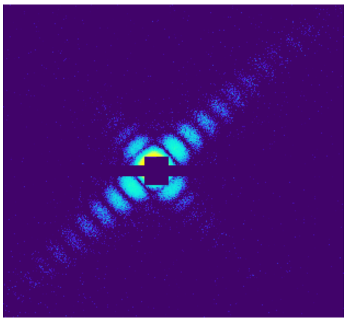


Figure 1.13: X-ray diffraction image of a gas phase cubic silver nanoparticle, measured at the endstation SQS at the EU-XFEL.

molecules as a function of photon energy has revealed a plethora of ultrafast relaxation channels, with very different couplings to molecular vibrations. In the beamtime at the FEL FLASH mentioned above measurements at higher field strengths permitted to study sequential multi-electron emission and the concomitant heating of the electronic system of lead and silver clusters.

X-ray diffraction experiments at the EU-XFEL on silica coated iron-oxide and nickel-coated silver particles as a function of photon energy were used to study the optical properties of highly excited matter.

Time-resolved pump-probe X-ray diffraction of large silver nanoparticles was employed to measure the development of the particles after weak to strong optical excitation in real time. Here a cooperation with Michael Moseler and his group was very helpful to understand the fascinating dynamics observed - effects ranging from melting, over cavitation driven fragmentation to phase explosion could be identified.

X-ray spectroscopy

X-ray spectroscopy via resonant excitation of core states yields very specific information about the local electronic structure at the position of the excited atom [bvi6]. In case of magnetic transition metal atoms it even allows to characterize their magnetic moments via magnetic dichroism [bvi10].

A large variety of pure and doped metal and semiconductor clusters have been studied at the synchrotron BESSY II. Recently small molecules like N_2^+ [bvi5] and biologically relevant larger molecules like pieces of DNA have been characterized as well.

Future Plans

The strongly enhanced resolution of the newly developed magnetic bottle spectrometer in combination with the very low temperatures (few K) of the clusters will be used to look at many effects which could

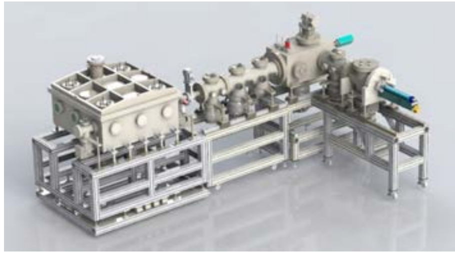


Figure 1.14: Storage ring setup for photoelectron spectroscopy on size-selected clusters currently commissioned at the TICNN, Tianjin, China.

not be resolved yet, ranging from vibrational excitation in large clusters over spin-orbit coupling effects to potential observation of Cooper pair formation in larger superconducting clusters. The new theoretical description of electron emission from simple metal clusters will be tested for a variety of systems with different strengths of ion-electron interaction.

A completely new experimental setup for X-ray photoelectron spectroscopy on size-selected gas phase ions at synchrotrons is currently built, funded by a BMBF project. Here ions will be stored and irradiated in a radio frequency ion trap; emitted electrons will be magnetically guided from the trap to an energy analyzer. This worldwide unique setup will permit to study core shell binding energies and especially electron emission dynamics in the high photon energy regime.

Photoelectron spectroscopy at the FEL FLASH will be continued; here pump-probe schemes will be used to study ultrafast electronic dynamics. Likewise time-resolved X-ray diffraction experiments will be continued to fully demonstrate the new phenomena discovered in the first experiments mentioned above.

In Freiburg in a cooperation with the group of Giuseppe Sansone attosecond streaking measurements will be used to characterize the plasmon excitation and its coupling to the electron emission channel in simple metal clusters.

Finally a cluster storage ring especially designed for angle resolved photoelectron spectroscopy experiments on stored size-selected clusters with high harmonics radiation from femtosecond lasers, which is currently being commissioned at the TICNN (Tianjin, China) within a cooperation project, will be used to study electronic and nuclear dynamics of a broad range of cluster systems.

1.2.6 Cluster and Synchrotron Spectroscopy – Group Lau

The group of **Tobias Lau** at Helmholtz-Zentrum Berlin was established in summer 2018, with a co-appointment at Universität Freiburg until January 2024. The group's main research focus is on electronic states and magnetic properties of transition metal clusters and transition metal centers in coordination entities. One goal of our current activities is to identify oxidation states and spin states of model systems and reaction intermediates that can be linked to relevant catalytic reactions. We also develop methods and instrumentation for x-ray spectroscopy of gaseous and liquid samples.

Our collaborations within Physikalisches Institut are with the groups of Bernd von Issendorff and Michael Moseler. An active collaboration, with co-supervision of a PhD student, also exists with the group of Ingo Krossing at Institut für Anorganische und Analytische Chemie. External collaborations, focusing mainly on theoretical x-ray absorption spectroscopy and electronic states, exist with the groups of Dimitrios Manganas at Max-Planck-Institut für Kohlenforschung Mülheim, Marcus Lundberg and Jan-Erik Rubensson at Uppsala University, Meiyuan Guo at SLAC, Hans Ågren at KTH Stockholm, and Sebastian Riedel at FU Berlin.

At BESSY II the group operates two endstations for x-ray spectroscopy of gaseous ions and liquid samples. We are currently commissioning a new elliptical undulator beamline for our liquid phase activities.

Research Report

Spin and orbital magnetic moments of transition metal clusters

XMCD reveals strong, and strongly varying, contributions of electronic orbital angular momentum to the total magnetic moment of small cobalt clusters in Fig. 1.15. Since the spin magnetic moment per atom is roughly constant, at $1\ \mu_B$ per 3d hole because of fully occupied majority states, this leads to a minimum magnetic moment for Co_2^+, contrary to the expectation of a steady increase towards the atomic value. This demonstrates once more that simple scaling laws cannot be applied in the small size regime. The orbital magnetic moment, indicative of the magnetic anisotropy energy, has an astonishingly large maximum value of $1.4 \pm 0.1\ \mu_B$ at five atoms per cluster. From this value we estimate a large magnetic anisotropy energy of 10 meV per atom.

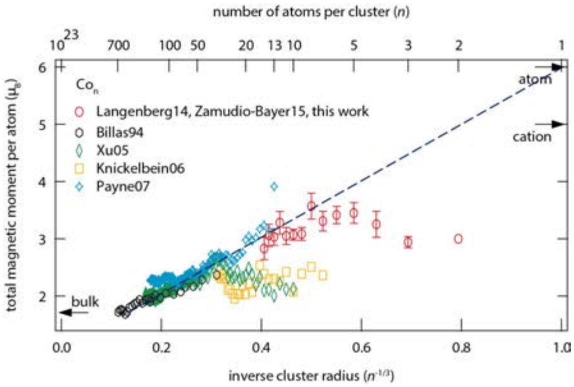


Figure 1.15: Total magnetic moment per atom, from Stern-Gerlach deflection and X-ray magnetic circular dichroism spectroscopy, with a strong deviation from the simple scaling-law behaviour observed for clusters smaller than ten atoms because of strong variations in the orbital magnetic moment.

Molecular ions

Core-excited final states of simple molecular ions have been studied since the beginning of x-ray spectroscopy with synchrotron radiation, but even simple molecular ions, such as N_2^+ or CO^+, have remained largely inaccessible so far, mostly because of low target densities. We have pioneered x-ray spectroscopy of molecular ions by use of our ion trap setup at BESSY II, and could recently record the first data for a variety of small molecular ions, revealing qualitative differences to their neutral counterparts because of the cationic charge, and typically an open shell, in their ground states. The open shell leads to strong enhancement of many-particle excitations below the ionization threshold, whereas the net positive charge transforms shape resonances, above threshold in the neutral molecule, to bound final states in the molecular ion. The description of these states still poses a

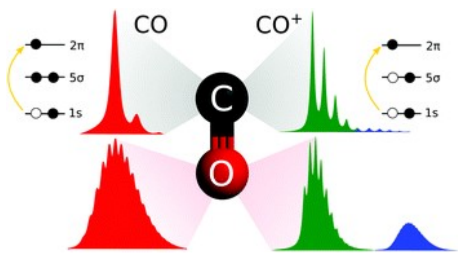


Figure 1.16: The localization of the 5σ molecular orbital at the carbon center in carbon monoxide plays an important role for the large differences in energy and intensity of two final states, associated with the 2π transition in the molecular ion, that can both be reached in oxygen and carbon 1s core-excited states.

challenge to theory, and our experimental data allows for a refinement of theoretical approaches, indicated in Fig. 1.16.

L-edge energy shifts as a quantitative method for the determination of oxidation states

In the thesis works of Tim Gitzinger and Max Flach, we have studied in detail the relationship of electronegativity difference, non-bonding 3d occupation at the metal center, and L-edge excitation energy, using diatomic transition metal halide cations as model systems, all of the same electronic ground state and symmetry within one series, shown for iron halides in Fig. 1.17. With a relative accuracy of 40 meV, we could determine significant L-edge excitation energy shifts, up to 40 %, within the same oxidation state, and relate this to fractional changes in 3d occupation. The results agree in order-of magnitude with the value that is expected from known shifts with integer oxidation states, but reveals further shifts within a given oxidation state because of higher resolution. This helps to better understand a strong variation that is reported in experimental data, and to more reliably determine oxidation states that are often inferred from L edge or K edge spectroscopy.

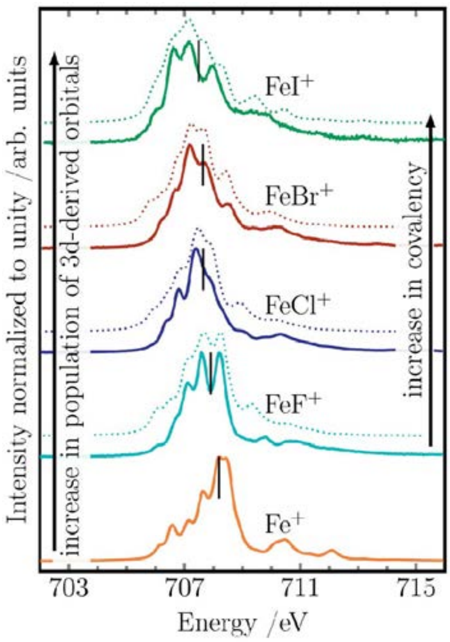


Figure 1.17: L_3 spectra of iron halide molecular ions, along with the iron cation reference spectrum. The shift of the median excitation, indicated by the dashed lines, to lower photon energy, is linked to an increase in 3d population at the metal site because of decreasing electronegativity difference from $[FeF]^+$ to $[FeI]^+$.

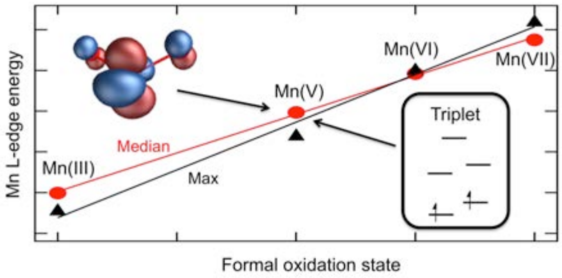


Figure 1.18: A combined experimental and theoretical x-ray absorption spectroscopy study identifies MnO_2^+ as a rare high-spin manganese(V) center, only the second of this kind, with potential relevance to water splitting in photosystem II.

Catalytically relevant oxidation states: water splitting

The oxygen evolving complex of photosystem II consists of a $CaMn_4O_5$ cluster. While the structure of this cluster, and many steps of the oxygen evolution reaction, are known, one important intermediate in the catalytic cycle is still unkown, and there is an ongoing debate about the mechanism and about the oxidation state, +4 or +5, of the participating manganese center. Calcium manganese oxide clusters can potentially contribute to the understanding of this reaction step. PhD student Olesya Ablyasova has successfully prepared a series of manganese oxide and calcium manganese oxide clusters that resemble the oxygen evolving complex of photosystem II. Water molecules are added to these clusters in a hexapole collision cell. On these model systems, oxidation states can be determined by manganese L edge x-ray absorption spectroscopy. Very recently, we have identified a high-spin manganese(V) center, cf. Fig. 1.18, in $[MnO_2]^+$, an important ingredient in one of the proposed mechanisms of water splitting by photosystem II.

Future Plans

Solvated transition metal ions: liquid jet and ion trap

Detailed studies of solvated transition metal ions and coordination entities will be performed in a combined electrospray ionisation/ion trap and liquid jet approach, where electrospray ionisation and quadrupole mass filtering will be used to prepare solvation shells with a well-defined number of solvent molecules around ions, whereas a liquid jet in transmission geometry will be used to study the fully solvated species. In preliminary studies, PhD student Max Flach has recently recorded the first L-edge spectra of the hexaaqua iron(II) ion for comparison with Fe^{2+} in aqueous solution. The gas-phase ap-

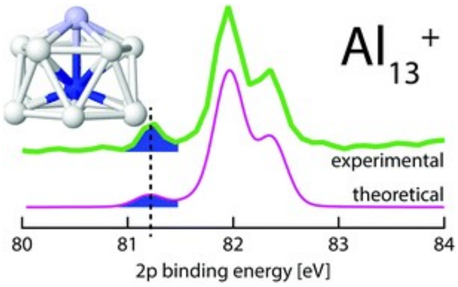


Figure 1.19: Experimental 2p electron binding energy spectrum of Al_{13}^{+}, as obtained from the photoionization efficiency curve in partial ion yield mode. The contribution of the central atom, well separated from the outer shell, is highlighted in blue. A dedicated XPS setup will allow us to directly access core level bindig energies of size-selected molecular, cluster, and complex ions.

proach also allows for a detailed study of the solvent molecules and their interaction with the solute, as this technique is essentially background free in contrast to studies in bulk solutions.

X-ray photoelectron spectroscopy

In collaboration with the group of Bernd von Issendorff and funded by BMBF, x-ray photoelectron spectroscopy will be performed on size-selected molecular, cluster, and complex ions, which are not accessible by x-ray photoelectron spectroscopy so far. A dedicated end station for this project, to be used at BESSY II, is currently set up in the laboratory of Bernd von Issendorff. Preliminary studies, making use of specific ion yield channels that represent ionization efficiency curves from which core-level binding energy spectra can be obtained, already demonstrate the potential of this method, as shown in Fig. 1.19 for the test case of aluminum clusters, where large chemical shifts were identified in experimental and computational spectroscopy, opposite in sign and larger by one order of magnitude than for bulk and surface aluminum.

Excited electronic states of transition metals

Within RTG 2717 DynCAM we will further investigate the dependence of L-edge excitation energy, oxidation state, and local 3d configuration in excited electronic states of transition metal ions. The aim is to separate the contributions of charge and configuration to the excitation energy by varying the 3d configuration within the same charge state. This will be done by preparing ground and metastable excited electronic states of transition metal ions in a magnetron discharge. Electronic states will be separated by ion mobility mass spectrometry.

1.2.7 Solar Physics – Group Berdyugina and von der Lühe (KIS)

The **Leibniz-Institut für Sonnenphysik (KIS) led by Svetlana Berdyugina and Oskar von der Lühe** is a member of the Leibniz Association. Until 2018 it was known as Kiepenheuer-Institut. The scientists at KIS conduct fundamental research in astrophysics, with particular emphasis on 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.

The institute operates the German solar telescopes at the Observatorio del Teide, Tenerife, Spain, including the 1.5-m telescope GREGOR, one of the world's most powerful solar telescopes, and the Vacuum Tower Telescope (VTT). KIS is about to contribute the cutting-edge technology Visible Tunable Filter (VTF) to the instrument suite of the Daniel K. Inuoye Solar Telescope (DKIST). With its 4-meter main mirror DKIST is the world-largest solar telescope that started science operations in 2021. The VTF instrument is among the largest Fabry-Perot interferometers ever built for astrophysics. Further highlights of the institute's work are the development of high-precision polarimeters for exoplanet studies (in cooperation with the Universities of Hawaii and of Turku).

In addition, among the recent developments at KIS is the establishment of a Science Data Centre (SDC) for accessing, processing, and analysing solar physics data.

Moreover, KIS plays a major role in international collaborative efforts, e.g., the High-resolution Solar Physics Network (SOLARNET), and the definition of the next generation of instrumentation for solar observations. In particular these are the 4-meter European Solar Telescope (EST) for high-resolution observations of the Sun, and the Solar Physics Research Integrated Network Group (SPRING) for synoptic observations.

KIS is involved in ESA's Solar Orbiter space mission, and awaits the third flight of the Sunrise balloon mission.

KIS contributes to the education of students at the University of Freiburg by offering lectures on experimental and theoretical astrophysics, term paper seminars, and hands-on training. Furthermore, KIS is frequently host of students working on their BSc, MSc, or PhD theses.

Research Report

Recent research highlights include:

- Studies of vortex motions and magnetic tornadoes on the Sun.
- Establishment of polarization measurements in molecular lines as diagnostics for stellar and sub-stellar magnetic fields.
- The solution of the radiative transfer equation in the magnetized solar atmosphere on a geometrical height scale.
- Studies on the thermal, magnetic, and dynamical structure of sunspots
- Measurements of the electric current vector in the lower solar atmosphere
- Helioseismic measurements of the solar interior and the solar atmosphere
- Studies on the topography, biosignatures, and artificial mega-structures on exoplanets
- Asteroseismic investigations of stellar magnetic cycles.

Future Plans

Currently, the institute is located at the Schlossberg in Freiburg. In 2023 it will move to a new building on the University Campus IV.

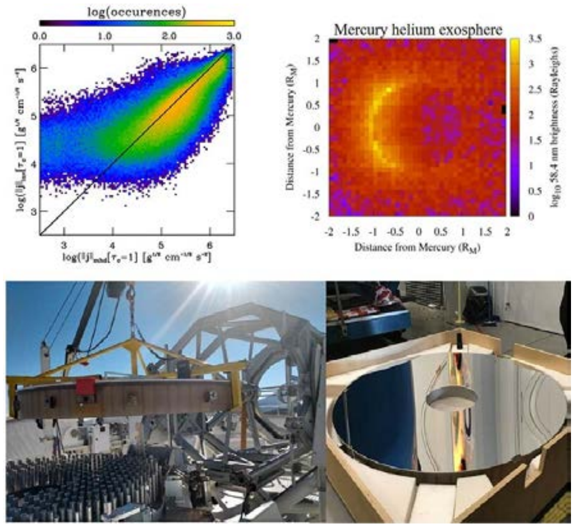


Figure 1.20: *Top left*: Results of a new method developed in international collaboration that allows to accurately determine electric currents on the solar surface. Electric currents form in the presence of non-potential configurations of the magnetic field and are believed to cause explosive events in the solar atmosphere. Therefore this method can potentially represent a major breakthrough in space weather forecasting. *Top right*: Emission from helium atoms in Mercury's exosphere at 58.4 nm was observed by the Mariner 10 spacecraft in the 1970s. This emission is due to resonant scattering of solar radiation on the helium atoms escaping from its solid surface and forming an exosphere. Using Monte-Carlo simulations, we demonstrated how Mercury's exospheric He I 58.4 nm emission varies due to the periodic changes in solar radiation and wind. The results indicate that the He I 58.4 nm brightness varies by between one and three orders of magnitude along the planet's orbit. These findings are strongly dependent on the intrinsic line width of the solar He I 58.4 nm emission. We expect that this variation will be observable by new missions, such as BepiColombo and Hisaki. Our results are also important for the characterization of exoplanets with ultraviolet space missions. *Bottom:* Impressions of the periodic recoating of the GREGOR main mirror at the IAC facility in La Laguna.

1.3 Important Publications and Conference Talks

Group Buhmann

Publications

[syb1] F. A. Burger, J. Fiedler, and S. Y. Buhmann, “Zero-point electromagnetic stress tensor for studying Casimir forces on colloidal particles in media”, Europhys. Lett. **121**, 24004 (2018).

The correct form of the electromagnetic stress tensor in media has been debated in the context of calculating the Casimir force and beyond. We resolve the debate by showing that only one of the competing approaches is consistent with a microscopic description.

[syb2] J. L. Hemmerich, R. Bennett, and S. Y. Buhmann, “The influence of retardation and dielectric environments on interatomic Coulombic decay”, Nature Commun. **9**, 2934 (2018).

We present the first relativistic model of interatomic Coulombic decay and show that the effect has a larger range than previously thought and that it is affected by dielectric environments such as liquid media and surfaces.

[syb3] S. Fuchs, R. Bennett, R. V. Krems, and S. Y. Buhmann, “Nonadditivity of optical and Casimir–Polder potentials”, Phys. Rev. Lett. **121**, 083603 (2018).

Contrary to current beliefs and practice, it is shown that atom–surface Casimir–Polder forces and optical light forces are not independent, so that new boundary-assisted light-forces can arise when a laser-driven atom is placed near a surface.

[syb4] R. Bennett, P. Votavová, P. Kolorenč, T. Miteva, N. Sisourat, and S. Y. Buhmann, “The virtual photon approximation for three-body interatomic Coulombic decay”, Phys. Rev. Lett. **122**, 153401 (2019).

We employ macroscopic quantum electrodynamics to establish a new analytical tool for describing the recently predicted many-body effects in interatomic Coulombic decay and establish its consistency with molecular dynamics simulations.

[syb5] S. Y. Buhmann, “Steifigkeit des leeren Raums”, Phys. J. **18**, 21 (2019).

In this perspective article, the recent first measurement of a Casimir torque in a liquid crystal setup is interpreted in terms of shearing the quantum vacuum.

[syb6] R. Bennett, Y. Gorbachev, and S. Y. Buhmann, “Symmetry-breaking in a condensate of light and its use as a quantum sensor”, Phys. Rev. Appl. **13**, 044031 (2020).

The sensitivity of a photonic Bose–Einstein condensate in finding and macroscopically occupying the lowest energy electromagnetic mode is exploited for the prediction of a quantum sensing application: the presence of chiral molecules in a dye-filled cavity can be observed via circular polarisation of the condensate.

[syb7] N. Gack, C. Reitz, J. L. Hemmerich, M. Könne, R. Bennett, J. Fiedler, H. Gleiter, S. Y. Buhmann, H. Hahn, and T. Reisinger, “Signature of short-Range Van der Waals forces observed in Poisson spot diffraction with indium atoms”, Phys. Rev. Lett. **125**, 050401 (2020).

An experimental observation of the Poisson-spot formed by scattering of an indium-atom matter wave off spherical particles is reported. The theoretical analysis shows first-time evidence for the influence of Casimir–Polder forces on Poisson-spot diffraction.

[syb8] R. Bennett and S. Y. Buhmann, “Inverse design of light-matter interactions in macroscopic QED”, New J. Phys. **22**, 093014 (2020).

The method of inverse design is combined with macroscopic quantum electrodynamics to provide a numerical tool for optimizing dielectric structures towards enhancing or suppressing a range of quantum electrodynamics effects. Application to resonance energy transfer reveals a range of novel structures that strongly outperform conventional geometries such as cavities.

[syb9] F. Lindel, R. Bennett, and S. Y. Buhmann, “Theory of polaritonic quantum-vacuum detection”, Phys. Rev. A **102**, 041701(R) (2020).

Novel electro-optic sampling experiments have provided a window for the direct detection of the electromagnetic quantum vacuum. We present a quantitative theoretical framework for predicting and interpreting such experiments.

[syb10] J. Klatt, C. M. Kropf, and S. Y. Buhmann, Open quantum systems' decay across time, Phys. Rev. Lett. **126**, 210401 (2021).
We discuss how two alternative descriptions of quantum open systems dynamics via the Markov approximation and linear response theory emerge as opposite limits on asymptotic timescales. This comprehensive view resolves a recent controversy about the velocity-dependence of quantum friction.

Conference Talks

1. S. Y. Buhmann, Forces of the quantum vacuum: from dispersion forces to quantum friction, Winter Colloquium of the Physics of Quantum Electronics, Snowbird, USA, January 2018.

2. S. Y. Buhmann, Collective atom–photon interactions in complex environments, Spring Meeting of the German Physical Society, Erlangen, Germany, March 2018.

3. S. Y. Buhmann, Macroscopic quantum electrodynamics: Engineering atom–field interactions, Molecular Polaritonics, Madrid, Spain, June 2019.

4. S. Y. Buhmann, Engineering Casimir forces: From topological insulators to (collective) photon recoil, Progress In Electromagnetics Research Symposium, Rome, Italy, June 2019.

5. S. Y. Buhmann, The influence of retardation, dielectric environments and mediating atoms on interatomic Coulombic decay, Progress In Electromagnetics Research Symposium, Rome, Italy, June 2019.

6. S. Y. Buhmann, The photonic Bose–Einstein condensate as a precision quantum sensor, Fall Meeting of the German Physical Society, Freiburg, Germany, September 2019.

7. A. Ērglis, Photonic Bose–Einstein condensation in planar cavity, 735^{th} WE-Heraeus-Seminar on Exploring Quantum Many-Body Physics with Ultracold Atoms and Molecules, Hanau, Germany (online), December 2020.

8. J. Franz, Purcell modification of Auger and interatomic Coulombic decay, Interatomic Coulombic Decay in External Environments conference (ICD-X), Glasgow, United Kingdom, September 2021.

9. J. Fiedler, The role of dispersion forces for matter-wave binary holography experiments, European Quantum Technologies Conference 2021, Dublin, Ireland, November 2021.

10. O. J. Franca Santiago, Transition radiation near topological insulators, Topological quantum matter: foundations and applications, Mexico City, Mexico (online), January 2022.

Group Breuer

Publications

[breuer1] A. Colla and H.-P. Breuer, "Exact Open System Approach to Strong Coupling Quantum Thermodynamics," arXiv:2109.11893v2 [quant-ph] 20 Oct 2021.
We develop a general theory describing the thermodynamical behavior of open quantum systems coupled to thermal baths beyond perturbation theory. Our approach is based on the exact time-local quantum master equation for the open system, and on a new principle of minimal dissipation. This principle leads to unique definitions for work, heat and entropy production, and enables us to formulate a first and second law of quantum thermodynamics.

[breuer2] A. Colla and H.-P. Breuer, "Entropy production and the role of correlations in quantum Brownian motion," Phys. Rev. A **104**, 052408 (2021).
We perform a study on quantum entropy production, different kinds of correlations, and their interplay in the driven Caldeira-Leggett model of quantum Brownian motion. The model, taken with a large but finite number of bath modes, is exactly solvable, and the assumption of a Gaussian initial state leads to an efficient numerical simulation of all desired observables in a wide range of model parameters.

[breuer3] S. Wenderoth, H.-P. Breuer and M. Thoss, “Non-Markovian effects in the spin-boson model at zero temperature,” Phys. Rev. A **104**, 012213 (2021).
We investigate memory effects in the spin-boson model using our measure for non-Markovianity based on the information exchange between an open system and its environment, employing the multilayer multiconfiguration time-dependent Hartree approach which allows an exact numerical simulation of the model at zero temperature for a broad range of system parameters.

[breuer4] S. Imai, N. Wyderka, A. Ketterer and O. Gühne, “Bound entanglement from randomized measurements,” Phys. Rev. Lett. **126**, 150501 (2021).
If only limited control over a multiparticle quantum system is available, a viable method to characterize correlations is to perform random measurements and consider the moments of the resulting probability distribution. We present systematic methods to analyze the different forms of entanglement with these moments in an optimized manner.

[breuer5] S. Einsiedler, A. Ketterer and H.-P. Breuer, “Non-Markovianity of quantum Brownian motion,” Phys. Rev. A **102**, 022228 (2020).
We study quantum non-Markovian dynamics of the Caldeira-Leggett model, a prototypical model for quantum Brownian motion describing a harmonic oscillator linearly coupled to a reservoir of harmonic oscillators. Employing the exact analytical solution of this model one can determine the size of memory effects for arbitrary couplings, temperatures, and frequency cutoffs, where quantum non-Markovianity is defined in terms of the flow of information between the open system and its environment quantified through the Bures metric.

[breuer6] D. Tamascelli, C. Benedetti, H.-P. Breuer and M. G. A. Paris, “Quantum probing beyond pure dephasing,” New J. Phys. **22**, 083027 (2020).
Quantum probing is the art of exploiting simple quantum systems interacting with a complex environment to extract precise information about environmental parameters, e.g. its temperature or its spectral density. Here we analyze the performance of a single-qubit probe in characterizing bosonic environments. In particular, we analyze the effects of tuning the interaction Hamiltonian between the probe and the environment, going beyond the traditional paradigm of pure dephasing.

[breuer7] B. Vacchini, H.-P. Breuer and A. Bassi (editors), “Advances in Open Systems and Fundamental Tests of Quantum Mechanics,” Proceedings of the 684. WE-Heraeus-Seminar, Bad Honnef, Germany, 2–5 December 2018 (Springer Nature Switzerland AG, 2019).
The book reports new results in open quantum systems, foundations of quantum mechanics and recent developments in advanced experiments testing quantum mechanics.

[breuer8] G. Amato, H.-P. Breuer and B. Vacchini, “Generalized trace distance approach to quantum non-Markovianity and detection of initial correlations,” Phys. Rev. A **98**, 012120 (2018).
A measure of quantum non-Markovianity for an open system dynamics, based on revivals of the distinguishability between system states, has been introduced in our group using the trace distance as quantifier for distinguishability. Here we show that this approach can be generalized by employing the trace norm of Helstrom matrices. We demonstrate that this approach is consistent with the original interpretation in terms of an information flow, and further analyze its performance in local detection schemes for initial correlations.

[breuer9] H.-P. Breuer, G. Amato and B. Vacchini, “Mixing-induced quantum non-Markovianity and information flow,” New J. Phys. **20**, 043007 (2018).
Mixing dynamical maps describing open quantum systems can lead from Markovian to non-Markovian processes. Here, we develop a natural interpretation of this feature in terms of the distinguishability of quantum states, system environment correlations and the information flow between system and environment.

[breuer10] M. Wittemer, G. Clos, H.-P. Breuer, U. Warring and T. Schätz, “Measurement of quantum memory effects and its fundamental limitations,” Phys. Rev. A **97**, 020102(R) (2018).
We discuss that projective measurements in quantum mechanics can lead to a nontrivial bias in non-Markovianity measures which quantify the flow of information between a system and its environment. In our trapped-ion system, we precisely quantify such bias and perform local quantum probing to demonstrate corresponding limitations. Our scalable experimental approach can provide a versatile reference, relevant for understanding more complex systems.

Conference Talks

1. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems, First National Conference and Workshop on Quantum Information and Open Quantum Systems, Azarbaijan Shahid Madani University, Tabriz, Iran, February 2018.

2. H.-P. Breuer, Mixing-induced quantum non-Markovianity, system-environment correlations and information flow, 50th Symposium on Mathematical Physics, Toruń, Poland, June 2018.

3. H.-P. Breuer, Non-Markovian Dynamics: Correlations, Information Flow and Memory in Open Quantum Systems, Plenarvortrag, DPG-Frühjahrstagung, Rostock, March 2019.

4. A. Ketterer, Entropic uncertainty relations from quantum designs, DPG-Frühjahrstagung, Rostock, March 2019.

5. A. Ketterer, Entropic uncertainty relations from quantum designs, Benasque Quantum Information Workshop, Benasque, June 2019.

6. A. Ketterer, Characterizing multiparticle entanglement with moments of random correlations, Central European Workshop on Quantum Optics (CEWQO), Paderborn, June 2019.

7. H.-P. Breuer, Quantum Theory of Open Systems, Festkolloquium Nico Giulini, ZARM, University of Bremen, October 2019.

8. H.-P. Breuer, Non-perturbative quantum non-Markovianity of the Caldeira-Leggett model, workshop on *Quantum Information Processing in Non-Markovian Quantum Complex Systems*, Nagoya University, Japan, December 2019.

9. H.-P. Breuer, Non-Markovian Quantum Dynamics of Open Systems: Information Flow, Memory Effects and Correlations, QQQ Workshop, Milan, Italy, February 2020.

10. A. Colla, Exact approach to strong-coupling quantum thermodynamics in open systems, International workshop “Openness as a resource: Accessing new quantum states with dissipation,” Max Planck Institute for the Physics of Complex Systems, Dresden, 31 January - 04 February 2022.

Mandates/Awards

1. Since 2018: Member of the steering committee of the Georg H. Endress PostDoc cluster of the universities Basel and Freiburg.

Group Buchleitner

Publications

[abu1] G. Sorelli, N. Leonhard, V.N. Shatokhin, C. Reinlein, A. Buchleitner, “Entanglement protection of high dimensional states by adaptive optics”, New J. Phys. **21**, 023003 (2019).
We demonstrate the potential of adaptive optics for secure quantum key distribution across turbulent atmosphere.

[abu2] T. Binninger, V.N. Shatokhin, A. Buchleitner, T. Wellens, “Nonlinear quantum transport of light in a cold atomic cloud”, Phys. Rev. A **100**, 033816 (2019)
We devise a scalable method to describe nonlinear radiation transport in a multiply scattering, dilute atomic medium.

[abu3] T. Giordani, F. Flamini, M. Pompilli, N. Viggianiello, N. Spagnolo, A. Crespi, R. Osellame, N. Wiebe, M. Walschaers, A. Buchleitner, F. Sciarrino, “Experimental statistical signature of many-body quantum interference”, Nature Photon. **12**, 173 (2018)
QOS’ C-data protocol to scalably certify many-particle interference across random multi-mode scatterers is experimentally demonstrated.

[abu4] T. Brünner, G. Dufour, A. Rodríguez, A. Buchleitner, "Signatures of indistinguishability in bosonic many-body dynamics", Phys. Rev. Lett. **120**, 210401 (2018)
We quantify the impact of the degree of indistinguishability of an interacting many-particle state's constituents on its dynamics.

[abu5] J. Lindinger, A. Buchleitner, A. Rodríguez, "Many-body multifractality throughout bosonic superfluid and Mott insulator phases", Phys. Rev. Lett. **122**, 106603 (2019)
We show that the Mott-superfluid transition of the Bose-Hubbard Hamiltonian has an unambiguous signature in the dependence of the system ground state's localisation properties, and notably of its dominant expansion coefficient alone, on the particles' interaction strength.

[abu6] L. Pausch, E.G. Carnio, A. Rodríguez, A. Buchleitner, "Chaos and ergodicity across the energy spectrum of interacting bosons", Phys. Rev. Lett. **126**, 150601 (2021)
The transition from the integrable to the ergodic phase of interacting bosons is quantified by the universal fluctuations of the associated eigenstates' localisation properties. Furthermore, the emergence of non-universal statistical features with increasing system size is demonstrated.

[abu7] C. Dittel, G. Dufour, M. Walschaers, G. Weihs, A. Buchleitner, R. Keil, "Totally destructive many-particle interference", Phys. Rev. Lett. **120**, 240404 (2018)
We unveil the general algebraic structure underlying the strict suppression of many-particle transition events across multimode unitaries.

[abu8] C. Dittel, G. Dufour, G. Weihs, A. Buchleitner, "Wave-particle duality of many-body quantum states", Phys. Rev. X **11** 031041 (2021)
We derive an inequality which quantifies the trade-off between which-way information and interference contrast on the level of many-body transition amplitudes.

[abu9] A.J.C. Woitizk, P.K. Barkoutsos, F. Wudarski, A. Buchleitner, I. Tavernelli, "Entanglement production and convergence properties of the variational quantum eigensolver", Phys. Rev. A **102**, 042402 (2020)
We scrutinize the functionality of hybrid quantum-classical optimization routines with respect to the type and level of entanglement generated by its quantum sub-unit.

Conference Talks

1. A. Rodríguez, Many-body Multifractality throughout the Superfluid to Mott Insulator Bosonic Phase Transition, International Workshop on Disordered Systems: From Localization to Thermalization and Topology, Center for Theoretical Physics of Complex Systems (PCS-IBS), Daejeon, Republic of Korea, 3-7 September 2018.

2. A. Buchleitner, Interference of indistinguishable particles: from dynamics to statistics, Workshop on Modern Aspects of Quantum Physics, Zagreb, Croatia, 1st-5 October 2018.

3. T. Wellens, Nonlinear quantum transport in a cold atomic cloud, Hauptvortrag, SAMOP Frühjahrstagung der Deutschen Physikalischen Gesellschaft, Rostock, 10-15 March 2019.

4. A. Rodríguez, Eigenstate complexity in Fock space for interacting bosons, CCPQ Workshop, Dynamics of Complex Quantum Systems, Cumberland Lodge, Windsor Great Park, United Kingdom, 5-8 August 2019.

5. A. Buchleitner, Quantum effects in "complex" systems, Workshop on communication technology transfer to ocean science, Crieff, Scotland, 18-21st August 2019.

6. A. Buchleitner, Quantum transport on disordered networks – from single to many particles, Quantum Effects in Biological Systems (QUEBS2019), Puebla, Mexico, 27 October-2nd November 2019.

7. A. Buchleitner, Quantum transport in complex systems: from single to many particles, VII Leopoldo García-Colín Mexican Meeting on Mathematical and Experimental Physics, Mexico-City, 16-23rd February 2020.

8. A. Buchleitner, Spectral properties, "quantum" phase transitions, many-particle localisation and interference in interacting many-particle systems, Workshop on Quantum Information Theory and Thermodynamics at the Nanoscale, Al Hoceima, Morocco, 2nd-6 March 2020.

9. V. Shatokhin, Stability of spatial eigenmodes of light in dynamic atmospheric turbulence, IEEE Photonics Society, Summer Topicals Meetings Series 2021, Virtual Conference, 19-21st July 2021.

10. L. Pausch, Chaos in the Bose-Hubbard model versus Gaussian orthogonal and embedded random matrix ensembles, 753. WE Heraeus-Seminar, Modern developments in quantum chaos, Bad Honnef, 20-24 September 2021.

Mandates/Awards

1. since 3/2021: Editor in Chief of New Journal of Physics
2. since 4/2021: Executive Board member for Scientific Programmes and Awards, German Physical Society
3. since 10/2019: Elected member of the Senate of the Albert-Ludwigs-Universität
4. since 2018: Co-Director of the Georg H. Endress PostDoc Cluster of the Universities Basel and Freiburg
5. since 2008: Personal mentor of the German National Academic Foundation

Group Sansone

Publications

[sans1] P. K. Maroju, C. Grazioli, M. Di Fraia., M. Moioli, D. Ertel, H. Ahmadi, O. Plekan, P. Finetti, E. Allaria, L. Giannessi, G. De Ninno, S. Spampinati, A. A. Lutman, R. J. Squibb, R. Feifel, P. Carpeggiani, M. Reduzzi, T. Mazza, M. Meyer, S. Bengtsson, N. Ibrakovic, E. R. Simpson, J. Mauritsson, T. Csizmadia, M. Dumergue, S. Kühn, N. G. Harshitha, D. You, K. Ueda, M. Labeye, J. E. Bækhøj, K. J. Schafer, E. V. Gryzlova, A. N. Grum-Grzhimailo, K. C. Prince, C. Callegari and G. Sansone, "Analysis of two-color photoelectron spectroscopy for attosecond metrology at seeded free-electron lasers", New Journal of Physics **23** (2021) 043046.
Detailed theoretical analysis of the novel metrology technique applied for the temporal reconstruction of trains of attosecond pulses using a the seeded free-electron laser FERMI.

[sans2] C. Callegari, A. N. Grum-Grzhimailo, K. L. Ishikawa, K. C. Prince, G. Sansone, and K. Ueda, "Atomic, molecular and optical physics applications of longitudinally coherent and narrow bandwidth Free-Electron Lasers", Physics Reports **904** (2021) 1-59.
Review on the most recent applications and experiments enabled by free-electron laser pulses characterized by longitudinal coherence.

[sans3] D. You, K. Ueda, E. V. Gryzlova, A. N. Grum-Grzhimailo, M. M. Popova, E. I. Staroselskaya, O. Tugs, Y. Orimo, T. Sato, K. L. Ishikawa, P. A. Carpeggiani, T. Csizmadia, M. Füle, G. Sansone, P. K. Maroju, A. D'Elia, T. Mazza, M. Meyer, C. Callegari, M. Di Fraia, O. Plekan, R. Richter, L. Giannessi, E. Allaria, G. De Ninno, M. Trovò, L. Badano, B. Diviacco, G. Gaio, D. Gauthier, N. Mirian, G. Penco, P. R. Ribič, S. Spampinati, C. Spezzani and K. C. Prince "New Method for Measuring Angle-Resolved Phases in Photoemission", Physical Review X **20** (2020) 031070.
Demonstration of a novel scheme for the characterization of attosecond time delays in photoionization, based on the combination of two coherent harmonics of the free-electron laser FERMI.

[sans4] P. K. Maroju, C. Grazioli, M. Di Fraia, M. Moioli, D. Ertel, H. Ahmadi, O. Plekan, P. Finetti, E. Allaria, L. Giannessi, G. De Ninno, C. Spezzani, G. Penco, S. Spampinati, A. Demidovich, M. B. Danailov, R. Borghes, G. Kourousias, C. E. Sanches Dos Reis, F. Billé, A. A. Lutman, R. J. Squibb, R. Feifel, P. Carpeggiani, M. Reduzzi, T. Mazza, M. Meyer, S. Bengtsson, N. Ibrakovic, E. R. Simpson, J. Mauritsson, T. Csizmadia, M. Dumergue, S. Kühn, H. Nandiga Gopalakrishna, D. You, K. Ueda, M. Labeye, J. E. Bækhøj, K. J. Schafer, E. V. Gryzlova, A. N. Grum-Grzhimailo, K. C. Prince, C. Callegari and G. Sansone "Attosecond pulse shaping using a seeded free-electron laser", Nature **578** (2020) 386-391.
First experimental demonstration of the generation of an attosecond pulse trains using a seeded free-electron laser. Moreover, the work shows the first demonstration of complete amplitude and phase shaping of an attosecond waveform.

[sans5] I. Orfanos, I. Makos, I. Liontos, E. Skantzakis, B. Major, A. Nayak, M. Dumergue, S. Kühn, S. Kahaly, K. Varju, G. Sansone, B. Witzel, C. Kalpouzos, L. A. A. Nikolopoulos, P. Tzallas and D. Charalambidis, ”Non-linear processes in the extreme ultraviolet”, Journal of Physics: Photonics **2** (2020) 042003.
Topical review on non-linear processes in the extreme ultraviolet and x-ray spectral range, driven by attosecond sources.

[sans6] H. Ahmadi, S. Kellerer, D. Ertel, M. Moioli, M. Reduzzi, P. K. Maroju, A. Jäger, R. N. Shah, J. Lutz, F. Frassetto, L. Poletto, F. Bragheri, R. Osellame, T. Pfeifer, C. D. Schröter, R. Moshammer and G. Sansone, ”Collinear setup for delay control in two-color attosecond measurements”, Journal of Physics: Photonics **2** (2020) 024006.
Demonstration of an ultrastable delay line for the implementation of pump-probe experiments with attosecond temporal resolution.

[sans7] A. Nayak, M. Dumergue, S. Kühn, S. Mondal, T. Csizmadia, N. G. Harshitha, M. Füle, M. Upadhyay Kahaly, B. Farkas, B. Major, V. Szaszkó-Bogár, P. Földi, S. Majorosi, N. Tsatrafyllis, E. Skantzakis, L. Neoričić, M. Shirozhan, G. Vampa, K. Varjú, P. Tzallas, G. Sansone, D. Charalambidis and S. Kahaly ”Saddle point approaches in strong field physics and generation of attosecond pulses” Physics Reports **833** (2019) 1-52.
Review on the applications of the stationary phase method and of the saddle-point equations for the theoretical description of the generation of attosecond pulses and of strong-field processes.

[sans8] M. Di Fraia, O. Plekan, C. Callegari, K. C. Prince, L. Giannessi, E. Allaria, L. Badano, G. De Ninno, M. Trovò, B. Diviacco, D. Gauthier, N. Mirian, G. Penco, P. R. Ribič, S. Spampinati, C. Spezzani, G. Gaio, Y. Orimo, O. Tugs, T. Sato, K. L. Ishikawa, P. A. Carpeggiani, T. Csizmadia, M. Füle, G. Sansone, P. Kumar Maroju, A. D’Elia, T. Mazza, M. Meyer, E. V. Gryzlova, A. N. Grum-Grzhimailo, D. You and K. Ueda, ”Complete Characterization of Phase and Amplitude of Bichromatic Extreme Ultraviolet Light”, Physical Review Letters **123** (2019) 213904.
Experimental demonstration of the complete temporal reconstruction of the electric field of a pulse in the extreme ultraviolet spectral range consisting of two harmonics of a fundamental frequency.

[sans9] P. A. Carpeggiani, E. V. Gryzlova, M. Reduzzi, A. Dubrouil, D. Facciálá, M. Negro, K. Ueda, S. M. Burkov, F. Frassetto, F. Stienkemeier, Y. Ovcharenko, M. Meyer, O. Plekan, P. Finetti, K. C. Prince, C. Callegari, A. N. Grum-Grzhimailo and G. Sansone, “Complete reconstruction of bound and unbound electronic wavefunctions in two-photon double ionization”, Nature Physics **15** (2019) 170-177.
First experimental demonstration of a complete experiment in two-photon double ionization of neon.

[sans10] L. Giannessi, E. Allaria, K. C. Prince, C. Callegari, G. Sansone, K. Ueda, T. Morishita, C. N. Liu, A. N. Grum-Grzhimailo, E. V. Gryzlova, N. Douguet and K. Bartschat ”Coherent control schemes for the photoionization of neon and helium in the Extreme Ultraviolet spectral region”, Scientific Reports **8** (2019) 7774.
Theoretical analysis of the applicability of coherent control schemes based on two and three-photon processes in the extreme ultraviolet range using seeded free-electron lasers.

Conference Talks

1. G. Sansone, “Shaping attosecond waveforms at free-electron lasers”, 52nd Conference of the European Group on Atomic Systems (EGAS), 6-8 July 2021 (on-line).

2. G. Sansone, “New Opportunities for Attosecond Experiments Using FELs”, Workshop Attosecond to Few-Femtosecond Ultrafast Science at Future FELs EuXFEL, 28-30 June 2021 (on-line)

3. G. Sansone, “Attosecond metrology at Free Electron Lasers”, Conference on Lasers and Electro-Optics Europe (CLEO/Europe) and the European Quantum Electronics Conference (EQEC) 2021, 20–24 June 2021 Munich, Germany (on-line).

4. G. Sansone, “Attosecond metrology at seeded free-electron lasers”, CLEO Laser Science to Photonic Application, 9-14 May 2021 San Jose, California, USA (on-line).

5. G. Sansone, “Synthesizing attosecond pulses at a seeded FEL”, 3rd ICEL Conference, 22-25 October 2019 Prague.

6. S. H. Ahmadi, P. A. Carpeggiani, M. Reduzzi, A. Comby, M. Nisoli, G. Sansone, F. Frassetto, L. Poletto, D. Hoff, G. Paulus, C.-D. Schröter, R. Moshammer, "Time-resolved petahertz spectroscopy", Quantum dynamics in tailored intense fields (QUTIF) International Conference, July 25-27, 2019, Oldenburg, Germany.
7. G. Sansone, "Temporal Characterization of FEL-driven Attosecond Pulses", 7th International Conference on Attosecond Science and Technology, 1-5 July 2019, Szeged Hungary.
8. P. K. Maroju, "Sub-femtosecond Timing Tool for Experiments with a Seeded Free Electron Laser", 7th International Conference on Attosecond Science and Technology, 1-5 July 2019, Szeged, Hungary.
9. G. Sansone, "Polychromatic photoionization of atoms in atto- and femtosecond domain" XXXIst International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC), 23-30 July 2019, Deuville, France.
10. P. K. Maroju, "Attosecond Pulse Shaping at FERMI FEL", The 5th International Symposium on Intense Short Wavelength Processes in Atoms and Molecules (ISWAMP), July 20-22 2019, Paris, France, 2019.

Mandates/Awards

1. Innovation Award on Synchrotron Radiation 2020 Helmholtz-Zentrum Berlin (HZB) for Giuseppe Sansone (price shared with Dr. L. Giannessi, Dr. C. Callegari, Dr. K. Prince).
2. Since 2020: Associate Editor of the Science Partner Journal "Ultrafast Science".
3. General Co-Chair (2020 and 2022) and Program Co-Chair (2018) of OSA/OPTICA Topical Meeting on High-Intensity Lasers and High-Field Phenomena (HILAS).
4. October 2019-September 2021: Dean of Studies of the Institute of Physics.
5. Since 2019: Member of the European XFEL User Organization Executive Committee.

Group Schaetz

Publications

[schae1] F. Schlawin, M. Gessner, A. Buchleitner, T. Schaetz, and S. S. Skourtis, "Continuously Parametrized Quantum Simulation of Molecular Electron-Transfer Reactions", Phys. Rev. X Quantum **2** (2021) 010312.
Our numerical simulations predict an unconventional quantum transfer regime, featuring a transition from quantum adiabatic to resonance-assisted transfer as a function of the donor-acceptor energy gap, which can be reached by increasing the electronic coupling at low temperatures.

[schae2] P. Weckesser, F. Thielemann, D. Wiater, A. Wojciechowska, L. Karpa, K. Jachymski, M. Tomza, T. Walker and T. Schaetz, "Observation of Feshbach resonances between a single ion and ultracold atoms", Nature **600** (2021) 429–433 [0 cit.]
We demonstrate Feshbach resonances between ions and atoms, using magnetically tunable interactions between $^{138}Ba^{+}$ ions and ^{6}Li atoms.

[schae3] J. Schmidt, P. Weckesser, F. Thielemann, T. Schaetz, L. Karpa, "Optical Traps for sympathetic Cooling of Ions with ultracold neutral Atoms", Phys. Rev. Lett. **124** (2020) 053402
We report the trapping of ultracold neutral Rb atoms and Ba^{+} ions in a common optical potential in absence of any radio frequency (rf) fields.

[schae4] P. Kiefer, F. Hakelberg, M. Wittemer, A. Bermdez, D. Porras, U. Warring, T. Schaetz, "Floquet-engineered vibrational dynamics in a two-dimensional array of trapped ions", Phys. Rev. Lett. **123** (2019) 213605
We demonstrate Floquet engineering in a basic yet scalable 2D architecture of individually trapped and controlled ions. Local parametric modulations of detuned trapping potentials steer the strength of long-range interion couplings and the related Peierls phase of the motional state.

[schae5] M. Wittemer, F. Hakelberg, P. Kiefer, J.-P. Schroeder, C. Fey, R. Schuetzhold, U. Warring, T. Schaetz, "Phonon pair creation by inflating quantum fluctuations in an ion trap", Phys. Rev. Lett. **123** (2019) 180502
We switch the trapping field of two ions sufficiently fast to tear apart quantum fluctuations, i.e., create pairs of phonons and, thereby, squeeze the ions' motional state. This process can be interpreted as an experimental analog to cosmological particle creation and is accompanied by the formation of spatial entanglement.

[schae6] F. Hakelberg, P. Kiefer, M. Wittemer, U. Warring, T. Schaetz, "Interference in a Prototype of a two-dimensional Ion Trap Array Quantum Simulator", Phys. Rev. Lett. **123** (2019) 100504
We operate a basic triangular array of three individually trapped ions based on scalable microfabrication technology. We demonstrate coherent coupling, tunable in real time and enabling interference in 2D, an essential building block for a reconfigurable quantum simulator.

[schae7] J. Schmidt, A. Lambrecht, P. Weckesser, M. Debatin, L. Karpa, T. Schaetz, "Optical Trapping of Ion Coulomb Crystals", Phys. Rev. X **8** (2018) 021028
We report on the trapping of multiple barium ions in a single-beam optical dipole trap without radio-frequency or additional magnetic fields. We study the persistence of order in ensembles of up to six ions within the optical trap, measure their temperature, and conclude that the ions form a linear chain, commonly called a one-dimensional Coulomb crystal.

[schae8] M. Wittemer, G. Clos, H.-P. Breuer, U. Warring, T. Schaetz, "Measurement of quantum memory effects and its fundamental limitations", Phys. Rev. A **97** (2018) 020102(R)
We discuss that the nature of projective measurements in quantum mechanics can lead to a nontrivial bias in non-Markovianity measures, quantifying the flow of information between a system and its environment. Consequently, in the current form, envisioned applications are fundamentally limited.

[schae9] P. Weckesser, F. Thielemann, D. Hoenig, A. Lambrecht, L. Karpa and T. Schaetz, "Trapping, shaping and isolating of an ion Coulomb crystals via state-selective optical potentials", Phys. Rev. A **103** (2018) 013112
For conventional ion traps, the trapping potential is close to independent of the electronic state, providing confinement for ions dependent primarily on their charge-to-mass ratio. In contrast, storing ions within an optical dipole trap results in state-dependent confinement. Here we experimentally study optical dipole potentials for $^{138}Ba^{+}$ ions stored within two distinctive traps operating at 532 and 1064 nm. We prepare the ions in either the electronic ground or one of the metastable excited states and probe the relative strength and polarity of the potential.

[schae10] U. Warring, F. Hakelberg, P. Kiefer, M. Wittemer, T. Schaetz, "Trapped Ion Architecture for Multi-Dimensional Quantum Simulations", Adv. Quantum Technol. (2020) 1900137
In this article, an overview of recent developments and demonstrations of prototype operations is given. The features and limitations of the architecture are discussed and crucial steps toward mid and long-term simulation applications are laid out.

Conference Talks

1. T. Schaetz,Optical Trapping of Ion Coulomb Crystals, Nature (Webinar sponsored by Andor), July, 2018.
2. T. Schaetz, Few-body and collective many-body behavior with charge impurities in atomic quantum gases, Sant Feliu de Guixols, Spain, July 2018.
3. T. Schaetz, Experimental Quantum Simulations in Arrays of Trapped Ions European Conference on Trapped Ions, Weizmann Institute, Israel, November 2018.
4. T. Schaetz, Experimental Quantum Simulations – Time Resolved Observation of Thermalization in an Isolated Quantum System, 684. WE-Heraeus Seminar on: Advances in open systems and fundamental tests of quantum mechanics, December 2018.
5. T. Schaetz, Optical Lattices for Trapping Atoms and Ions, Workshop: Compound Quantum Systems, Lorentz Centre, Netherlands, May 2019.
6. T. Schaetz, Optical Lattices for Trapping Atoms and Ions Gordon Conference "Atomic Physics Gordon Research Conference, Salve Regina University, USA, June 2019.

7. T. Schaetz, Optical Traps for Ions & Ultracold Atoms and the Onset of Sympathetic Cooling, ITAMP Workshop: Cold Ion Many-Body Physics, Cambridge, USA, October 2019.

8. T. Schaetz, Phonon Pair Creation, Royal Society, London, UK, December 2019.

9. T. Schaetz, Wäre die Welt nicht einfacher ohne Quanten zu verstehen? Campus Talk (ARD alpha), March 2020.

10. T. Schaetz, Optical Traps for Ions & Ultracold Atoms and the Onset of Sympathetic Cooling, Winter School on Physics with Trapped Charged Particles, Les Houches, February 2021.

Mandates/Awards

1. 10.2016 - 09.2018: Managing Director of the Institute of Physics, University of Freiburg.

2. Since 2017: Member of the steering committee of the Freiburg-Basel Cluster of Excellence Quantum Science and Quantum Computing funded by the Georg H. Endress Foundation.

3. Since 2018: Member of the steering committee of the doctoral training programme QUSTEC (Quantum Science ans Technologies at the European Campus)set up by the European Grouping of Territorial Cooperation (EGTC) Eucor – The European Campus.

4. Since 2020: speaker of the knot at the University of Freiburg within the competence network Quantum Technolgy in the state of Baden-Württemberg.

5. Since 2015–1/2021: ERC Consolidator Grant: 648330 TIAMO, Trapping Ions and Atoms Optically.

Group Stienkemeier

Publications

[sti1] D. Uhl, U. Bangert, L. Bruder, and F. Stienkemeier, "Coherent optical 2D photoelectron spectroscopy", Optica **8** (2021) 1316-1324.
Coherent 2D optical spectroscopy was combined for the first time with photoelectron spectroscopy as a probe. The highly differential photoelectron detection enables the selective probing of specific electronic contributions and increased the experimental sensitivity by two orders of magnitude.

[sti2] S. Izadnia, A. C. LaForge, F. Stienkemeier, J. R. Cheeseman, J. Bloino, J. Cheramy, W. Jäger, and Y. Xu, "Unusual binary aggregates of perylene bisimide revealed by their electronic transitions in helium nanodroplets and DFT calculations", Phys. Chem. Chem. Phys. **23** (2021) 13862-13872.
The vibronic spectra of dimers of perylene bisimide synthezised with superfluid helium nanodroplets were measured in high resolution. A comparison with extensive vibronic DFT calculations confirmed the formation of unusal T-shaped geometric structures.

[sti3] C. Medina, D. Schomas, N. Rendler, M. Debatin, D. Uhl, A. Ngai, L. Ben Ltaief, M. Dumergue, Z. Filus, B. Farkas, R. Flender, L. Haizer, B. Kiss, M. Kurucz, B. Major, S. Toth, F. Stienkemeier, R. Moshammer, T. Pfeifer, S. R. Krishnan, A. Heidenreich, M. Mudrich, "Single-shot electron imaging of dopant-induced nanoplasmas", New J. Phys., **23 (5)** (2021) 053011.
Single-shot electron velocity-map images of nanoplasmas generated from doped helium nanodroplets and neon clusters by intense near-infrared and mid-infrared laser pulse are measured and the kinetic energy distributions are analyzed in comparison with molecular dynamics calculations.

[sti4] A. C. LaForge, R. Michiels, Y. Ovcharenko, A. Ngai, J. M. Escartín, N. Berrah, C. Callegari , A. Clark, M. Coreno, R. Cucini, M. Di Fraia, M. Drabbels, E. Fasshauer, P. Finetti, L. Giannessi, C. Grazioli, D. Iablonskyi, B. Langbehn, T. Nishiyama, V. Oliver, P. Piseri, O. Plekan, K. C. Prince, D. Rupp, S. Stranges, K. Ueda, N. Sisourat, J. Eloranta, M. Pi, M. Barranco, F. Stienkemeier, T. Möller, M. Mudrich, "Ultrafast Resonant Interatomic Coulombic Decay Induced by Quantum Fluid Dynamicsc", Phys. Rev. X, **11 (2)** (2021) 021011.

The timescale of interatomic Coulombic decay (ICD) in helium nanodroplets is measured using a high-resolution, tunable, extreme ultraviolet free-electron laser. Using a combination of time-dependent density functional theory and ab initio quantum chemistry calculations, a mechanisms of an ultrafast decay process has been found, where pairs of excited helium atoms in one droplet strongly attract each other and form merging void bubbles, which drastically accelerates ICD.

[sti5] A. Wituschek, L. Bruder, E. Allaria, U. Bangert, M. Binz, R. Borghes, C. Callegari, G. Cerullo, P. Cinquegrana, L. Giannessi, M. Danailov, A. Demidovich, M. Di Fraia, M. Drabbels, R. Feifel, T. Laarmann, R. Michiels, N. S. Mirian, M. Mudrich, I. Nikolov, F. H. O'Shea, G. Penco, P. Piseri, O. Plekan, K. C. Prince, A. Przystawik, P. R. Ribič, G. Sansone, P. Sigalotti, S. Spampinati, C. Spezzani, R. J. Squibb, S. Stranges, D. Uhl, and F. Stienkemeier, "Tracking attosecond electronic coherences using phase-manipulated extreme ultraviolet pulses", Nat. Commun. **11** (2020) 883.
A new method for interferometry in the XUV spectral domain was established. Phase cycling of a free electron laser was implemented and electronic wave packet interferometry was performed to track the coherence decay of an electronic wave packet at a Fano resonance in the time domain.

[sti6] M. Mudrich, A. C. LaForge, A. Ciavardini, P. O'Keeffe, C. Callegari, M. Coreno, A. Demidovich, M. Devetta, M. Di Fraia, M. Drabbels, P. Finetti, O. Gessner, C. Grazioli, A. Hernando, D. M. Neumark, Y. Ovcharenko, P. Piseri, O. Plekan, K. C. Prince, R. Richter, M. P. Ziemkiewicz, T. Möller, J. Eloranta, M. Pi, M. Barranco, and F. Stienkemeier, "Ultrafast relaxation of photoexcited superfluid He nanodroplets", Nat. Commun. **11** (2020) 112.
Using ultrafast XUV laser pulses the relaxation processes upon electronic excitation of helium nanodroplets are tracked in real time. Supported by TDFT calculations the full relaxation pathway is identified in detail, including inter-band relaxation, nano-bubble formation, collaps and ejection of excited helium atoms off the surface of the droplet.

[sti7] L. Bruder, A. Eisfeld, U. Bangert, M. Binz, M. Jakob, D. Uhl, M. Schulz-Weiling, E. R. Grant, and F. Stienkemeier, "Delocalized excitons and interaction effects in extremely dilute thermal ensembles", Phys. Chem. Chem. Phys. **21** (2019) 2276-2282.
A highly sensitive detection of interparticle interactions was developed based on coherent nonlinear spectroscopy. The new method revealed dipolar interactions in extremely dilute thermal alkali atom vapors with a mean interparticle distance of up to 27 μm. This regime was previously not accessible by the frequency-domain methods form the ultracold and quantum optics community.

[sti8] A. C. LaForge, R. Michiels, M. Bohlen, C. Callegari, A. Clark, A. von Conta, M. Coreno, M. Di Fraia, M. Drabbels, M. Huppert, P. Finetti, J. Ma, M. Mudrich, V. Oliver, O. Plekan, K. C. Prince, M. Shcherbinin, S. Stranges, V. Svoboda, H. J. Wörner, and F. Stienkemeier, "Real-Time Dynamics of the Formation of Hydrated Electrons upon Irradiation of Water Clusters with Extreme Ultraviolet Light", Phys. Rev. Lett. **122** (2019) 133001.
The initial steps in the formation of solvated electrons in water were studied by time-resolved photo-electron spectroscopy using femtosecond XUV laser pulses from the free-electron laser FERMI, revealing in particular a prominent formation of excited hydrogen atoms.

[sti9] A. C. LaForge, M. Shcherbinin, F. Stienkemeier, R. Richter, R. Moshammer, T. Pfeifer, and M. Mudrich, "Highly efficient double ionization of mixed alkali dimers by intermolecular Coulombic decay", Nat. Phys. **15** (2019) 247–250.
A new decay mechanism leading to the double ionization of alkali dimers by intermolecular energy transfer from excited helium was found. The efficiency is equal or even greater compared to single ionization, and is similar to the well-known shake-off mechanism observed in double Auger decay and single-photon double ionization.

[sti10] L. Bruder, U. Bangert, M. Binz, D. Uhl, R. Vexiau, N. Bouloufa-Maafa, O. Dulieu, F. Stienkemeier, "Coherent multidimensional spectroscopy of dilute gas-phase nanosystems", Nat. Commun. **9** (2018) 4823.
Coherent 2D spectroscopy was applied for the first time to isolated, cold molecular species prepared in a cluster-beam experiment. This provides an important extension of 2D spectroscopy from the predominantly studied condensed phase to well-defined model systems in the gas phase. The ultrafast in rubidium dimer and trimers dissolved in superfluid helium droplets were studied.

Conference Talks

1. F. Stienkemeier, “2-Dimensional Electronic Spectroscopy of Gas Phase Samples”, Gordon Research Conference on Photoionization and Photodetachment, Galveston, USA, February 2018.

2. F. Stienkemeier, “Two-dimensional electronic spectroscopy of cold, controlled systems”, 49th Annual Meeting DAMOP 2018 (Division of Atomic, Molecular and Optical Physics), Ft. Lauredale, Florida, USA, May 2018.

3. U. Bangert, “Two-dimensional electronic spectroscopy of molecules in helium nanodroplet isolation”, 28th International Symposium on Molecular Beams, Edinburgh, United Kingdom, June 2019.

4. L. Bruder, “Tracking electronic coherences in the XUV spectral range”, 11th Ringberg Workshop: Hard X-ray XFELs, Tegernsee, Germany, June 2020.

5. F. Stienkemeier, “Coherent Multidimensional Spectroscopy of Cluster Beams”, Gordon Research Conference on Molecular and Ionic Clusters, Ventura, USA, February 2020.

6. F. Stienkemeier, “Multidimensional spectroscopy and ultrafast dynamcis in nanoclusters”, Physical Chemistry Seminar, University of California, Berkeley, CA, USA, February 2020.

7. F. Stienkemeier, “Multidimensional spectroscopy and ultrafast dynamics”, Photon Science Seminar at the SLAC National Accelerator Laboratory, Menlo Park, USA, February 2020.

8. F. Stienkemeier, “Phase cycling and coherent spectroscopy in the XUV domain”, First WavemiX workshop on Non-linear X-ray spectroscopy, Paul Scherrer Institut, Switzerland, January 2021.

9. L. Bruder, “Coherent multidimensional spectroscopy of cluster beams”, International Symposium of Molecular Beams (ISMB 2021) (virt. conf.), July 2021.

10. L. Bruder, “Extending coherent nonlinear spectroscopy to new samples and light sources”, Ultrafast Dynamic Imaging of Matter (UFDIM), (virt. conf.), September 2021.

Mandates/Awards

1. F. Stienkemeier, since 4/2019: Board member of the Atomic, Molecular and Optical Physics Division (AMOPD) and representative of the Chemical and Molecular Physics Section (CMPS) of the European Physical Society (EPS).

2. F. Stienkemeier, Member of the Council of the German Physical Society, 2012 - 2018.

3. F. Stienkemeier, since 05/18 Member of the European XFEL Proposal Review Panel SQS.

4. F. Stienkemeier, Spokesperson of the DFG-funded International Research Training Group *Cold Controlled Ensembles in Physics and Chemistry* (IRTG 2079).

5. F. Stienkemeier, ERC Advanced Grant, European Research Council, “COCONIS” (Coherent Multidimensional Spectroscopy of Controlled Isolated Systems), 09/2016 - 08/2021

Group Dulitz

Publications

[du1] N. Rendler, A. Scognamiglio, M. Barranco, M. Pi, N. Halberstadt, K. Dulitz, and F. Stienkemeier, “Dynamics of photoexcited Cs atoms attached to helium nanodroplets”, J. Phys. Chem. A **125** (2021) 9048-9059.
The desorption and re-adsorption dynamics of laser-excited Cs atoms as well as CsHe exciplex formation on the surface of He nanodroplets are measured using femtosecond pump–probe velocity map imaging spectroscopy and ion time-of-flight spectrometry.

[du2] P. Straňák, L. Ploenes, S. Hofsäss, K. Dulitz, F. Stienkemeier, and S. Willitsch, "Development and characterization of high-repetition-rate sources for supersonic beams of fluorine radicals", Rev. Sci. Instrum. **92** (2021) 103203.
Comparison between a dielectric-barrier discharge source and a plate discharge source for the generation of supersonic beams of F radicals.

[du3] T. Sixt, J. Guan, A. Tsoukala, S. Hofsäss, T. Muthu-Arachchige, F. Stienkemeier, and K. Dulitz, "Preparation of individual magnetic sub-levels of ^{4}He(2^3S$_1$) in a supersonic beam using laser optical pumping and magnetic hexapole focusing", Rev. Sci. Instrum. **92** (2021) 073203.
Comparison between laser-optical pumping and magnetic hexapole focusing for the magnetic-sub-level preparation of metastable ^{4}He in the 2^3S$_1$ level in a supersonic beam.

[du4] J. D. Asmussen, R. Michiels, K. Dulitz, N. Ngai, U. Bangert, M. Barranco, M. Binz, L. Bruder, M. Danailov, M. Di Fraia, J. Eloranta, R. Feifel, L. Giannessi, M. Pi, O. Plekan, K. C. Prince, R. J. Squibb, D. Uhl, A. Wituschek, M. Zangrando, C. Callegari, F. Stienkemeier, and M. Mudrich, "Unravelling the full relaxation dynamics of superexcited helium nanodroplets", Phys. Chem. Chem. Phys. **23** (2021) 15138-15149.
Investigation of the relaxation dynamics of superexcited superfluid He nanodroplets using extreme-ultraviolet femtosecond electron and ion spectroscopy complemented by time-dependent density functional theory.

[du5] J. Guan, T. Sixt, D. Dulitz, and F. Stienkemeier, "Sensitive detection of metastable NO and N_2 by reactive collisions with laser-excited Li", J. Phys. B: At. Mol. Opt. **53** (2020) 245201.
Experimental demonstration of the sensitive detection of NO molecules in the a$^4\Pi_i$ state, generated inside a pulsed supersonic expansion, by reactive collisions with Li atoms in the 2^2P$_{3/2}$ state.

[du6] K. Dulitz, T. Sixt, J. Guan, J. Grzesiak, M. Debatin, and F. Stienkemeier, "Suppression of Penning ionization by orbital angular momentum conservation", Phys. Rev. A **102** (2020) 022818.
It is demonstrated experimentally that Penning ionization is suppressed in collisions between metastable He and laser-excited Li atoms. The suppression is due to the conservation of both the total electron spin and Λ, i.e., the projection of the total molecular orbital angular momentum along the internuclear axis. The results suggest that Λ conservation is applicable not only to the He-Li system, but also to other autoionizing systems in which the spin-orbit coupling in the entrance and exit channels is weak.

[du7] K. Dulitz, M. van den Beld-Serrano, and F. Stienkemeier, "Single-source, collinear merged-beam experiment for the study of reactive neutral–neutral collisions", J. Phys. Chem. A **124** (2020) 3484-3493.
Proposal for a collinear merged-beam method and an intrabeam-scattering technique as experimental techniques for studying reactive collisions between neutral species.

[du8] J. Guan, V. Behrendt, P. Shen, S. Hofsäss, T. Muthu-Arachchige, J. Grzesiak, F. Stienkemeier, and K. Dulitz, "Optical quenching of metastable helium atoms using excitation to the $4P$ state", Phys. Rev. Appl. **11** (2019) 054073.
Presentation of a new and efficient scheme for the depopulation of the 2^1S$_0$ state of He in a supersonic beam which is based on the laser excitation of the 4^1P$_1 \leftarrow 2^1$S$_0$ transition followed by spontaneous decay into the 1^1S$_0$ ground state.

[du9] J. Grzesiak, T. Momose, F. Stienkemeier, M. Mudrich, and K. Dulitz, "Penning collisions between supersonically expanded metastable He atoms and laser-cooled Li atoms", J. Chem. Phys. **150** (2019) 034201.
Description of an experimental setup for the study of chemi-ionization processes composed of a discharge source for supersonic beams of metastable He atoms and a magneto-optical trap for ultracold Li atoms. A multi-pulse ion-time-of-flight scheme for the detection of the charged reaction products is presented. Metastable He-Li chemi-ionization is used to determine the temperature of the ultracold Li atoms; and the influence of elastic He-Li collisions on the steady-state Li atom number in the MOT is determined.

[du10] J. Grzesiak, M. Vashishta, P. Djuricanin, F. Stienkemeier, M. Mudrich, K. Dulitz, and T. Momose, "Production of rotationally cold methyl radicals in pulsed supersonic beams", Rev. Sci. Instrum. **89** (2018) 113103.
Comparison between a plate discharge source and a dielectric barrier discharge source for the production of rotationally cold, pulsed supersonic beams of methyl radicals.

Conference Talks

1. K. Dulitz, “Quantum-state controlled chemi-ionization reactions”, 32nd International Conference on Photonic, Electronic and Atomic Collisions (ViCPEAC 2021), (virt. conf.), July 2021.

2. K. Dulitz, “Kontrolle chemischer Reaktionen auf Quantenbasis”, 23. Steinheimer Gespräche des Fonds der Chemischen Industrie für den Hochschullehrernachwuchs, (virt. conf.), June 2021.

3. K. Dulitz, “Quantum-state controlled Penning collisions between metastable He atoms and ultracold Li atoms”, New Horizons in Chemical Physics Symposium, Merton College Oxford, UK, April 2019.

4. K. Dulitz, “Towards the study of quantum-state-selected Penning reactions”, 101st Canadian Chemistry Conference and Exhibition (CSC2018), Edmonton, Canada, May 2018.

5. K. Dulitz, “Towards the study of quantum-state-selected Penning reactions”, Cold and Controlled Molecules and Ions (CCMI) conference, Athens/GA, USA, March 2018.

6. K. Dulitz, “Towards the study of quantum-state-selected Penning reactions”, DPG Spring Meeting, Erlangen, Germany, March 2018.

Mandates/Awards

1. Since 01/2021: Guest Editor for the focus issue “Cold and Ultracold Chemistry of Atoms, Molecules and Ions” by the New Journal of Physics

2. Since 04/2018: Member of the Advisory Panel for the international conference series Cold and Controlled Molecules and Ions (CCMI)

3. 03/2018–09/2021: Liebig Fellowship, Fonds der Chemischen Industrie

Group von Issendorff

Publications

[bvi1] A. Piechaczek, C. Bartels, C. Hock, J.-M. Rost, and B. von Issendorff, “Decoherence-Induced Universality in Simple Metal Cluster Photoelectron Angular Distributions”, Phys. Rev. Lett. **126** (2021) 233201.
Simple metal clusters are demonstrated to exhibit universal photoelectron angular distributions independent of cluster size and material and the initial state of the electron, which can be explained by a simple quantum model in which decoherence quenches interference and therefore leads to semiclassical behaviour.

[bvi2] K. Majer, L. Ma, and B. von Issendorff “Photoelectron Spectroscopy of Large Water Cluster Anions”, J. Phys. Chem. A **125** (2021) 8426–8433.
Measurement of photoelectron spectra of water cluster anions with up to 1100 molecules permits to determine the bonding motif of the solvated electron and yields a precise value for the binding energy extrapolation to the bulk.

[bvi3] R.C. Couto, W. Hua, R. Lindblad, L. Kjellsson, S.L. Sorensen, M. Kubin, C. Bülow, M. Timm, V. Zamudio-Bayer, B. von Issendorff, J. Söderström, J.T. Lau, J.-E. Rubensson, H. Ågren and V. Carravetta “Breaking inversion symmetry by protonation: experimental and theoretical NEXAFS study of the diazynium ion, N_2H^+”, Phys. Chem. Chem. Phys., 2021,23, 17166-17176.
Attachment of a proton to a nitrogen molecule makes dark states bright, by lifting symmetry imposed selection rules.

[bvi4] D. Sankar De, B. Schaefer, B. von Issendorff, and S. Goedecker “Nonexistence of the decahedral Si20H20 cage: Levinthal’s paradox revisited”, Phys. Rev. B **101** (2020) 214303.
The complex energetic landscape of Si20H20 is responsible for the fact that the fullerene cage-like structure does not form spontaneously despite being the lowest energy structure.

[bvi5] R. Lindblad, L. Kjellsson, R. C. Couto, M. Timm, C. Bülow, V. Zamudio-Bayer, M. Lundberg, B. von Issendorff, J. T. Lau, S. L. Sorensen, V. Carravetta, H. Ågren, and J.-E. Rubensson, "X-Ray Absorption Spectrum of the N_2^+ Molecular Ion", Phys. Rev. Lett. **124** (2020) 203001.
Vibrationally resolved x-ray absorption spectra permit to sensitively check calculated potential energy curves and demonstrate a complete breakdown of the single particle picture for higher excitation energies.

[bvi6] M. Walter, M. Vogel, V. Zamudio-Bayer, R. Lindblad, T. Reichenbach, K. Hirsch, A. Langenberg, J. Rittmann, A. Kulesza, R. Mitrić, M. Moseler, T. Möller, B. von Issendorff, J. T. Lau "Experimental and theoretical 2p core-level spectra of size-selected gas-phase aluminum and silicon cluster cations: chemical shifts, geometric structure, and coordination-dependent screening", Phys. Chem. Chem. Phys. **21** (2019) 6651.
High charge state fragment abundance as a function of photon energy yields core level binding energies like x-ray photoelectron spectroscopy, allowing to determine position dependent chemical shifts.

[bvi7] X. Wu, X. Liang, Q. Du, J. Zhao , M. Chen, M. Lin, J. Wang, G. Yin, L. Ma, R. B. King and B. von Issendorff, "Medium-sized Si_n^- (n=14-20) clusters: a combined study of photoelectron spectroscopy and DFT calculations", J. Phys.: Condens. Matter **30** (2018) 354002.
Determination of geometric structures of small silicon clusters based on improved experimental and theoretical methods.

[bvi8] A. Aguado, A. Vega, A. Lebon and B. von Issendorff, "Are zinc clusters really amorphous? A detailed protocol for locating global minimum structures of clusters", Nanoscale **10** 10, (2018) 19162.
Application of an improved structure search scheme employing an optimized classical potential to the complex structures of zinc clusters.

[bvi9] C. Yu, R. Schira, H. Brune, B. von Issendorff, F. Rabilloudband, W. Harbich, "Optical properties of size selected neutral Ag clusters: electronic shell structures and the surface plasmon resonance", Nanoscale **10** (2018) 20821.
High resolution absorption spectra of size selected silver clusters in a neon matrix in good agreement with calculations.

[bvi10] V. Zamudio-Bayer, K. Hirsch, A. Langenberg, A. Ławicki, A. Terasaki, B. von Issendorff, J. T. Lau, "Large orbital magnetic moments of small, free cobalt cluster ions Co_n^+ with $n \leq 9$", J. Phys.: Condens. Matter **30** (2018), 464002.
XMCD spectra measured on size selected cobalt cluster cations in a cryogenic ion trap reveal both spin and orbital magnetic moments, which reveal a cluster specific larger contribution of the latter.

Conference Talks

1. B. v. Issendorff, Structure and dynamics of simple metal clusters QINO Seminar, Uni Wien, Vienna, Austria, October 2021.
2. B. v. Issendorff, Small is beautiful: structure and dynamics of clusters Egas 52, Zagreb, Croatia (online), July 2021.
3. B. v. Issendorff, Study of gas phase metal clusters using free electron lasers, S3C, Davos, Switzerland, February 2020.
4. B. v. Issendorff, Structure and dynamics of metal clusters: old and new tales, 705. WE Heraeus Seminar (Clustertreffen), Bad Honnef, Germany, September 2019.
5. B. v. Issendorff, Structure and dynamics of gas phase metal clusters, ESD 8, Tianjin, China, August 2019.
6. B. v. Issendorff, Small is beautiful: study of the structure and dynamics of clusters, Physics Colloquium Uni Innsbruck, Innsbruck, Austria, June 2019.
7. B. v. Issendorff, X-ray spectroscopy and imaging of free metal clusters, CFEL Molecular Physics Seminar, Hamburg, Germany, June 2018.

Group Lau

Publications

[lau1] R. C. Couto, W. Hua, R. Lindblad, L. Kjellsson, S. L. Sorensen, M. Kubin, C. Bülow, M. Timm, V. Zamudio-Bayer, B. von Issendorff, J. Söderström, J. T. Lau, J.-E. Rubensson, H. Ågren, V. Carravetta, "Breaking inversion symmetry by protonation: experimental and theoretical NEXAFS study of the diazynium ion, N_2H^+", Phys. Chem. Chem. Phys. **23** (2021) 17166.
Protonation of the dinitrogen molecule breaks inversion symmetry and leads to final states that are symmetry-forbidden in the corresponding neutral molecule.

[lau2] X. Wang, S. Rathnachalam, K. Bijlsma, W. Li, R. Hoekstra, M. Kubin, M. Timm, B. von Issendorff, V. Zamudio-Bayer, J. T. Lau, S. Faraji, T. Schlathölter, "Site-selective soft X-ray absorption as a tool to study protonation and electronic structure of gas-phase DNA", Phys. Chem. Chem. Phys. **23** (2021) 11900.
Protonation sites of gas-phase oligonucleotides are identified in a combined experimental and theoretical x-ray absorption spectroscopy study in our cryogenic ion trap.

[lau3] K. Schubert, M. Guo, K. Atak, S. Dörner, C. Bülow, B. von Issendorff, S. Klumpp, J. T. Lau, P. S. Miedema, T. Schlathölter, S. Techert, M. Timm, X. Wang, V. Zamudio-Bayer, L. Schwob, S. Bari, "The electronic structure and deexcitation pathways of an isolated metalloporphyrin ion resolved by metal L-edge spectroscopy", Chem. Sci. **12** (2021) 3966.
The electronic state of the cobalt(III) protoporphyrin IX cation is determined from L-edge x–ray absorption spectroscopy in the gas phase, enabled by our combination of electrospray ionization and cryogenic ion trapping

[lau4] R. C. Couto, L. Kjellsson, H. Ågren, V. Carravetta, S. L. Sorensen, M. Kubin, C. Bülow, M. Timm, V. Zamudio-Bayer, B. von Issendorff, J. T. Lau, J. Söderström, J.-E. Rubensson, R. Lindblad, "The carbon and oxygen K-edge NEXAFS spectra of CO^+", Phys. Chem. Chem. Phys. **22** (2020) 16215.
The strong localization of the 5σ orbital at the carbon center in CO^+ affects Coulomb and exchange energy in core-excited states that can be monitored via 2π splittings and intensity ratios at carbon and oxygen $1s$ core excitation.

[lau5] R. Lindblad, L. Kjellsson, R. C. Couto, M. Timm, C. Bülow, V. Zamudio-Bayer, M. Lundberg, B. von Issendorff, J. T. Lau, S. L. Sorensen, V. Carravetta, H. Ågren, J.-E. Rubensson, "X-ray absorption spectrum of the N_2^+ molecular ion", Phys. Rev. Lett. **124** (2020) 203001.
Surprisingly little data exists about core-excited states of even very simple diatomic molecules. The positive charge of the cation leads to numerous bound excited states at significantly higher energies than in the neutral species, corresponding to multiparticle excited states that are a challenge to theory.

[lau6] L. Schwob, S. Dörner, K. Atak, K. Schubert, M. Timm, C. Bülow, V. Zamudio-Bayer, B. von Issendorff, J. T. Lau, S. A. Techert, S. Bari, "Site-selective dissociation upon sulfur L-edge X-ray absorption in a gas-phase protonated peptide", J. Phys. Chem. Lett. **11** (2020) 1215.
Site-specific dissociation induced by element-specific core excitation. Protonation in the electrospray ionization process allows for ion mass selection and trapping.

[lau7] M. Walter, M. Vogel, V. Zamudio-Bayer, R. Lindblad, T. Reichenbach, K. Hirsch, A. Langenberg, J. Rittmann, A. Kulesza, R. Mitrić, M. Moseler, T. Möller, B. von Issendorff, J. T. Lau, "Experimental and theoretical 2p core-level spectra of size-selected gas-phase aluminum and silicon cluster cations: chemical shifts, geometric structure, and coordination-dependent screening", Phys. Chem. Chem. Phys. **21** (2019) 6651.
The particular energy dependence of product ions allows for the determination of core-level binding energies from ion yield spectroscopy, and reveals large chemical shifts of opposite sign for both elements. In collaboration with the Moseler group for computational spectra that fit the experimental data very well.

[lau8] V. Zamudio-Bayer, K. Hirsch, A. Langenberg, A. Lawicki, A. Terasaki, B. von Issendorff, J. T. Lau, "Large orbital magnetic moments in small, free cobalt cluster ions Co_n^+ with $n \leq 9$", J. Phys.: Condens. Matter **30** (2018) 464002.
Unexpectedly large orbital magnetic moments of small cobalt clusters hint at large magnetic anisotropy energy.

[lau9] S. C. Meier, A. Holz, J. Kulenkampff, A. Schmidt, D. Kratzert, D. Himmel, D. Schmitz, E.-W. Scheidt, W. Scherer, C. Bülow, M. Timm, R. Lindblad, S. T. Akin, V. Zamudio-Bayer, B. von Issendorff, M. A. Duncan, J. T. Lau, I. Krossing, “Access to the bis-benzene cobalt(I) sandwich cation and its derivatives: synthons for a ”naked” cobalt(I) source?”, Angew. Chem. Int. Ed. **57** (2018) 9310.
Spin and orbital resolved magnetic moments of the gas-phase species helped to understand electronic properties of condensed phase. In collaboration with Krossing lab at Institut für Angewandte Chemie, who report on synthesis and properties.

[lau10] S. Bari, D. Egorov, T. L. C. Jansen, R. Boll, R. Hoekstra, S. Techert, V. Zamudio-Bayer, C. Bülow, R. Lindblad, G. Leistner, A. Lawicki, K. Hirsch, P. S. Miedema, B. von Issendorff, J. T. Lau, T. Schlathölter, “Soft x-ray spectroscopy as a probe for gas-phase protein structure: electron impact ionization from within”, Chem Eur. J. **24** (2018) 7631.
Secondary ionization efficiency depends on the trajectory of photoelectrons through gas-phase peptides. This effect is used as a coarse probe of gas-phase protein structure. Electrospray ionization is key to addressing ionic samples prepared from solvated species.

Conference Talks

1. M. da Silva Santos, High-resolution x-ray absorption spectroscopy in a cryogenic ion trap as a tool to investigate 3d metal-oxygen bonds, Cluster Meeting 2021, Prague, Czech Republic, July 2021
2. M. da Silva Santos, Study of chemical bonds in metal-oxygen systems based on X-ray absorption spectroscopy, Seminar Anorganische Chemie, Freiburg, October 2021
3. J. T. Lau, Oxidation states and charge transfer, S3C, Davos, Switzerland, February 2020.
4. J. T. Lau, Discussion leader and introduction to magnetic clusters, Clusters and Nanostructures GRC, Les Diablerets, Switzerland, June 2019
5. J.T. Lau, Molecular iron oxides: iron in the unusual +7 oxidation state, Matter, Materials, and Life – Helmholtz Programme Workshop, Dresden, February 2019
6. J. T. Lau, Single Center Iron Oxide Clusters: Iron in the Remarkable +7 Oxidation State, ISSPIC IXX, Hangzhou, China, August 2018
7. J. T. Lau, Molecular Iron Oxides: Iron in the Remarkable +7 Oxidation State, International Bunsen Discussion Meeting on Gas-Phase Model Systems for Catalysis, Ulm, June 2018
8. J. T. Lau, Soft x-ray spectroscopy of gaseous ions in cryogenic ion traps and strong magnetic fields: unusual oxidation states and magnetic properties, Conference on Theoretical X-ray spectroscopy, Uppsala, Sweden, March 2018
9. J. T. Lau, Magnetic properties and unusual oxidation states of inorganic and organometallic clusters: soft x-ray spectroscopy of gaseous ions in cryogenic ion traps and strong magnetic fields, Zintl-Kolloquium, Darmstadt, January 2018

Mandates/Awards

1. Since 02/2021: Spokesperson, Photon Science Division, HZB
2. Since 12/2018: Chairperson, LDM Programme Advisory Committee, MAX IV, Lund, Sweden

Leibniz Institute for Solar Physics (KIS)

Publications

[kis1] Kleint, L., Wheatland, M., Mastrano, A., McCauley, P., ”Nonlinear force-free modeling of flare-related magnetic field changes at the photosphere and chromosphere”, Astrophys. J. **865** (2018) 146

[kis2] Löhner-Böttcher, J., Schmidt, W., Stief, F., Steinmetz, T., Holzwarth, R., ”Convective blueshifts in the solar atmosphere, I. Absolute measurements with LARS of the spectral lines at 6302 Å”, Astron. Astrophys. **611** (2018) A4

[kis3] Schubert, M., Kentischer, T., von der Lühe, O., ”Simulation algorithm to model the visible tunable filter for the Daniel K. Inouye Solar Telescope”, J. Astron. Telescopes, Instruments, and Systems **3** (2018) 045002

[kis4] Strecker, H., Bello González, N., ”Evolution of the flow field in decaying active regions. Transition from a moat flow to a supergranular flow”, Astron. Astrophys. **620** (2018) A122

[kis5] Gorobets, A.Y., Berdyugina, S.V., ”Stochastic entropy production in the quiet Sun magnetic fields”, Monthly Notices Roy. Astr. Soc. **483** (2019) L69

[kis6] Afram, N., Berdyugina, S.V., ”Complexity of magnetic fields on red dwarfs”, Astron. Astrophys. **629** (2019) A83

[kis7] Fischer, C.E., Vigeesh, G. Lindner, P., Borrero, J.M., Calvo, F., Steiner, O., ”Interaction of magnetic fields with a vortex tube at solar subgranular scale”, Astroph. J. Lett. **903** (2020) L10

[kis8] Kleint, L, Berkefeld, T., Esteves, M., et al., ”GREGOR: Optics redesign and updates from 2018-2020”, Astron. Astrophys. **641** (2020) A27

[kis9] Judge, P., Kleint, L., Leenaarts, J., et al., ”New light on an old problem of the cores of solar resonance lines”, Astrophys. J. **901** (2020) 32

[kis10] Palacios, J., Utz, D., Hofmeister, S., et al., ”Magnetic flux emergence in a coronal hole”, Solar Phys. **295** (2020) 64

1.4 Bachelor, Master and PhD Theses

Group Buchleitner

Habilitations

1. Stefan Y. Buhmann, “Signatures of the quantum vacuum”, 2019.
2. Robert Bennett, “Designing light matter interactions”, 2021.

PhD Theses

1. Giulio Amato, “Many-particle quantum transport between finite reservoirs”, 2021.
2. Giacomo Sorelli, “Quantum state transfer in diffractive and refractive media”, 2019. `https://10.6094/UNIFR/150962`
3. Tobias Brünner, “Signatures of partial distinguishability in the dynamics of interacting bosons”, 2018. `https://10.6094/UNIFR/16683`

Diploma/Master Theses/Zulassungsarbeiten

1. Christian Haen, “Distinguishability-induced quantum-to-classical transitions in many-body interference”, 2020.
2. Jaewoon Lee, “Trapped-ion implementation of electron transfer processes”, 2020.
3. Benedikt Ames, “Dynamical detection of dipole-dipole interactions in dilute atomic gases”, 2019.
4. Eric Brunner, “Many-body interference, partial distinguishability and entanglement”, 2019.
5. Joachim R. Welz, “A universal quantum circuit for variational quantum algorithms”, 2019.
6. Maximilian Dirkman, “Thermodynamics of the micromaser”, 2019.
7. Andreas J.C. Woitzik, “Entanglement in quantum-classical variational algorithms”, 2018.
8. Frank Schäfer, “Dynamics and spectral structure of strongly interacting bosons in a double well”, 2018.
9. Katharina Hess, “Excitation transfer in ultracold Rydberg atoms”, 2018.
10. Jonathan Brugger, “Quantum annealing and disorder: a statistical analysis”, 2018.
11. Jonas Mielke, “Spectral structure of the 2D Bose-Hubbard model dressed by a quantized cavity field”, 2018.
12. Timon Eichhorn, “Transport of high-dimensional photonic states across a turbulent atmosphere”, 2018.

Bachelor Theses

1. Katrina Wharam, “Open quantum systems composed of many partially distinguishable particles”, 2021.
2. Tom Hoger, “Tunneling of a composite particle on a one-dimensional lattice”, 2021.
3. Stefanie Emig, “Violation of Bell inequality in Analogue Gravity”, 2021.
4. Robin Grether, “Analysis of the Tunnel Effect for a Quantum Walker”, 2021.
5. Michael Minke, “Extracting particle distinguishability from imperfect output event suppression in many-particle interference”, 2020.
6. Niklas Neubrand, “First detection time statistics of many partially distinguishable particles”, 2020.
7. Clément Canard, “Collective dephasing of symmetric multipartite state”, 2019.

8. Sabrina Unmüßig, “Entanglement dynamics of orbital angular momentum qubit states upon diffraction at “cake-slice” aperture”, 2019.
9. Marianne Schneider, “Fock space localization of many-body states in the titled Bose-Hubbard model”, 2019.
10. Wiebke Wirtz, “Investigating the accuracy of analytical optical models to determine the generation current density of silicon solar cells from spectral reflectance and transmittance measurements”, 2019.
11. Simon Strnad, “Quantum simulations of Floquet systems”, 2019.
12. Clara Fuchs, “Estimation of ground state energies in quantum circuits”, 2018.
13. Jan Schuler, “Spatial eigenmodes of atmospheric turbulence”, 2018.

Group Breuer

Master Theses

1. Sophia Ohnemus, “Probing Multiparticle Correlations in Random Quantum Circuits with Randomized Measurements,” 2021.
2. Somar Kalthoum, “Spin star system with Heisenberg interaction: Memory effects and entropy production,” 2021.
3. Tom Endres, “Quantum Thermodynamics of a Driven Damped Quantum Harmonic Oscillator,” 2021.
4. Joshua Reinacher, “Probing moments of multipartite density matrices with randomized measurements,” 2020.
5. Simon Einsiedler, “Non-perturbative approach to non-Markovianity and entropy production in the Caldeira-Leggett model,” 2020.
   `https://freidok.uni-freiburg.de/data/165942`
6. Nico Krause, “Entropy Production in Open Quantum Systems,” 2019.
   `https://freidok.uni-freiburg.de/data/151968`
7. Rodrigo Miguel Gómez, “Role of system-environment correlations in quantum open system dynamics,” 2019.
   `https://freidok.uni-freiburg.de/data/150939`
8. Martin Streif, “Non-exponential decay of a two-level system interacting with a bosonic reservoir,” 2018.

Bachelor Theses

1. Uwe Holm, “Exact approach to the thermodynamics of an open two-level quantum system,” 2021.
2. Felix Riesterer, “Quantum Thermodynamic Processes: The Swap Engine,” 2021.
3. Tobias Nauck, “Statistical characterization of multipartite entanglement based on finite samples of randomized measurements,” 2020.
   `https://freidok.uni-freiburg.de/data/219670`
4. Michael Krebsbach, “Characterization of bipartite entanglement with moments of randomized measurements,” 2019.
   `https://freidok.uni-freiburg.de/data/150706`

Group Buhmann

PhD Theses

1. Pablo Barcellona, “Photon-mediated interactions in macroscopic environments”, 2018.
2. Sebastian Fuchs, “Control of dispersion interactions of atoms near surfaces”, 2018.

Master Theses

1. Severin Bang, “Superradiant enhancement of resonance energy transfer”, 2019.
2. Frieder Lindel, “Probing the quantum vacuum using nonlinear crystals: A macroscopic quantum electrodynamics perspective”, 2019.
3. Nico Strauß, “Quantum friction and internal atomic dynamics”, 2019.
4. David Steinbrecht, “Macroscopic quantum electrodynamics theory of photonic Bose–Einstein condensation”, 2020.

Group Sansone

PhD Theses

1. P. K. Maroju, “Attosecond pulse shaping at a seeded free-electron laser: towards attosecond time-resolved experiments at the free-electron lasers”, 2021.
   https://freidok.uni-freiburg.de/data/220018/

Master Theses

1. J. Lutz, “Construction and characterization of an attosecond ultra-stable delay line for time resolved experiments”, 2019.
2. A.-L. Jäger, “Temporal pulse compression using a hollow-core fibre system”, 2019.
3. S. Kellerer, “Construction and characterization of an attosecond ultrastable delay line for time resolved experiments”, 2019.

Bachelor Theses

1. J. Schreck, “Covariance based reconstruction of attosecond pulses”, 2020.
2. M. Schmoll, “Measurement of sideband oscillations in two-color photoionization”, 2020.
3. M. Van der Hoeven, “Temporal characterization of amplified femtosecond pulses”, 2019.

Group Schaetz

Habilitations

1. L. Karpa, “Optical dipole traps for ultra-cold ion-atom interactions”, 2019.

PhD Theses

1. J. Schmidt, “Optical trapping of ion Coulomb crystals”, 2018.
2. M. Wittemer, “Particle creation and memory effects in a trapped ion quantum simulator”, 2019.
3. F. Hakelberg, “Controlled Inter-Site Coupling in a two-dimensional Ion Trap Array”, 2019.
4. P. Kiefer, “Floquet engineering in a two-dimensional array of trapped ions”, 2020.
5. P. Weckesser, “Feshbach resonances between a single ion and ultra-cold atoms”, 2021.

Master Theses

1. F. Thielemann, “A Lithium Setup for Ultra-cold Atom-Ion Experiments”, 2018.
2. A. Hasenfratz, “Design and characterization of a frequency doubling stage”, 2018.
3. S. Schnell, “Motional coherence of a single trapped ion in the classical regime”, 2018.
4. D. Palani, “Benchmarking Micro-Diamonds for Sensing Applications”, 2019.
5. I. Lindemann, “Creation and characterization of ultra-cold Lithium atoms in a Dipole trap”, 2019.
6. F. Hasse, “Optical Temperature Measurement of Single Ions”, 2019.
7. K. Lok Lam, “Scanning Transfer Cavity Lock for long term Laser Frequency Drift Stabilization”, 2020.
8. R. Thomm, “State detection of Magnesium ions”, 2021.
9. L. Guth, “Assembling and Benchmarking the Next Generation of Solid-State Laser Systems for Controlling Trapped Magnesium Ions”, 2021.

Bachelor Theses

1. O. Orlov, “Diamanten-Spektroskopie”, 2018.
2. L. Restat, “Analyse eines Faltungsnetzwerks zum Optimieren von Kontrollparametern”, 2018.
3. F. Richter, “Aufbau einer optischen Dipolfalle für Barium-Ionen”, 2018.
4. K. Waescher, “Realisierung und Charakterisierung einer Dipolfalle für ultrakalte Lithium Atome”, 2019.
5. L. Guth, “Aufbau und Charakterisierung eines Vier-Quadranten-Photonendetektionssystems zur parallelen Zustandsanalyse von Magnesiumionen”, 2019.
6. M. Jaud, “Kohärente Manipulation eines spinpolarisierten Ensembles von ultrakalten Li Atomen”, 2020.
7. C. Richter, “Ein Hochleistungs-Radiofrequenz-Aufbau zur Spektroskopie eines ultrakalten Atom-Ionen-Gemischs”, 2020.
8. A. Spiess, “Optische Spinpolarisation eines einzelnen Barium-Ions für ultrakalte Atom-Ionen Experimente”, 2021.
9. S. Schell, “Magnetfeld Charakterisierung zur experimentellen Untersuchung von Mikrodiamanten”, 2021.

Group Stienkemeier

PhD Theses

1. Marcel Binz, “Phase-modulated coherent spectroscopy of rubidium: High-intensity effects and the interaction with helium nanodroplets”, 2021.
`https://freidok.uni-freiburg.de/data/218338/`
2. Rupert Michiels, “Time-resolved photoelectron and photoion spectroscopy of atomic and molecular clusters using XUV radiation”, 2021.
`https://freidok.uni-freiburg.de/data/220423/`
3. Andreas Wituschek, “Phase-modulated coherent time-domain spectroscopy in the extreme ultraviolet regime”, 2020.
`https://freidok.uni-freiburg.de/data/175730/`

4. Dominik Schomas, “Helium und Neon Nanoplasmas Ignited by Ultrashort NIR, MIR and X-Ray Laser Pulses”, 2019.
`https://freidok.uni-freiburg.de/data/151512/`

5. Sharareh Izadnia, “Fluorescence Lifetime Reduction Mechanisms of Organic Complexes Studied by Cluster Isolation Spectroscopy”, 2018.
`https://freidok.uni-freiburg.de/data/16006/`

Master Theses

1. Lars-Stephan Klein, “Characterization and Optimization of Ultrashort Pulses for Phase-modulated Spectroscopy”, 2021.

2. Elena Leißler, “Construction and characterisation of a source and doping chamber for phase-modulated spectroscopy”, 2020.

3. Aaron Ngai, “Charge-Transfer in the Auger-decay-induced Fragmentation of Iodomethane”, 2020.

4. Cristian E. Hernadez Medina, “Single Shot Electron Imaging of He and Ne Clusters under Strong Mid-Infrared Laser Fields”, 2019.

5. Jakob Krull, “Preparation and Testing of a Pulsed Nozzle for Molecular Jets for Photon-Induced Charge Transfer Experiments”, 2019.

6. Max Jakob, “Construction and Characterisation of a Magnetic Bottle Spectrometer for Two-Dimensional Electronic Spectroscopy”, 2018.

Bachelor Theses

1. Nicolai Gölz, “Implementierung einer automatisierten Leistungssteuerung von Laserstrahlung mittels akusto-optischer Modulatoren”, 2020.

2. Robin v. d.Neut , “Messung von Laserstabilität mit Hilfe eines weiterentwickelten Beamprofilers”, 2020.

3. Santana Andreo, A, “Beam profiler system”, 2019.

4. Andreas Göppentin, “Aufbau und Charakterisierung einer Molekularstrahlquelle”, 2019.

5. Niels Sorgenfrei , “Über die Optimierung gepulster Cluster-Düsen des CRUCS-Designs”, 2019.

6. Lars-Stephan Klein , “Aufbau eines kompakten Interferometers für phasenmodulierte Wellenpaket-Interferometrie”, 2018.

Group Dulitz

Master Theses

1. Lasse Bienkowski, “Design and setup of an apparatus for the coherent control of helium autoionization”, 2021.

2. Simon Hofsäss, “A source of magnetic-quantum-state-selected metastable helium for Penning reaction studies”, 2018.

3. Vivien Behrendt, “Optical Depletion of Metastable Helium Atoms for Penning Reaction Studies”, 2018.

Bachelor Theses

1. Leon Göpfert , “Aufbau und Charakterisierung eines Diodenlasersystems zur Absorptionsabbildung von ultrakalten Lithium-Atomen”, 2021.

Group von Issendorff

PhD Theses

1. Simon Dold, Time-resolved imaging of laser-induced phase transitions in free silver nanoclusters, 2020. `https://freidok.uni-freiburg.de/data/175263`

Bachelor Theses

1. Elena Leißler, Hochaufgelöste Photoelektronenspektroskopie an tiefkalten, massenselektierten Niob-Clustern, 2018

2. Philipp Elsässer, Aufbau eines neuartigen Photoelektronenspektrometers zur Messung von Elektronenzuständen in Atomen und Clustern, 2019

3. Emanuel Tzivakis, Charakterisierung eines Clusterstrahls mit Laserstreuung, 2019

4. Timo Lang, Konstruktion einer Ionenfalle für Photoelektronenspektroskopie am Synchrotron, 2020.

Group Lau

Master Theses

1. Max Flach, "Einfluss der Elektronegativität der Halogene auf das Röntgenabsorptionsspektrum bei Eisenhalogenidmolekülen", TU Berlin, 2020.

Bachelor Theses

1. Tim Gitzinger, "Metal L-edge energy shift analysis of diatomic nickel, copper, and iron halides", 2019.

Leibniz Institute for Solar Physics (KIS)

PhD Theses

1. Rene Kiefer, "Seismic investigations of solar and stellar magnetic activity", 2018. `https://freidok.uni-freiburg.de/pers/23507`

2. Sebastian Hoch, "Multi-Spektrale Photometrie der Sonne mit hoher räumlicher und zeitlicher Auflösung", 2019.

3. Hanna Strecker, "On the decay of sunspots", 2020. `https://freidok.uni-freiburg.de/data/165760`

4. Andriy Gorobets, "Stochastic analysis of the quiet Sun magnetic field evolution", 2020. `https://freidok.uni-freiburg.de/data/167239`

5. Matthias Waidele, "Helioseismology of sunspots - On the detection of subsurface structure and svolution", 2021.

Master Theses

1. Monika Ellwarth, "Exploding Granules in the Solar Atmosphere Formation of Intergranular Lanes and Acoustic Events", 2018.
2. Philip Lindner, "The vertical component of the magnetic field as a criterion for the stability of sunspot umbrae and pores - An observational investigation", 2018.
3. Erik Nebelo, "Center-to-limb variation of chromospheric lines", 2018.
4. Markus Schmassmann, "On the magnetic field at the umbral boundary of sunspots – Time series analysis of a sunspot over two disc passages with HMI/SDO", 2018.
5. Valentin Hoffmann, "Aufbau und Beleuchtung einer adaptiven Optik in Analogie zur adaptiven Optik am Sonnenteleskop GREGOR", 2019.
6. Wolfgang Breu, "Global helioseismology of the solar meridional flow", 2019.
7. P. Christian, "Investigating polarimetry as a technique for remote sensing of life", 2019.
8. Jessica Denise Schäper, "Asteroseismic study of gravitational Waves", 2019.
9. Patrick Jürgens, "Helioseismology of the Sun: Differential rotation and banded zonal flow", 2019.
10. Pascal Weyer, "Seismology of the solar magnetic field by means of tensor generalized spherical harmonics", 2020.
11. Franziska Morawietz, "Maneuver detection for space situational awareness", 2020.
12. Thibaut Klinger, "Two component inversion of a sunspot penumbra", 2021.
13. Sarah Fuchs, "Polarisation und Stellar-Interferometrie", 2021.
14. Daniel Konrad Pitters, "Effects of solar evolution on finite acquisition time of VTF", 2021.
15. Lars Ruder, "Temperaturstruktur eines Sonnenflecks", 2021.

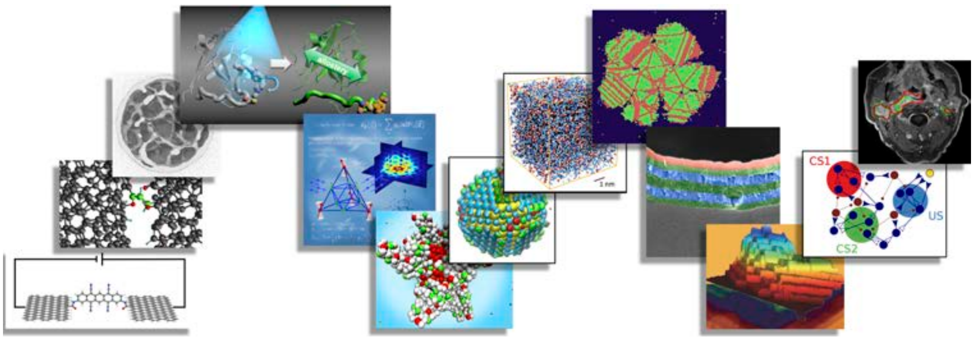
Bachelor Theses

1. Akira Kamijo, "Bestimmung der solaren meridionalen Strömung", 2018.
2. Thibault Klinger, "Untersuchung von Geschwindigkeit und Magnetfeld in der Penumbra eines Sonnenflecks", 2018.
3. Severin Küsel, "Sichtlinienfunktion in der Fourier-Legendre-Helioseismologie", 2018.
4. Joshua Elias Reinacher, "Auswirkung des globalen Magnetfeldes auf die Schwingungsmoden der Sonne", 2018.
5. Moritz Benedikt Spannenkrebs, "Helioseismologische Untersuchung der Sonnenatmosphäre - Bestimmung akustischer Cut-Off-Frequenzen", 2018.
6. Sophie Schmiz, "Newly formed intergranular lanes in the solar atmosphere", 2019.
7. Thomas Otto Winterhalder, "Helioseismology of the solar magnetic field", 2019.
8. Sarah Fuchs, "Photometrie der solaren Feinstruktur in verschiedenen Wellenlängen", 2019.
9. Simon Lentz, "Helioseismologie der meridionalen Strömung", 2019.
10. C. Lautenbacher, "Influence of mode bases on image reconstruction with GREGOR", 2019.
11. Stefan Haulitschke, "Solare Fizeau-Interferometrie mit GREGOR", 2020.
12. Simon Kiesner, "Oszillationen im Roten Riesen und Weißen Zwergen", 2020.

13. Lars Ruder, ”Thermale Eigenschaften der solaren Feinstruktur”, 2020.
14. Paul Martin Fleing, ”Messung der meridionalen Strömung mit Hilfe der Fourier-Hankel-Analyse”, 2020.
15. Leon Roman Ecker, ”The mass of the supermassive black hole of the BCG (brightest cluster galaxy) of Abell 498/592”, 2021.
16. Adrian Schad, ”Messung der Sonnenrotation mit Intensitätsdaten von HMI und MDI”, 2021.

Chapter 2

Condensed Matter and Applied Physics



- **Experimental Polymer Physics**
  Prof. G. Reiter
- **Nanophysics and Molecular Magnets**
  Prof. O. Waldmann
- **Solar Energy – Materials and Technology**
  Prof. A. Bett (IoP, Fraunhofer ISE)
- **Applied Theoretical Physics – Computational Physics**
  Prof. J. Dzubiella
- **Functional Nanosystems**
  Prof. M. Moseler (IoP, Fraunhofer IWM)
- **Materials Modelling**
  apl. Prof. C. Elsässer (Fraunhofer IWM)
- **Spectroscopy of Optical Materials**
  PD F. Kühnemann (Fraunhofer IPM)
- **Statistical Physics of Soft Matter and Complex Systems**
  Prof. T. Schilling
- **Biomolecular Dynamics**
  Prof. G. Stock
- **Theoretical Condensed Matter Physics**
  Prof. M. Thoss
- **Dynamics in the Life Sciences**
  Prof. J. Timmer
- **Bio and Nanophotonics**
  Prof. A. Rohrbach
  (Faculty of Engineering, co-opted)
- **Medical Physics**
  Prof. J. Hennig (Uni Hospital, co-opted)
  Prof. M. Bock (Uni Hospital, co-opted)
- **Computational Neurosciences**
  Prof. S. Rotter
  (Faculty of Biology, co-opted)

Chapter caption: Images representing the diversity of our research, spanning from low-dimensional nanoscopic systems (left) to complex macroscopic systems (right), in the field of Condensed Matter and Applied Physics.

2.1 Overview

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

The research area comprises eight groups located at the Institute of Physics (IoP), working on: Nanophysics and Molecular Magnetism (**O. Waldmann**), Theoretical Condensed Matter Physics (**M. Thoss**), Biomolecular Dynamics (**G. Stock**), Applied Theoretical Physics - Computational Physics, (**J. Dzubiella**, newly appointed in 04/2018), Experimental Polymer Physics (**G. Reiter**), Theoretical Physics of Soft Matter and Complex Systems (**T. Schilling)**, Functional Nanosystems (**M. Moseler**), and Dynamic Processes in the Life Sciences (**J. Timmer**).

In addition, there are three co-opted members of the IoP, working on Bio- and Nanophotonics (**A. Rohrbach**, Microsystems Engineering, Faculty of Engineering), Neurobiology and Biophysics (**S. Rotter**, Faculty of Biology), and Medical Physics, (**J. Hennig**, **M. Bock**, Faculty of Medicine), and three members from Fraunhofer Institutes, **C. Elsässer** (Mechanics of Materials - IWM), **F. Kühnemann** (Phyiscal Measurement Techniques - IPM), and **A. Bett** (Solar Energy Systems - ISE). Bett joined the Institute of Physics in 04/2020 and is director of the Fraunhofer Institute for Solar Energy Systems. J. Wagner (apl. Prof.) who was a member of the IoP and the head of the Optoelectronics Research Unit at the Fraunhofer Institute for Applied Solid State Physics (IAF) retired at the beginning of the reporting period in early 2018.

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

There is obvious overlap with the research of the colleagues in the area of "Atomic, Molecular and Optical Sciences". In contrast to their work, however, our focus is on the understanding, tailoring and harnessing of the emerging complex quantum states and classical excitations, transport processes, novel functions, and information processing capabilities. These depend on the structures, topologies of the interaction pathways, and external fields or embedding environments, and naturally feature a wide spectrum of scales and systems. The cover figure on the previous page aims at sketching this richness in scales, displaying the variety of condensed matter systems and soft materials involving a few interacting units at nanoscales up to ensembles and networks on macroscales, as being investigated in the Condensed Matter and Applied Physics research area.

The various ongoing research activities have been arranged in this chapter into the three topical sections 'Transport and Dynamics in Matter' (2.2), 'Functional Materials' (2.3), and 'Biological Systems' (2.4), with the understanding that a group's research cannot always be strictly attributed to one or the other. The research in our area has a wide, interdisciplinary spectrum and connects physics with (macromolecular) chemistry, biology, and applied sciences as well as engineering.

The research activities presented in Section 2.2 primarily focus on transport and dynamics in nanoscale systems. This includes, for example, experimental and numerical studies of spin excitations and magnetic relaxation dynamics in molecular nanomagnets as well as theoretical modeling of advanced quantum mechanical phenomena in low-dimensional systems, such as complex quantum many-body states and excitations, quantum dynamics and transport as well as environmental effects such as dissipation, decoherence and relaxation in open systems. The research in this topic also involves time-dependent structural dynamics of biomolecular systems such as solvated proteins, in particular nonequilibrium transport processes such as energy transfer and intramolecular signal transduction addressed by multi-scale simulations. The systems and materials studied thus range from one and two dimensional carbon based materials, nano-and-micro structured semiconducting and optical materials, self-assembled monolayers and magnetic molecules to biological macromolecules and synthetic polymers.

The Section 2.3 describes experimental and theoretical research activities which are primarily devoted to the relation of the electronic, molecular, and geometric 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. This includes, for example, the 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 nanoclusters, semiconductors, complex solvents and liquids, supra-molecular architectures, polymer films, conducting polymers and silicon, as well as typical soft matter systems, such as colloids, liquid crystals and soft composites are investigated in order to eventually establish structure-property-function relationships. Here, the new appointment Dzubiella adds complementary expertise in the computational physics of applied (soft matter) physics systems, e.g., functional electrolytes and polymers, to the field, bridging physics to chemistry and the applied sciences in Freiburg. The new joint appointment Bett (Fraunhofer ISE) focuses on the physics and optimization of photovoltaic devices, improving bulk material as well as interface and heterojunction properties using tools such as luminescence spectroscopy. Both additions extend the research at the IoP towards the development of energy storage and conversion materials.

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, for example, proteins and their interactions, biological cells, bio-mimetic systems and synthetic cell systems up to ensembles of neurons, the brain, and the dynamics and functions of whole organs. They focus on understanding the microscopic mechanisms underlying these complex systems, their information processing and response, neuronal dynamics and coordinated activity, on one hand using tools of computational, mathematical and statistical physics, on the other hand state-of-the art photonic and cross-sectional imaging technologies. Applications range from addressing questions in basic science to specific biological problems up to clinical studies and medical treatments.

Collaborative Research:

In the following we briefly describe ongoing, collaborative research and training initiatives in which this research area is participating. In the framework of the last round of the German Excellence Initiative for German universities – initiated by the German Council of Science and Humanities & the German Research Foundation (DFG) – the University of Freiburg was successful in two Clusters of Excellence. Our research area is strongly represented in these clusters as well as in other collaborative, third party funded research structures within the university and on (inter)national levels.

Moseler, Reiter, Schilling and Dzubiella are members of the Cluster of Excellence ”Living, adaptive and energy-autonomous Material Systems” (livMatS), in which they employ and develop physics approaches, such as polymer physics, nonequilibrium statistical physics, and large-scale particle-resolved computer simulations to rationalize the bottom-up design and the longevity of soft, adaptive ’living’ materials. Timmer is member of the Cluster of Excellence ”Center for Biological Signalling Studies (CIBSS), where he contributes with mathematical models of biological dynamics to pave the way for medical applications. Both clusters embrace six faculties of the university and foster inter- and transdisciplinary research frameworks.

Reiter was the speaker of the in 09/2019 terminated International Research Training Group (IRTG) 1642 “Soft Matter Science: Concepts for the Design of Functional Materials” and principal investigator (PI) of the DFG-funded transregio collaborative research center (CRC-Transregio) 141: “Biological Design and Integrative Structures - Analysis, Simulation and Implementation in Architecture” (until 06/2019), and participated in the International Training Networks (ITNs) ’PlaMatSu’ and ’Photo-Emulsion’, as well as in the the DFG Priority Program (SPP 2171) ”Dynamic Wetting of Flexible, Adaptive and Switchable Surfaces”. Timmer is PI of the CRC-transregio 179: ”Determinants and dynamics of elimination versus persistence of hepatitis virus infection” and the CRC 1381 ”Dynamic organisation of cellular machineries: From biogenesis and modular assembly to function”, and coordinator of the collaborative research project ’NephrESA’ of the German Federal Ministry of Education and Research (BMBF). Thoss was principal investigator in the collaborative research center (CRC 953) ’Synthetic carbon allotropes’ (until 12/2019) and the IRTG ’Cold controlled ensembles in physics and chemistry’. Dzubiella and M. Walter (Moseler group) are PIs and collaboration partners in the DFG Priority Program SPP 2248 ”Polymer-based batteries”. The research area participates in the centre of excellence for ’Quantum Science and Quantum Computing’, the doctoral training program QUSTEC, and the new RTG ’Dynamics of controlled atomic and molecular systems’ (see AMO section 1.1).

DFG-funded Research Unit (RU) FOR 5099: ”Reducing Complexity in Nonequilibrium Systems” (funding period 2020-2024): In the reporting period our research area utilized the recently achieved ’critical mass’ of theorists from the recent appointments

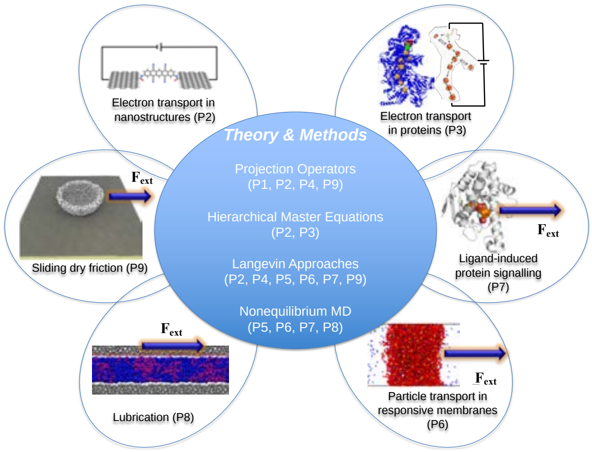


Figure 2.1: Overview and interrelation of projects of the DFG Research Unit FOR 5099 "Reducing complexity in nonequilibrium systems".

(Thoss and Schilling in the last reporting period; Dzubiella in 04/2018) to establish the DFG Research Unit FOR 5099 which started in 10/2020. This initiative of the IoP obtained a total of three million Euros funding over the next four years. Apart from spokesperson Stock and deputy spokesperson Thoss, the Research Unit includes PIs Breuer, Dzubiella, Moseler, and Schilling from the IoP, as well as three more PIs from Chemistry (Koslowski), Engineering (Pastewka), and Fraunhofer IWM (Falk), thus fostering interdisciplinary collaborations in this field. The overarching goal of the Research Unit FOR 5099 is to develop efficient and accurate theories as well as models and computational methods that employ a reduced description to treat nonequilibrium processes in complex systems. An overview and the interrelation between the research projects is sketched in Fig. 2.1.

Future developments and plans

The faculty of Mathematics and Physics is preparing pre-proposals for two applications for Clusters of Excellence in the framework of the upcoming excellence initiative. One of these cluster proposals has been initialized by Tanja Schilling together with Andreas Buchleitner from the section of atomic, molecular and optical sciences and Angelika Rohde from the Institute of Mathematics. The topic of the cluster will be model reduction and uncertainty prediction of complex systems. Most professors from the condensed matter section have joined the consortium of the pre-proposal.

2.2 Transport and Dynamics in Matter

2.2.1 Nanophysics and Molecular Nanomagnets – Group Waldmann

The **Nanophysics and Molecular Magnetism Group of Oliver Waldmann** investigates the spin excitations and magnetic relaxation dynamics in so-called molecular nanomagnets. These magnetic materials consist of molecules containing a dozen or so magnetic metal ions and organic ligands. The ligands play a three-fold role: Via complex bonds they hold together the molecule in a well-defined structure, which is precisely known from x-ray crystallography. They also permit magnetic exchange interactions between the magnetic metal ions in a molecule, such that these clusters are essentially quantum many-body systems of a dozen interacting spin centers. Lastly, the ligands act as "chicken fat" enclosing the magnetic core, and magnetic interactions between different molecules in a sample are negligibly small. These features make the molecular nanomagnets ideal model systems for studying magnetism at the nano scale, and distinguishes them in the class of magnetic nanoparticles.

In the Waldmann group the magnetic properties of molecular nanomagnets are experimentally studied and numerically simulated, with focus on two types of systems, which are associated to very different sets of questions: First, molecules are investigated in which the isotropic Heisenberg exchange is the dominant interaction term. These systems represent experimental model systems for nanosized quantum many-spin systems, and the ground state and low-energy spin excitations are the targets of study. The second type are the so called single molecule magnets (SMMs), which exhibit slow magnetic relaxation and quantum tunneling of the magnetisation at low temperatures. SMMs contain highly-anisotropic metal ions such as lanthanides, which dominate their magnetism. Experimentally the group is specialized in spectroscopic techniques such as inelastic neutron scattering (INS), but also applies thermodynamic techniques such as magnetometry.

Research Report

Ferromagnetic Spin Waves in Molecular Spin Clusters

We undertook in-depth investigations of the magnetic energies and wave functions in the general class of ferromagnetic spin clusters. Here, "ferromagnetic" does not relate to ferromagnetism as seen in extended systems, but refers to a spin ground state with the maximal total spin quantum number possible in a given small finite spin cluster. In this situation the well known spin wave theories can - with proper modifications - be applied, and the low-lying states exactly be calculated.

In a first work we have compiled the scarce literature on the cluster spin wave theories and extended them to a systematic frame work [waldm2]. In particular a simple yet insightful graphical representation of the spin wave excitations was developed, which should be of value especially to experimentalists. In a further work we investigated the spectroscopic intensities, as observable for instance in inelastic neutron scattering experiments [waldm3]. We showed that the magnetic wave functions in these systems can be directly and unambiguously reconstructed from the experimental intensities via a procedure which could be described as a sort of generalized Fourier transform taking into account the crystal structure of the molecule, Fig. 2.2. This is a most remarkable experimental opportunity, since so far "only" transition matrix elements were determined, but not the composition of a magnetic many-body wave function itself.

Figure 2.2: Graphical illustration of the INS approach to experimentally determine magnetic wave functions.

3d-4f Single Molecule Magnets

In the recent years our main attention had been on investigating 3d-4f SMMs. Incorporating 4f metal ions into SMMs has been shown to vastly improve, e.g., their blocking temperature, which is the temperature below which their intriguing properties such as slow relaxation of the magnetization occur. Raising the blocking temperatures is not only of much scientific interest, but also of relevance for potential applications. Most progress has been made for 4f clusters, where blocking temperatures above liquid-nitrogen temperatures were reported. However, the progress in this area is much hampered by a substantial lack of experimental tools which can be applied for studying the magnetic excitations. Important techniques such as electron magnetic resonance spectroscopy do not generally work here because transitions are highly forbidden. Also, the standard magnetic measurements are generally featureless and their information content small. In addition, the ligand spheres enclosing the 4f metal ions exhibit no symmetry, and the ligand field models which are used to describe the magnetism of lanthanide ions do then involve 27 independent parameters, per ion. That is, one faces the situation of a lack of detailed experimental information and a simultaneous "explosion" in the number of parameters in the models. Moreover, even for relatively small clusters the numerical simulations become quite time consuming on today's PCs. All this seriously hampers the type of detail investigations known in other areas of research. Our efforts aim at tackling these challenges.

Experimentally we concentrate on 3d-4f clusters. These are generally not as good SMMs as 4f clusters, and from this perspective of less scientific interest. However, while the 4f metal ions continue to contribute nearly zero magnetic scattering intensity at low temperatures, this is not so for the 3d metal centers, and the magnetic excitations become indeed observable. As model systems we choose so-called 3d-4f "butterflies" and "squares". This work is undertaken in cooperation with the chemistry group of A. K. Powell, KIT, Karlsruhe, who provide us with samples. These molecules consist of two 3d metal centers and two lanthanide centers, which are arranged in a square like fashion with cross couplings. The lanthanide ions can be chemically easily substituted, which yields series of structurally related clusters. This in principle permits what we call a "linked fit", where all data of all members of a family are fitted simultaneously, to provide the experimental information for determining a large number of model parameters. Unfortunately, this alone is not sufficient to yield reasonable fits as has been also observed by other researches in the few attempts which were reported in the literature. Additional measures need to be taken (see below). On these compounds we could indeed record high-quality experimental INS data, which are shown for the example of a family of "butterflies" in Fig. 2.3.

Our simulations are based on diagonalizing the

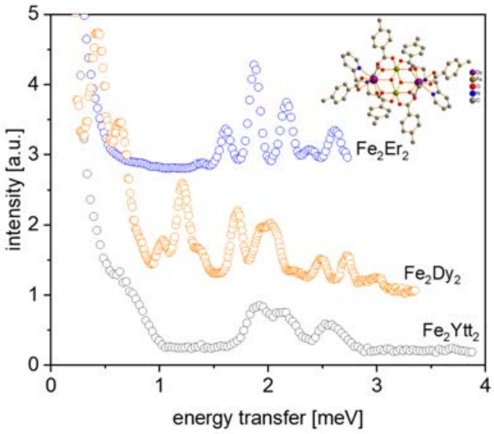


Figure 2.3: Experimental INS spectra at low temperatures for a family of "butterflies"; shown are data for the three members Fe_2Dy_2, Fe_2Er_2, Fe_2Yt_2. Experimental details are omitted. Inset: Crystal structure of a Fe_2Dy_2 "butterfly" SMM.

spin Hamiltonian which is used for describing the magnetism. We estimated a simulation time of 11 years for fitting the magnetization data of a Fe_2Dy_2 cluster on a modern PC. A diagonalization itself takes just ca 10 s for a Hilbert space dimension of ca 10000. However, about 50 million have to be done for modelling the data and doing the fitting. We recently could improve the simulation time by a factor 50, by exploiting that the magnetization curves are recorded at low temperatures where only a small number of low-lying states contribute, which permitted using sparse matrix diagonalization techniques. We are working on improving our algorithms by another factor of 5-10, which would finally make such fits practical.

Concerning models, we decided to look at the problem from a "black box" perspective. That is, we relaxed from requiring the models to yield physically or chemically relevant insight. While this is what would ultimately be desired, it is what obviously made the analyzes fail for the systems of interest as described before. Instead, the aim is to identify models which are successful in modeling the full set of experimental data (linked fit). In the context of machine learning and neural networks this is known as parameter reduction or finding a feature space of lower dimension. We in fact exploited neural networks to this extend. This was however not very successful since the neural networks tended to produce non-physical curves. We developed a "simulation-embedded" autoencoder, which worked reasonably well for simple systems, but computation time was huge and made it impracticable.

Our current best approach consists of using established chemical models such as the angular overlap model (AOM) for reducing the parameter space, but ignoring any chemical relevance which is usually given to these models; we consider them as adjustable black boxes for generating 27 Hamiltonian parameters from just a few input parameters. This approach indeed allowed us to achieve, for the first time, a linked fit to the susceptibility and magnetization curves of two related clusters (Al_2Er_2 and Al_2Dy_2), Fig. 2.4. We consider this a very significant success; similar achievements were not yet reported in the literature.

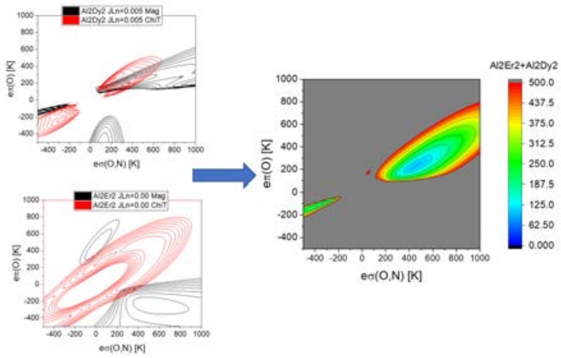


Figure 2.4: Chi^2 landscapes of a "linked fit", which included the temperature dependent susceptibility curves and magnetization curves of two related 3d-4f clusters. Left: Chi^2 landscape for each data set. Right: Resulting overall Chi^2 landscape, showing one distinct minimum.

Future Plans

We obviously intend to continue our efforts in developing approaches for simulating, fitting, analyzing and better interpreting the magnetism in lanthanide-based SMMs. The goal would be a complete and satisfying analysis of the experimental magnetic and INS data for the family of "butterflies" and "squares" described before.

As mentioned before, only few experimental techniques are suitable for investigating the magnetic energies in poly-nuclear lanthanide-based molecular clusters. The technique of high-field torque magnetometry at very low temperatures (30 T, 50 mK) has however largely gone unnoticed. Our group has strong expertise in this technique, and it had some popularity a decade ago. In one of our works we demonstrated that high-field torque at low temperatures allows us to infer quasi-spectroscopic details on the magnetic ground state of molecular clusters. Our plan is to revive this approach and to apply it to 3d-4f SMMs of interest today.

2.2.2 Theoretical Condensed Matter Physics – Group Thoss

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

Another line of research in theoretical condensed matter physics is followed by Junichi Okamoto, a senior postdoc in the Thoss group, who has been a G.H. Endress fellow since 2019. The focus of his research is light-induced dynamics in strongly correlated materials, such as high-Tc superconductors and ferroelectric compounds.

Research Report

Quantum Transport in Nanostructures

One of our main research activities concerns the theory and simulation of quantum transport in nanostructures. An example is charge transport in single molecule junctions, where single molecules are bound to metal or semiconductor electrodes. These systems combine the possibility to study fundamental aspects of nonequilibrium many-body quantum physics at the nanoscale with the perspective for technological applications in nanoelectronic devices. Employing a combination of first principles electronic structure methods and state-of-the-art transport theory, we have analyzed transport mechanisms in molecular junctions including electronic-vibrational and electron-electron interaction as well as fluctuations and noise phenomena. Moreover, we have devised novel schemes for molecular transistors based on proton transfer reactions (see Fig. 2.2.2) [thoss1].

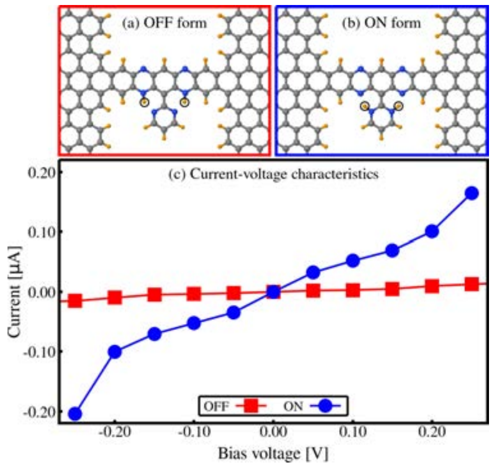


Figure 2.5: Molecule-graphene nanojunction functioning as a molecular transistor controlled by proton transfer. Shown are a clip of the device region in the OFF (a) and ON (b) forms of the junction as well as current-voltage characteristics (c) in these two forms. Hydrogen atoms are highlighted in orange color for better visibility in panels (a) and (b). The black circles mark the active protons. Adapted from [thoss1].

Another focus of our studies of charge transport in molecular junctions in recent years was the investigation of current-induced rupture of chemical bonds. The understanding of the underlying mechanisms is crucial for the design of molecular junctions, which are stable at higher bias voltages. To study this process, we developed a quantum master equation method based on the hierarchical equation of motion approach, which allows a numerically exact simulation of the process. In extensive studies we could show that, depending on the specific situation, different mechanisms are dominating, including the population of anti-bonding electronic states and current-induced heating resulting in vibrational ladder climbing. Furthermore, in a close collaboration with the group of U. Peskin (Technion - Israel Institute of Technology) we devised schemes which may enhance the stability of molecular junctions.

Light-induced Processes

The availability of ultrashort laser pulses, which have reached the subfemtosecond time scale, allows studies of ultrafast processes in atoms, molecules and condensed matter in 'real time'. Of primary interest in molecular systems and condensed matter is the unraveling of electronic and nuclear motion and their mutual correlation. Our theoretical work in this area concentrates on the simulation and analysis of time-dependent non-Born-Oppenheimer processes and their role in photoinduced charge and energy transport in molecular materials. To this end, we use a combination of high-level electronic structure calculations employing multireference perturbation theory and quantum dynamical approaches based on tensor network methods.

A focus of our work in the reporting period was the process of singlet fission, a multiple exciton generation process in molecular materials which involves the transformation of an optically excited singlet exciton into two triplet excitons. This process is both of fundamental interest to understand basic mechanisms of photophysical processes in molecular materials and has the potential to increase the efficiency of novel solar cells beyond the Shockley-Queisser limit. Together with the experimental groups of D. Guldi (Universität Erlangen-Nürnberg), R. Tykwinski (University of Alberta, Canada), and M. Wasielewski (Northwestern University, USA) as well as the theory group of P. Coto (Materials Physics Center (CSIC), Donostia-San Sebastian, Spain), we studied the process of intramolecular singlet fission in pentacene dimers with different linker groups [thoss3]. The studies revealed insight into the mechanisms of singlet fission in conjugated and non-conjugated dimers (see Fig. 2.2.2) [thoss4].

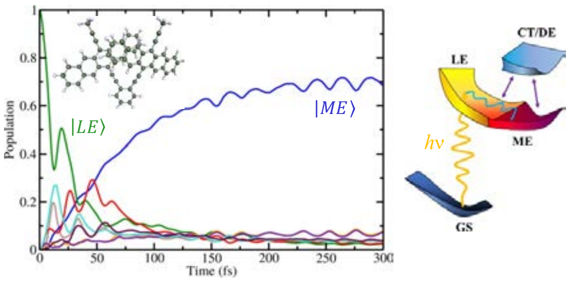


Figure 2.6: Quantum dynamical simulation of light-induced intramolecular singlet fission in a covalently linked pentacene dimer. Shown are the populations of the relevant electronic states including the initially populated locally excited (LE) state and the multiexciton (ME) state (left panel) as well as the scheme of the singlet fission process (right panel). The transition from the LE to the ME state proceeds predominantly via an indirect mechanism involving charge transfer (CT) and doubly excited (DE) states and is facilitated by vibronic coupling. Adapted from [thoss4].

Fundamental Aspects of Quantum Dynamics in Many-Body Systems

In addition to first-principles simulations of specific systems, the Thoss group also investigates fundamental aspects of nonequilibrium quantum dynamics in many-body systems employing generic models such as the spin-boson model, Anderson-type impurity models as well as other many-body models with electron-electron and electron-phonon interaction. Recent studies in this area include the investigation of localization dynamics in many-body quantum systems and electronic transport through correlated electron systems. Moreover, we have devised an approach to investigate open questions in the field of quantum thermodynamics of strongly coupled systems under nonequlibrium conditions and applied it to analyze the physics of externally driven nanosystems [thoss6]. Furthermore, in a collaboration with the group of H.-P. Breuer at the Institute of Physics within the DFG Research Unit 'Reducing complexity of nonequilibrium system', we have investigated non-Markovian effects in the spin-boson model at zero temperature revealing a rich physical behavior [thoss7].

Development of Numerical Methods for Quantum Dynamics in Many-Body Systems

Theoretical studies of quantum dynamics in condensed matter or molecular systems require accurate methods capable of describing many-body quantum systems out of equilibrium. The range of methods developed and used in the Thoss group comprises quantum dynamical methods based on wave functions, density matrix theory and nonequilibrium Green's functions. Examples include the multilayer multiconguration time-dependent Hartree method and hierarchical quantum master equations based on the hierarchical equation of motion approach [thoss8]. These dynamical methods are combined with a first-principles description of the electronic structure using density functional theory and wave-function based approaches.

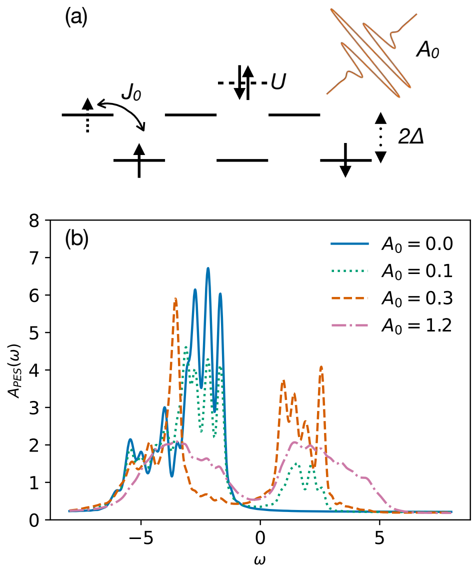


Figure 2.7: (a) Scheme of an ionic Hubbard model, which describes a light-induced paraelectric-ferroelectric transition. (b) Nonequilibrium photoemission spectrum after pump pulses with driving strength A_0. As the driving strength increases, more weights are transferred to the upper electronic band.

Strongly Correlated Materials

The research of J. Okamoto, who is a senior postdoc in the Thoss group, focuses on light-induced dynamics in strongly correlated materials. In particular, motivated by recent pump-probe experiments using ultrafast lasers, he has investigated the underlying mechanism of light-induced phase transitions. A theoretical challenge in this context lies in the strong interactions in the system, which requires non-perturbative methods to properly describe the microscopic quantum dynamics. The studies have identified multi-photon absorption processes leading to light-induced phase transitions and revealed nonequilibrium spectroscopic features accompanying them. The simulations also found intriguing dynamics due to the interference of multi-photon excited states, which may be used to control the many-body quantum phases [thoss9]. Furthermore, in a close collaboration with the group of L. Mathey (University of Hamburg), possible mechanisms to dynamically control the Josephson currents in high-Tc superconductors and two coupled Bose-Einstein condensates were proposed [thoss10].

Future Plans

The future research plans of the Thoss group involve a variety of different directions. In the field of charge transport in nanostructures, this includes the further analysis of current induced reactive processes in molecular junctions and the study of fluctuations. Furthermore, in a project pursued within the Research Unit 'Reducing complexity of nonequilibrium systems', the goal is to understand current-induced forces and electronic friction. As a new topic, we plan to investigate is the phenomenon of chirality induced spin selectivity in molecular nanostructures. This phenomenon describes an unusually large spin polarization of the charge current passing through a chiral molecule and was observed experimentally in a variety of systems.

The study of singlet fission in molecular materials will be continued and extended. In particular, longer-time spin mixing processes caused by spin-dipole coupling shall be explored within a newly funded DFG project. Furthermore, within the framework of the Research Training Group 'Dynamics of controlled atomic and molecular system', photoinuced charge transfer processes in building blocks of molecular materials will be investigated in collaboration with the experimental groups of F. Stienkemeier and L. Bruder.

We also plan to investigate interesting open question in the field of quantum thermodynamics. This includes the study of driven quantum nanosystems as well as thermodynamic uncertainty relations. in particular in non-Markovian quantum systems strongly coupled to environments.

2.2.3 Biomolecular Dynamics – Group Stock

The Biomolecular Dynamics Group of Prof. **Gerhard Stock** is concerned with the theory and computation of structure, dynamics and function of biomolecules, driven by the ultimate goal of a truly microscopic understanding of the underlying physics. In particular we study nonequilibrium transport processes such as energy transfer and intramolecular signaling or allosteric communication. Because state-of-the-art molecular dynamics (MD) simulations and multidimensional experiments generate an enormous amount of data, a main objective is to derive simple "post-simulation models" that explain the essential dynamics of the process. The group provides a link between the molecular physics research and the biophysics/polymer research of the Institute and also connects to the Physical Chemistry groups the Chemistry department. Most of our research projects during the reporting period can be summarized in the following topics.

Nonequilibrium allosteric communication

Information transfer within cells on the molecular level occurs via a mechanism called allostery, where binding of signaling molecules to a protein cause subsequent structural changes traveling through this protein to a distant site. The physical mechanism though which allostery takes place is under hot debate. Computational investigations of allosteric communication require the characterization of both structural and dynamical changes of the target protein via nonequilibrium experiments and MD simulations [stock2, stock4] In close collaboration with the group of Peter Hamm (Zürich) who study the process using time-resolved infrared spectroscopy experiments, we have developed a time-dependent picture of the allosteric communication in PDZ domains [stock2, stock7] as well as the the S protein [stock5]. Moreover we studied the hierarchical dynamics in allostery from nano- to milliseconds following ATP hydrolysis of chaperone protein Hsp90, which was done in collaboration with the Hugel group (Freiburg) performing single-molecule FRET experiments [stock8]. Our extensive nonequilibrium MD simulations have revealed that allostery amounts to the propagation of structural and dynamical changes, that are genuinely nonlinear and can occur in a nonlocal fashion.

Considering PDZ2 domain as an example, we have linked an azobenzene photoswitch to a peptide ligand in a way that its binding affinity to the PDZ2 domain changes upon switching, thus initiating an allosteric transition in the PDZ2 domain protein [stock7]. The subsequent response of the protein, covering four decades of time ranging from 1 ns to 10 μs, can be rationalized by a remodelling of its rugged free energy landscape, with very subtle shifts in the populations of a small number of structurally well defined states (Fig. 2.2.3). These findings lead to the insight that structurally and dynamically driven allostery, often discussed as limiting scenarios of allosteric communication, actually go hand-in-hand, allowing the protein to adapt its free energy landscape to incoming signals.

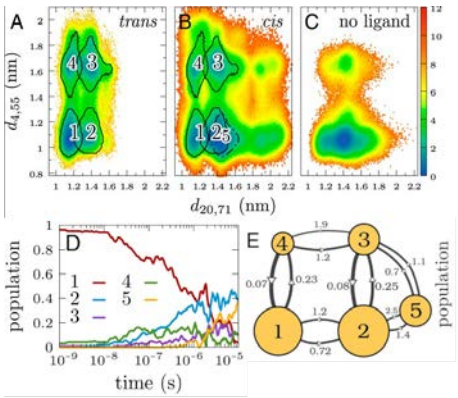


Figure 2.8: Allosteric communication in a photoswitchable PDZ2 domain. Free energy landscapes obtained from the (A) *trans*, (B) *cis* and (C) ligand-free MD simulations of PDZ2, plotted as a function of two essential inter-residue distances. (D) Time evolution of the state populations reflecting the allosteric transition, as obtained from a Markov state model (E) [stock7].

Protein energy transport

Vibrational energy transport is essential for protein function. It is responsible for efficient energy dissipation in reaction sites, and has been linked to pathways of allosteric communication. While it is understood that energy transfer occurs via the protein backbone as well as via non-covalent contacts, little is known about the transfer competition of these two transport channels, which determines the pathways. To tackle this problem, we have performed extensive nonequilibrium MD simulations and developed a master equation approach that is based on inter-residue, residue-solvent and heater-residue energy transfer rates which closely reproduces the results of the all-atom simulations. On the experimental side, the group of Jens Bredenbeck (Frankfurt) equipped the β-hairpin fold of a tryptophan zipper with pairs of non-canonical amino acids, one serving as a energy injector and one as a energy sensor in a femtosecond pump probe experiment. The compelling agreement of experiment and simulation (Fig. 2.2.3) allowed us to identify the energy transport pathways of the protein via a Monte-Carlo Markov Chain simulations of the master equation. Our joint experimental/computational endeavor revealed the efficiency of backbone vs. contact transport, showing that even if cutting short backbone stretches of only 3 to 4 amino acids in a protein, hydrogen bonds may be the dominant energy pathway [stock10].

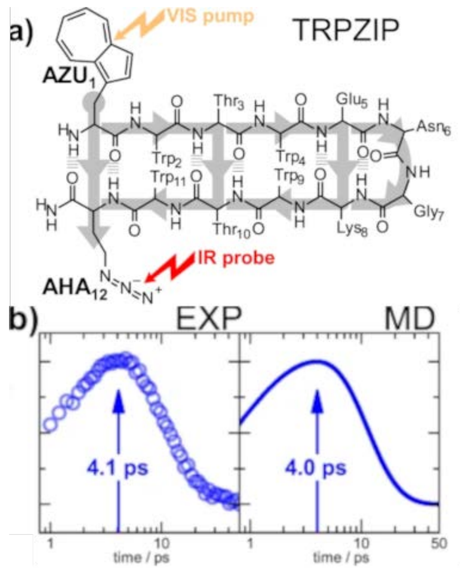


Figure 2.9: Vibrational energy transport in TrpZip2. (a) Energy is injected into the system via azulenylalanine (Azu) and propagates along various possible pathways to azidohomoalanine (Aha). (b) Comparison of experimental and simulated signals [stock10].

Dissipation corrected targeted MD

Current state-of-the-art MD simulation methods and hardware are capable to simulate molecular processes on timescales up to milliseconds, while the biologically relevant range of timescales reaches from microseconds to minutes. To enforce structural changes on such timescales, biased MD simulation methods have been developed, which aim at predicting free energies along a predefined reaction coordinate. A problem with this type of simulation and analysis is that the resulting free energies only allow limited inference of the unbiased system's dynamics and nonequilibrium effects such as dissipation, as fast degrees of freedom have been integrated out. To allow such a coarse-graining of system dynamics, we have developed dissipation-corrected targeted MD [stock3]. Combining the Jarzynski equality and a Markovian Langevin equation, we derived an expression for a dissipation correction that can be calculated on-the-fly for nonequilibrium pulling simulations. Our approach does not only result in the free energy profile, but in friction factors, as well, the latter allowing insights into fast dynamics not contained in the free energy and fluctuations along the biasing coordinate as well as their molecular origin. Furthermore, both quantities can serve as input for integration of a Langevin equation, speeding up calculations of system dynamics by several orders of magnitude. Combination with our approach of temperature boosted Langevin equation simulations finally allows to access timescales of up to minutes, which we demonstrated for the example of binding and unbinding of drug-like molecules to and from their host proteins [stock6].

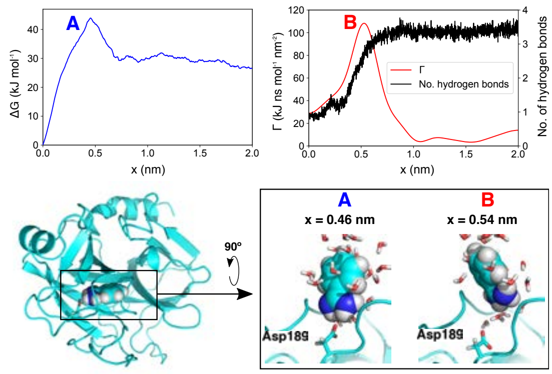


Figure 2.10: dcTMD analysis of free energy (blue) and friction profile (red) from biased unbinding of a ligand from its binding protein. While the free energy transition state **A** represents a strained electrostatic interaction between protein and ligand, the peak friction **B** comes from water molecules rushing into the binding site [stock6].

Learning of collective variables and coarse grained dynamical models

While classical MD simulations describe the motion of biomolecular systems in terms of usually thousands of atoms, their essential dynamics takes place on a way smaller, latent space, characterized by only few collective variables. Choosing these variables such that they encompass the system's main statistical and dynamical features, biomolecular processes can be described in terms of the corresponding free energy landscape, visualizing the metastable states of the systems and the pathways between these states. In the last decade, we have developed various methods to identify collective variables and metastable states (e.g., using machine learning), which subsequently can be employed to construct a Langevin or a Markov state model of the dynamics [stock1]. In particular we have investigated (generalized) Langevin equations accounting for nonequilibrium processes, and considered various practical implementations and applications [stock9].

Future Plans

Apart from a consequential continuation of our research lines, we also plan to follow various new paths. Concerning allostery, for example, we will extend our studies to PDZ domains with two clearly defined functional site such as photoswitchable PDZ3 and a PDZ tandem. As a new topic, we will consider cooperative allosteric transitions, which may be described by an Ising-type model. As a new prime application for dissipation corrected targeted MD we will consider molecular friction in complex fluids and study processes such as shear thinning of lubricants. Moreover, we will extend the theoretical framework of the approach towards non-Markov and multi-path processes and investigate possible contributions of polarization effects to intermolecular friction. Using machine learning methods such as Leiden clustering, we will established community-detection driven correlation analysis as a new approach of nonlinear dimensionality reduction. Combined with improved clustering methods, we will be in a position to establish a comprehensive trajectory analysis of protein folding, which may serve as a reference for future method developments.

2.3 Functional Materials

2.3.1 Applied Theoretical Physics - Computational Physics – Group Dzubiella

The **Applied Theoretical Physics Group of Joachim Dzubiella** has joined the Institute of Physics in April 2018. The Dzubiella group investigates the properties of soft matter and functional materials relevant for applications, such as molecular solvents, electrolytes, associating biological and synthetic polymers as well as dispersions of functional nanoparticles and colloids. We employ statistical physics approaches combined with multi-scale computer simulation techniques, such as all-atom molecular dynamics (MD) or coarse-grained Langevin dynamics type of simulations. Dzubiella also heads the joint research group (JRG) "Simulations of Energy Materials" which constitutes a formal cooperation between the Helmholtz-Zentrum Berlin (HZB) and the University of Freiburg (2018-2023). The JRG focuses on functional interfaces that are important for energy storage and conversion materials. In particular, we look at solid/liquid interfaces between (semi-)conducting electrode surfaces and electrolyte solvents, in collaboration with experimentalists.

The group is shareholder of the computing cluster NEMO and NEMO II. Our research has been funded from Freiburg, HZB, an ERC Consolidator grant (2015-2020) which moved from Berlin to Freiburg, an industry cooperation (Covestro, Leverkusen), and projects funded by the German Science Foundation (DFG). In particular, Dzubiella is PI in the DFG Priority Program "Polymer-based Batteries" (SPP2248) and the Research Unit (RU) FOR5099 "Reducing Complexity of Nonequilibrium Systems" centered in our institute. Our past research can be summarized by the following three topics, all situated at the interface between chemical physics, soft matter physics, and materials science. Our future plan is to connect us stronger and bridge physics with the applied sciences and engineering in Freiburg.

Research Report

ERC project: Nanoreactors and responsive polymers

In the ERC project "Multiscale modelling of stimuli-responsive nanoreactors" (2015-2020) we studied so-called nanoreactors in close collaboration with experimentalists at the HZB. In these nanoreactors, catalytically active metal nanoparticles are embedded in a stimuli-responsive polymer matrix, see Fig. 2.11 for an overview. The polymer controls the partitioning and mobility of the reactants close to the catalytic site and with thus the *permeability* and the catalytic activity of the system. Since the polymers are stimuli-responsive the catalytic activity can be tuned and switched by external triggers, such as pH or temperature; the nanoreactor can also respond to the reaction itself and thus create a feedback loop. In the project, we integrated scale-bridging microscopic and chemically-specific solvation and adsorption effects into macroscopic rate laws, taking into account the diffusion-influenced transport through polymer membranes. Nanoreactors thus open up new design routes in nano-catalysis science to create highly selective, programmable 'colloidal enzymes'.

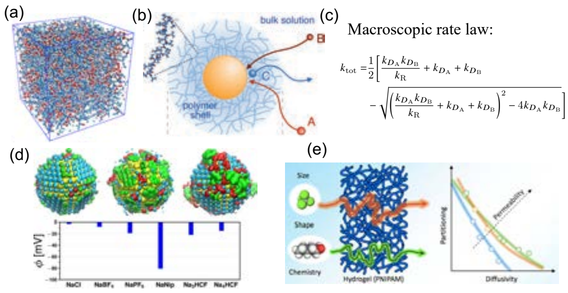


Figure 2.11: (a) All-atom MD simulation of an aqueous responsive polymer network. (b) Example architecture of a nanoreactor: a catalytic metal nanoparticle (yellow) is embedded in a polymer network, catalyzing a bimolecular reaction A+B→C. (c) A m acroscopic rate law which depends on polymer permeabilities. (d) Electrolyte solvation structure and surface potential of metal nanoparticles. (e) Molecular partitioning, diffusivity, and permeability in polymer networks is chemically specific but can be categorized.

In particular, we developed methodologies to include the high polarization of metal nanoparticles into simulations, revealing the complex heterogeneities of aqueous and ionic solvation and reactant adsorption at the catalytically active, facetted metal nanoparticles [dzu10]. We calculated diffusion and excess adsorption of molecules around cross-linkers and in collapsed polymers. Two breakthrough findings provided a completely new view on how charged reactants and salt penetrate polymer membranes [dzu3] and on chemical categories of membrane permeability [dzu9]. We determined how membrane permeability is determined generically from microscopic interactions and membrane topology [dzu6]. Finally, we introduced the action of permeability into diffusion-influenced rate theory for a general class of nanoreactors, which helped to understand and experimentally design a new form of of nanoreactors. Currently we are focussing on the development of self-regulating feedback loops in nanoreactors (see Master thesis Rolf Schimmer).

Complex electrolytes in bulk and at interfaces

Dense electrolytes with complex molecular structure are an integral component in electrochemical storage and conversion devices which we study using atomistic simulations in connection with statistical physics approaches, see Fig. 2.12 for an overview. Together with experimental partners we uncovered and rationalized the existence of an aqueous biphasic system in a concentrated mixture of simple but battery-application-relevant salts in water [dzu4]. Moreover, large-scale all-atom simulations on solvated, very dense electrolytes revealed correlation length behavior according to theoretical predictions, not experimental conjectures, contributing significantly to a controversial discussion in literature [dzu8]. Within our cooperation with the HZB and a project in the DFG-SPP2248, a strong focus of our research was on next-generation lithium-sulfur (Li-S) batteries. Using newly developed MD for polysulfides (PS) in electrolyte solutions of lithium salts in organic solvent mixtures, we investigated conductivities, diffusion coefficients, solvation structures, and clustering behavior and verified our simulation model with experimental measurements. Our results showed that in particular (unwanted) PS aggregation and clustering behavior are significantly influenced by the chain length of PS and the addition of specific salts [dzu5]. These findings are now supported by neutron scattering experiments. Furthermore, we recently studied the vulcanization process of polymer cathodes by electronic stability calculations and a statistical mechanics model of sulfur distributions, experimentally supported by Raman spectroscopy.

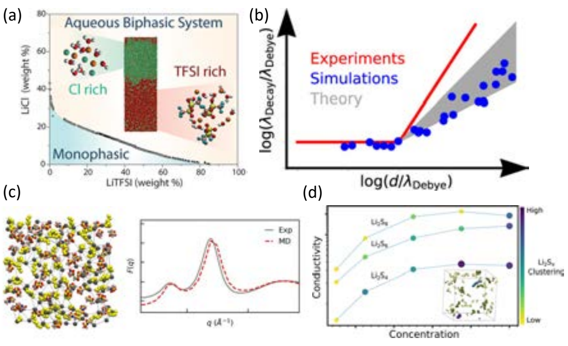


Figure 2.12: (a) Phase diagram of the aqueous biphasic system. (b) Correlation (decay) lengths behavior in dense electrolytes. (c) MD and neutron scattering (Exp.) of polysulfide electrolyte solutions in Li/S batteries. (d) Conductivity and clustering of polysulfides in battery electrolytes.

Protein-Polyelectrolyte complexation

Macromolecular polyelectrolytes (PEs), such as dendritic PEs or PE nanogels (nanometer-sized networks) have high potential in medical applications, e.g., to function as drug candidates or carrier systems. In cooperation with experimental partners in Berlin we studied the interaction of proteins such as human serum albumin (HSA) and lysozyme with linear polyelectrolytes, charged dendrimers such as dendritic polyglycerol sulfate (cf. Fig. 2.13), charged networks, and polyelectrolyte brushes [dzu1]. In all cases, we combined experimental work with MD simulations and mean-field theories. In particular, isothermal titration calorimetry (ITC) has been employed to obtain the respective binding constants and the Gibbs free energy of binding. MD simulations demonstrated that the entropic 'counterion release mechanism' is the main driving force for the binding of proteins to strongly charged polyelectrolytes. In several cases, the binding constant could be calculated from simulations to very good approximation, see Fig. 2.13. We also predicted the kinetics of protein uptake by microgels for a given system by applying dynamic density functional theory [dzu2]. We thus demonstrated by direct comparison of theory with experiments a comprehensive understanding of the interaction of proteins with charged polymers. We discussed possible implications for applications, such as drug design, in the literature.

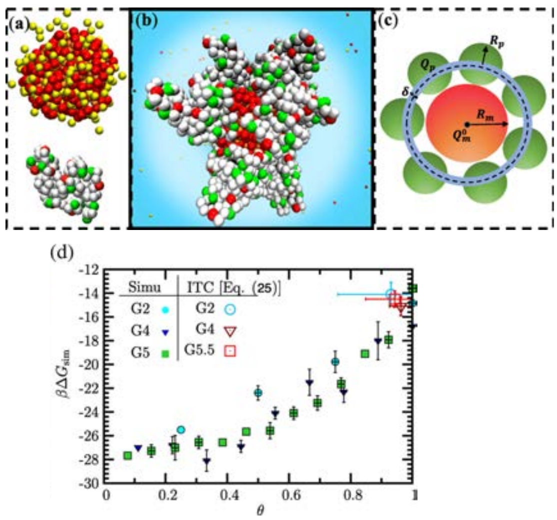


Figure 2.13: (a) Coarse-grained simulation model of dendritic polyglycerol sulfate (dPGS; top) and lysozyme (bottom). (b) Lysozyme adsorbed on dPGS, forming a 'protein corona', see sketch in (c). Simulated binding free energies agree will with ITC measurements.

Future Plans

Most of the above projects have been initiated in Berlin and have been fading out recently, in particular the ERC and the protein-PE projects. We are currently discussing whether our formal connection to the HZB will be continued. Quite certainly, however, the cooperation within the electrolyte-related battery research (SPP 2248) we plan to continue. Here, we started a new cooperation in Freiburg with Michael Walter (Group Moseler, Functional Nanosystems, Fraunhofer) on the theoretical prediction of X-ray spectroscopy of Li-S batteries. Meanwhile, more connections have been formed in Freiburg in this transition phase, in particular within the Institutes of Physics, and other institutes, such as Chemistry, Engineering and Fraunhofer (E.g., within RU FOR5099 and the LivMats Cluster.) Future plans are directed in strengthening these new connections in the field of applied physics / materials, two examples of which are as follows:

Active and adaptive responsive materials

In the LivMats Cluster materials are developed which exhibit life-like behavior, featuring response, (collective) learning and adaption, signalling, and feedback. We have recently developed a 'Responsive Colloids' model and made the first steps towards non-motile activity (Master theses Gaindrik and Göth) and a coarse-grained active switching model [dzu7]. Future studies will deal with the exciting questions how to include learning and adaptivity, e.g., in response to external triggers, into these nonequilibrium materials. We are currently identifying possible experimental cooperations within LivMats. Nonequilibrium theory development will also be in strong mutual benefit within our RU FOR5099.

Control of nonequilibrium polymers

Experiments from Prof. Reiter (Polymer Physics) in our institute show exciting phenomena of nonequilibrium polymers, e.g., a strong mechanical action when nonequilibrium 'free energy' is released in a controlled relaxation. Inspired by this, we recently showed by simulations that indeed in fast polymer synthesis and processing, some 'extra' free energy can be stored in the system and quantified it. How to control nonequilibrium polymers inspires many new theoretical and experimental questions on nonequilibrium materials, which are also relevant for the LivMats cluster and the RU FOR5099. Currently some synergistic and collaborative projects in these directions are discussed, including our neighboring partners in France (Strasbourg and Mulhouse).

2.3.2 Experimental Polymer Physics – Group Reiter

Research of the **Experimental Polymer Physics Group headed by Günter Reiter** focusses on "Soft Matter" and is based on links between Physics, Macromolecular Chemistry, Biology, Life Sciences, and Applied Sciences. The goal of the scientific studies is to gain a profound understanding, detailed physical description and a high control of dynamics and structure-forming processes in complex molecular systems and materials, some of which are inspired by processes in nature.

In an interdisciplinary approach, physics of polymers and soft matter provides one of the foundations with respect to fundamental and conceptual questions of innovative materials research. The scientific approach of the Reiter group centers on issues related to the properties of molecules on surfaces and interfaces, materials in flow, growth and structure formation processes, and functional materials based on complex, nanostructured systems. Here, the emphasis is on the study of the fundamental molecular interactions that control organization and structure formation and therefore determine the hierarchical organization of complex and functional macromolecules over many length scales up to macroscopic sizes.

Prof. Reiter was heading the International Research and Training Group (IRTG) Soft Matter Science, the Experimental Polymer Physics Group is part or has been participated in the International Training Networks (ITNs) "PlaMatSu" and "Photo-Emulsion", the priority program (SPP) "Dynamic Wetting of Flexible, Adaptive and Switchable Surfaces", and the Cluster of Excellence "Living, Adaptive and Energy-autonomous Materials Systems (*liv*MatS)".

Research of the group can be divided into subthemes, as illustrated by the examples presented below.

Research Report

Molecular interactions, light and structure formation

One of the main scientific activities refers to investigations of the relation between structural organization controlled by crystallization and opto-electronic properties of conjugated polymers. In the most recent experiments, the main focus is on analyzing the influence of illumination by visible light on crystallization of thin molten films of conjugated polymers and its impact on photoluminescence [reiter1,reiter3]. Using a microscope setup for temperature-dependent characterization of molten polymer films, the influence of white light illumination on the crystallization behavior of poly(3-(2,5-dioctylphenyl)thiophene)

(PDOPT) and poly(3-hexylthiophene) (P3HT) was examined. A reduction in nucleation density and crystal growth rate due to illumination was observed, with the magnitude of the reduction increasing with the increase in light intensity. Melting of samples previously crystallized under illumination and recrystallization of these samples in the dark showed complete reversibility of the crystallization behavior, implying that these illumination-induced changes in crystallization behavior were not permanent. It can be hypothesized, that the absorption of photons by conjugated polymers leads to a stiffening of the chain, possibly reducing the diffusivity of the polymer. This effect in turn slows down the growth rate of crystals and reduces the nucleation probability. It is likely that many other conjugated polymers will show similar or related illumination-induced phenomena which impact crystallization and opto-electronic properties.

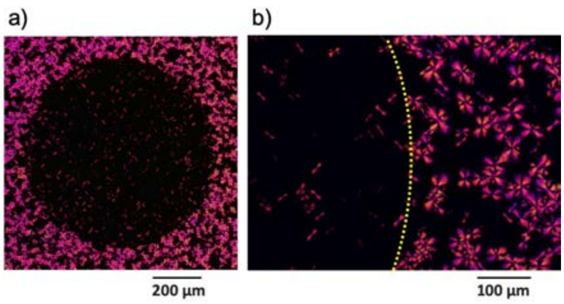


Figure 2.14: Optical micrographs (crossed polarizers), showing that size and number density of spherulitic crystals were reduced upon illumination with white light. (a) Large-scale image demonstrating that the illuminated circular region with a diameter of ca. 1.5 mm contained fewer and smaller spherulites. (b) Zoomed-in image which focusses on the boundary between the illuminated (left) and non-illuminated (right) region, indicated by the curved dotted line.

Phase transitions and growth processes in complex systems

The group has extensive experience in the study of polymer crystallization processes. One focus is on complex crystal morphologies that are critical for properties and performance of polymer materials.

In a recent study [reiter4], stacks of crystalline lamellae with a uniquely aligned hexagonal shape were obtained by isothermal crystallization of isotactic polystyrene at a temperature close to its melting point. The height of the stacks of uniquely oriented hexagonal lamellae, referred to as ”3D (three-dimensional) single crystals”, reached several micrometers, corresponding to hundreds of crystalline lamellae arranged on top of each other. There, the mechanism of self-induced nucleation enabled the transfer of the orientation of the basal lamellar crystal to all other lamellae in the stack. The unique alignment of all lamellae was reflected in the fact that observed cracks formed preferentially along the diagonal of the hexagonal stack. The cracks were caused by a mismatch of the thermal expansion coefficients of the substrate and the ”3D single crystals” during quenching from crystallization temperature to room temperature. The presented growth mechanisms of the ”3D single crystals” should also be observable for all crystallizable polymers, including block copolymers containing a non-crystallizable block.

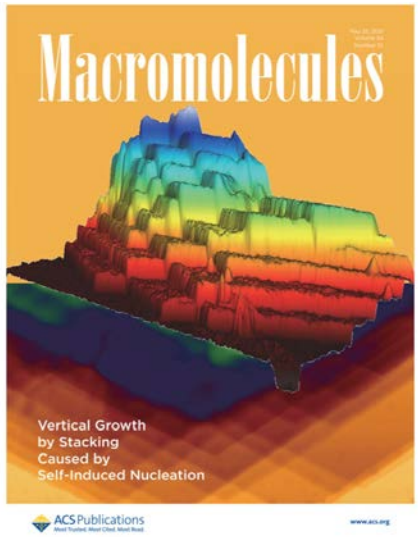


Figure 2.15: 3D AFM height image showing the crystal morphology of “3D single crystals” of iPS.

Polymers in thin films and at homogenous and structured interfaces

Using the group’s expertise on dewetting of thin polymer films, the origin of symmetry breaking for moving circular contact lines of dewetting polystyrene films suspended on a periodic array of elastic pillars was investigated [reiter5]. Here, dewetting force fields driving the polymer flow were perturbed by elastic micro-pillars arranged in a regular square pattern. Elastic restoring forces of deformed pillars locally balanced driving capillary forces and could be used for a spatially resolved analysis of the acting forces. The interactions of the elastic pillars with the dewetting film broke the circular symmetry of expanding dewetting holes. Even at sizes much larger than the characteristic period of the pillar array, the observed envelope of the dewetting holes reflected the symmetry of the underlying square pattern. These observations show that periodic perturbations in a driving force field can produce a well-defined pattern with lower symmetry. For the studied system, we succeeded in squaring the circle.

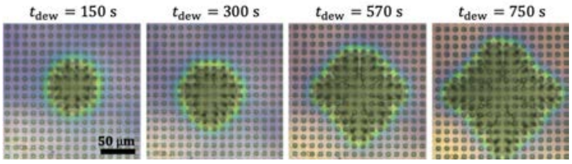


Figure 2.16: "Squaring the circle". Dewetting of a 400 nm thick film of polystyrene performed at a dewetting temperature $T = 180°$C on top of an array of deformable pillars for different values of dewetting times.

Elasto-fluid dynamics in microfluidics

Responsive and adaptive soft material systems at the micro- and mesoscale, which can deform dynamically and periodically under the influence of fluid flow and respond differently to distinctive stimuli, are of great importance for a variety of exciting new applications in soft robotics and in life sciences. Therefore, we develop, study, and analyze physical strategies for adaptive control, manipulation, and monitoring of single- and multiphase fluid flows in microfluidic networks for directed information and material transport. In detail, we investigate and determine the critical physical parameters of the interactions, instabilities, correlations and synchronizations of soft elastic thin walls mediated by the surrounding fluids, which on the one hand has significant impact on the dynamics of the fluids and on the other hand shows that the dynamics of the fluids have a direct influence on the interacting thin walls.

Moreover, inspired by tubular networks in nature, such as blood vessels in animals and conduction vessels in plants, we develop and analyze the physics of embedded microfluidic networks in soft material systems. Due to the specific dendritic architecture of these microfluidic networks and the local elastic properties, material and information transport within these material systems can be controlled depending on the implemented response and adaptability to internal and external stimuli.

Future Plans

Often, macromolecules in many polymer-based materials are subjected to rapid changes and strong forces during the processing stages. Accordingly, polymers are often unable to reach equilibrium and have to adopt non-equilibrium conformations. Therefore, in most cases, it is not possible to establish predictable and quantitative relations between processing conditions and resulting properties of polymer films. In order to design polymers with desirable properties and tunable performance in the future, we aim to develop a basic quantitative understanding of how processing pathways determine variations in molecular conformations and how these, in turn, determine the properties of the materials. In this spirit, we plan to combine systematic experiments, simulations and theory that will lead to a comprehensive fundamental understanding and quantitative processing-property correlations allowing for a predictive power of nonequilibrium behavior of polymers.

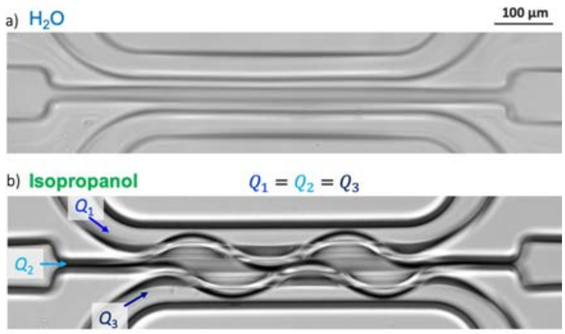


Figure 2.17: Interactions between two statically buckled membranes: a) Micrograph of three channels separated by thin membranes filled with water. b) Micrograph of correlated buckling membranes due to the volume flows of isopropanol.

The experiments of suspended polymer materials on elastically deformable pillar arrays will be extended, e.g., to characterize and directly measure residual stresses in nonequilibrated thin polymer films and measure the tension of polymer filaments, which are formed by dewetting processes. Furthermore, the strategy of guiding moving contact lines by periodic perturbations represents a promising approach for controlled material transport and the design of adaptive and programmable materials surfaces.

In addition, we plan to use elasto-fluid dynamics coupling in fluid networks to enable and analyze correlated and synchronized flows. These complex interaction patterns in flow networks will be used for peristaltic pumping and local pruning and thus for the development of simple logic gates and circuits as well as systems to emulate biophysical processes.

2.3.3 Statistical Physics of Soft Matter and Complex Systems – Group Schilling

The "Schilling group" are 15 theoreticians who work in the field of statistical physics. We develop methods to coarse-grain systems out of thermal equilibrium, we study percolation problems, and we predict the phase behaviour and phase transition dynamics of colloidal systems, liquid crystals and ionic fluids.

Our portfolio of methods consists of projection operator formalisms, density functional theory (DFT), Monte Carlo simulation and Molecular Dynamics simulation. A part of our work is carried out on high performance computing infrastructure. We are using the local computing cluster NEMO and we will be share-holders of NEMO II, which is currently being built. We develop new simulation methods and code, but we also frequently work with computer algebra or pen and paper.

All work presented here has been carried out in the context of seven DFG-funded projects, which we got granted within this reporting period.

Research Report

Coarse-grained dynamics out of thermal equilibrium

With the notable exception of elementary particles, physical systems are hardly ever described in terms of all their microscopic degrees of freedom. Instead physicists rely on effective models, which are often based on phenomenological considerations. The use of these models is justified if the processes of interest occur on time-, length-, and energy-scales that can be clearly separated from the microscopic scales. However, in principle we should be able to derive each effective model rigorously by integrating out irrelevant degrees of freedom from the underlying microscopic dynamics. And it would be useful to have systematic procedures that work even if the scales are not well separated.

The process of integrating out degrees of freedom is called *coarse-graining*. If a system is out of thermal equilibrium, the task of coarse-graining becomes particularly difficult, because the microscopic density of states evolves in time.

In the past five years our group has made several contributions to fundamental research on coarse-graining. We used time-dependent projection operator formalisms to derive exact equations of motion for systems under time-dependent external driving [schill1, schill2]. One central result of this work is that coarse-grained equations of motion which contain a potential of mean force (or a derivative of a "free energy landscape") as the non-linear drift are in general not compatible with the second fluctuation dissipation theorem. Hence we argue that the stochastic interpretation of the non-linear generalized Langevin equation is far from obvious, and that the wide-spread strategy to produce coarse-grained non-equilibrium models by adding colored noise to the dynamics is disputable.

Langevin-type models are frequently used in biomolecular modeling, the modeling of phase transitions (e.g. in phase field models) and of chemical reactions (e.g. in Grote-Hynes theory). Thus we expect our results to have an impact on modeling in a wide range of branches of physics.

Based on our theoretical work, we developed new numerical methods to construct coarse-grained models using experimental data or data from simulations [schill3, schill4]. In ref. [schill3] we introduced a method to compute memory kernels and then analyzed the kinetics of the crystallization transition in an undercooled melt. We observed that, contrary to one basic assumption of most theories on crystallization, the crystal nucleation process was not Markovian. In ref. [schill4] we analyzed the dissociation process of NaCl in water and observed signatures of the dynamics of the hydration shells in the memory kernel of the coarse-grained evolution equation. This piece of work was carried out in collaboration with the Stock group in the context of the research unit FOR 5099.

Percolation

Clustering of particles into connected aggregates is a process that occurs frequently in nature as well as in materials processing. The formation of a system spanning cluster is called *percolation*. The conditions under which percolation occurs are of particular technological interest, as such a cluster might support mechanical stress or allow the transport of charges through an otherwise insulating material.

The Schilling group has been working on percolation problems for 15 years. In the reporting period we did research on the aggregation and percolation behaviour of rod-like, plate-like and fractal filler particles in composite materials as well as on the closely related mathematical problem of epidemic modelling [schill5] (here the similarity stems from the fact that in the case of a pandemic, "clustering" refers to contacts between individuals and the "percolation event" is the spread of a disease across an entire population).

The spatial restrictions of this report do not allow us to present all these projects, therefore we just give two examples: We observed that percolation in the nematic liquid crystal phase shows re-entrant behaviour [schill6], and we developed a new theoretical approach that allows to relate the connectivity properties of a system to its pair-correlation function [schill7]. This approach enables us to solve a large class of percolation problems based on information on the thermal structure of a system.

Phase transition kinetics

In the reporting period we studied phase transition kinetics in various soft matter systems, such as liquid crystals, ionic liquids, active particles and colloidal suspensions. As we cannot report on all projects here, we focus on two examples: The liquid-to-crystal transition in suspensions of colloidal hard spheres and phase separation in active particles.

Hard spheres are the simplest system which undergoes a liquid-to-crystal transition. Therefore they serve frequently as a model in statistical physics and in the materials sciences. Yet, the most basic aspect of their phase transition kinetics still poses an unsolved problem: experimentally observed and numerically predicted crystal nucleation rates differ by ten orders of magnitude (see fig. 2.18 top panel). Based on large scale molecular dynamics simulations we propose the hypothesis that this discrepancy is due to a misinterpretation of the experimental scattering data. We argue that the formation of polycrystalline samples has not been taken into account correctly when the scattering data was analyzed. We show that all data (experimental and numerical) collapses onto a single curve, if crystal domain growth is correctly accounted for (see fig. 2.18 bottom panel). The remaining discrepancy between the curves in fig. 2.18 is due to different degrees of polydispersity in the experimental realizations.

The second example is phase separation in suspensions of active particles. The term active matter describes systems of particles that have a self-propulsion mechanism as e.g. schools of fish, flocks of birds or colonies of bacteria. The particles in these systems dissipate energy such that systems are always out of equilibrium. For this reason they show interesting effects driven by the particles motility as, for instance,motility induced phase separation. We developed a theoretical description of this phase separation [schill8].

Structure & thermodynamics of electric double layers

Electric double layers (EDLs) occur where mobile ionic charges in electrolytes arrange to screen particle or surface charges. They exist at electrodes in capacitors, around colloidal particles, and in cells and nerves.

We are interested in the electrostatic screening of surface or particle charges and we use primitive models of charged hard spheres to model the mobile ions.

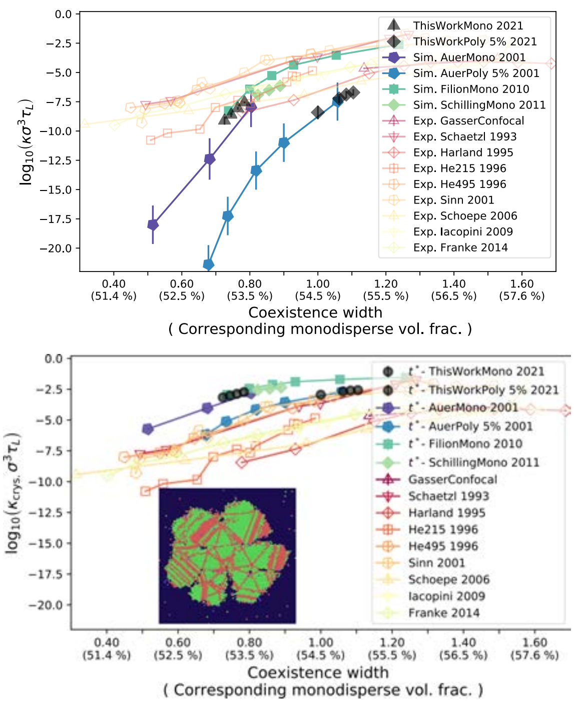


Figure 2.18: Top: Crystal nucleation rates as had been published up to 2021. Note the 10-orders of magnitude discrepancy between theory and experiment. Bottom: Same data as above, but analyzed taking into account the polycrystalline structure of the nuclei (see snapshot in the inset). The gap between theory and experiment is closed. (The data has not been published yet, the manuscript is still under review.)

In the reporting period, we studied the structure established in EDLs and the heat production in EDLs during electrode (surface) charging in the framework of DFT. Furthermore, we developed improved approximations for electrostatic DFT approaches.

One goal was and still is the theoretical description of underscreening, an experimentally measured strong increase of the electrostatic screening length with increasing ion concentration. This increase contrasts the monotonic concentration dependence of the Debye screening length of point-like ions. In collaboration with scientists from Utrecht (The Netherlands) and Cambridge (United Kingdom) we tackled the theoretical description of screening by the means of molecular dynamics simulations, machine learning methods, and classical density functional theory (DFT). We demonstrated that underscreening, as experimentally measured, cannot be explained within the primitive model [schill9].

However, a weak increase of the screening length follows even from theoretical considerations. For this weak screening, measurements reported an additional structural switch in the oscillatory behaviour of the screening length. Using a newly developed DFT approach, we explained this switch in the screening behaviour and related it to the fundamental nature of the underlying long-range correlations [schill10].

Future Plans

Power functionals and projection operators

Recently, two distinct pathways to non-equilibrium coarse-graining have been developed: Power Functional Theory (PFT) which is inspired by Density Functional Theory, and time-dependent projection operator formalisms. Both pathways are in principle exact, thus despite the rather different look of the resulting equations, they must be equivalent. However, to our knowledge the relation between them has not been analyzed yet.

In general, it is not possible to solve either of these theories exactly and approximations are needed. Probably the different mathematical structure of the two approaches will allow for different types of approximations. In the coming years we will analyze the potential of a combination of PFT and projection operator formalisms to construct approximative models for practical application problems in soft matter physics. In particular we will study the dynamics of phase transitions and the mechanical properties of complex fluids.

Next to practical applications, this approach will also allow us to study basic questions of non-equilibrium physics as we can e.g. construct the equation of motion for the heat dissipated in a driven system. We have recently started working on these questions in the context of the research unit FOR5099.

Percolation

We recently introduced a new criterion that allows to compute the percolation thresholds of a large class of systems exactly and to find controlled approximations for systems, which cannot be solved exactly. The basic idea of our approach is to construct a sequence of neighbourhoods on graphs, such that the percolation problem can be mapped to a branching process. In the future we will use this method to study percolation and transport in composite materials as well as in biological systems. One potential context for this work is the collaboration which we recently established with the institute of biology in Freiburg to study the swimming pattern of bacteria in confined geometries. Another context is our long standing collaboration on composite materials with the Leibniz Institute for New Materials.

2.3.4 Functional Nanosystems – Group Moseler

As a **member of the Physics Institute and the Fraunhofer IWM Michael Moseler** and his coworkers bridge the gap between fundamental and applied theoretical material physics. By modelling and understanding the basic mechanisms in materials and components the **Simulation and Modelling of Functional Nanosystems Group of Prof. Moseler** collaborates with academic and industrial partners in research and development. The work of the group covers classical molecular dynamics simulations [mos1, mos3, mos6, mos7, mos9, mos10] and quantum chemistry calculations [mos2, mos4, mos5, mos8] of nanomaterials [mos2, mos5] and tribological systems [mos1, mos3, mos4, mos7, mos8, mos9]. Tribology (the science of friction, lubrication as well as wear) is inherently multiscale ranging from atomic scale energy dissipation mechanisms up to earth quake dynamics. In Moseler's group multiscale modelling is invoked to bridge the gap between atomistic mechanisms and their consequences for macroscale devices by a a combination of contact mechanics [mos4, mos8], continuum fluid calculations [mos1] and the above mentioned molecular level simulations. In the last years the group's special focus was on CO_2 hydrogenation mechanisms on ZnO/Cu catalysts [mos2, mos5], on the tribochemistry of hard carbon coatings [mos4, mos8], on tribo-induced non-equilibrium phase transitions in silicon, carbon and polymers [mos3, mos9, mos10] as well as on the nanorheological properties of lubricants [mos1, mos7, mos9].

Research Report

Growing crystalline silicon nanostructures by means of tribology.

Despite the central role of silicon in microelectronics, its machining and fabrication with nanoscale precision remains challenging. Moseler's group has studied diamond cubic silicon crystals under combined compressive and shear stress by means of reactive molecular dynamics [mos3]. The simulation show that a possible localized plastic deformation mechanism leads to formation of localized amorphous regions. The growth of these amorphous shear bands is limited by a competing shear-induced recrystallization process resulting a steady-state value in their thickness. Based on this observation, the research group proposed a novel concept called "Triboepitaxy" to mechanically grow epitaxial silicon nanostructures without the need of elevated temperatures or impurities [mos10]. By mutual sliding of two silicon crystals with different shear elastic responses, the amorphous region can move along a preferential direction while maintaining its constant thickness, causing the crystal with lowest elastic energy density to grow at the expense of the other. Thus, the direct deposition of crystalline silicon nanofilms is technologically feasible (Fig. 2.19).

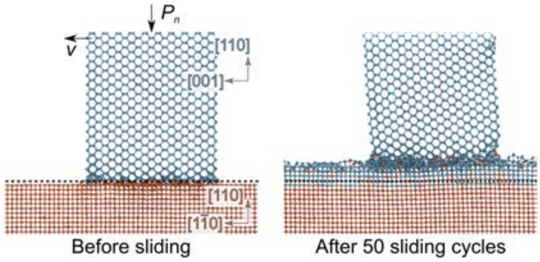


Figure 2.19: By rubbing a suitably oriented crystalline silicon nanotip (blue) under a normal load P_n and with velocity v against a silicon substrate (orange), crystalline nanostructures can be deposited on the substrate. The color of the atoms refers to the crystal they belonged to prior to sliding. See Ref. [mos10] for details.

Understanding the tribochemistry of tetrahedral amorphous carbon coatings (ta-C).

Ta-C is an excellent solid lubricant that exhibits high wear resistance and superlubricity (i.e., friction coefficient μ below 0.01) under boundary lubrication with organic friction modifiers including oleic acid and glycerol. Such hard carbon materials are increasingly applied as protective coatings in machines lubricated with traditional oils containing zinc dialkyldithiophosphate (ZDDP). Despite its importance in applied tribology, the tribochemistry of ta-C coatings is still elusive. Moseler's group has made first important steps towards a mechanistic understanding of ta-C lubricated by organic friction modifiers [mos4] and by ZDDP [mos8]. Tight-binding calculations of lubricated ta-C/ta-C tribopairs unveil universal tribochemical mechanisms explaining superlubricity [mos4] and wear [mos8]. Due to the simultaneous presence of multiple reactive centers unsaturated fatty acids, glycerol and ZDDP can concurrently chemisorb on both ta-C surfaces. Sliding induces mechanical strain and triggers a cascade of molecular fragmentation reactions releasing functional groups. Passivating H and OH groups combined with graphenoid surface terminations cause superlubricity [mos4], while sulfur release contaminates the ta-C resulting in its massive wear [mos8] (see Fig. 2.20 for a scheme that summarizes the ZDDP simulation results).

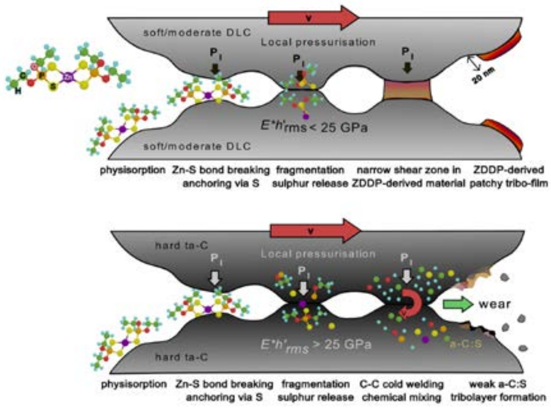


Figure 2.20: Schematic representation of likely scenarios for carbon coatings lubricated by ZDDP-additivated oils. The upper panel shows the formation of ZDDP-derived patchy antiwear tribofilms on soft carbon coatings (when $E \cdot h'_{rms}$ <25 GPa), the lower panel the wear of hard ta-C coatings. See Ref. [mos8] for details.

Future Plans

Molecular dynamics simulation of phase explosions in clusters.

In collaboration with Bernd von Issendorff, the Moseler group has started to study ultrafast phase transitions in silver clusters. Clusters that are subject to FEL laser pulses show an interesting fragmentation behavior. Classical molecular dynamics can help to explain the observed fragment distributions.

Understanding energy dissipation in dry friction.

Within the Research Unit 5099, Moseler's group performs molecular dynamics simulations of realistic material systems that are subject to unlubricated sliding. In collaboration with the experimental nanotribology group of Roland Bennwitz (INM, Saarbrücken), the friction mechanisms acting between a tip sliding against a graphene layer supported by SiC are considered. Depending on the load acting on the tip, various friction regimes and tribo-induced phase transitions can be observed – including the formation of monolayer diamond.

2.3.5 Materials Modelling – Group Elsässer (Fraunhofer IWM)

The theory group **"Materials Modelling" at Fraunhofer IWM of Christian Elsässer (scientific coordinator "Emerging Topics", strategy staff) and Daniel Urban (group leader)** explores material behaviors and predicts material properties using theoretical models and computational methods of solid-state physics and mechanics of materials. At the Institute of Physics Christian Elsässer is Adjunct Professor for Physics since 2007. He is Associated Member at the Freiburg Materials Research Centre (FMF) and Member at the Freiburg Center for Interactive Materials and Bioinspired Technologies (FIT).

Our ambition is to design compositions and structures of materials for targeted properties and functions. We identify the effects of crystal defects and microstructures on the macroscopic behavior of materials. This enables the effective and efficient use of material and energy resources in order to achieve long-term improvements to technical systems. The research field of our theory group is summarized in the following sentences. Some of our topics are reported in the ten selected publications listed below. More information on further topics is provided on our Fraunhofer IWM webpage: `https://www.iwm.fraunhofer.de/en/services/assessment-materials-lifetime-concepts/materials-modeling.html`

Screening, exploringand designing novel materials with tailored structural and functional properties

There is great demand in industry for designing novel materials, driven by strict technical challenges, economic concerns, or legal constraints. As a result, new materials must both have tailored physical properties and be compatible with established or new manufacture processes [elsae1]. Furthermore, they should be made of inexpensive raw materials

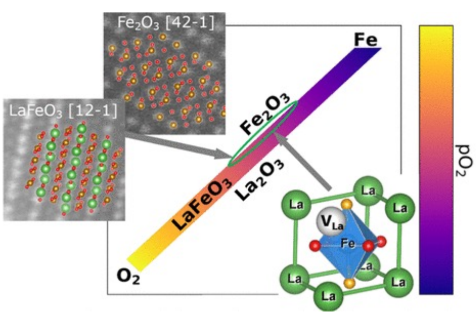


Figure 2.21: Phase stability diagram for LaFeO3, a functional oxide-perovskite material for high-temperature fuel cells [elsae10].

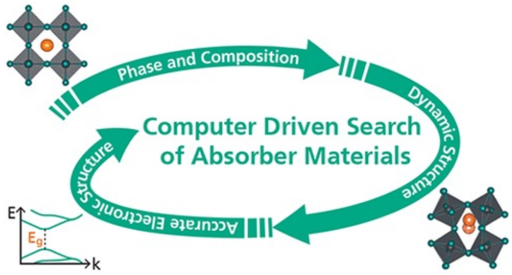


Figure 2.22: Computational workflow to search for functional halide-perovskite materials for solar cells [elsae8].

and contain few - ideally zero - critical elements. Dependencies on fluctuating material prices and market monopolies should also be avoided. The design of novel materials in principle faces the need for expensive and tedious experimental synthesis series. At this point, a computational high-throughput screening approach is employed to speed up the development of novel materials. Advanced simulation methods and growing computer capacities enable a large variety of structures and compositions to be virtually screened and predictions of their properties to be made. Various options can be tested systematically in an efficient manner. The basis for this is given by extensive theoretical material-property data. Data analysis tools exploit information in this database and help to steer and extend the search directions. Materials with promising properties can subsequently be investigated in depth and eventually synthesized experimentally. Our techniques are suited to a wide range of material classes.

We employ our methods for example to the search for permanent-magnet materials that contain less amounts of rare-earth elements [elsae2], to the exploration of chemical, kinetic, or mechanical properties of ion-conducting compounds for solid-state lithium-ion batteries [elsae3] and solid-oxide fuel cells [elsae9], to predict opto-electronic properties hybrid-perovskite-absorber [elsae8] and transparent-conductor-electrode materials for solar cells [elsae4, elsae5], or to investigate properties of defects and dopants of wide-bandgap semiconductors for piezoelectric actuators [elsae7] and magnetic quantum sensors [elsae6]. Currently, driven by the National Hydrogen Strategy in Germany and many related global initiatives, we are extending our research efforts at Fraunhofer IWM in the theoretical physics and experimental mechanics to the modelling and simulation of microstructural interactions and damage mechanisms of hydrogen in steels [elsae10], which influence the stability and durability of tubes and tanks of future hydrogen-gas transport and storage infrastructures.

2.3.6 Solar Energy - Materials and Technology – Group Bett (Fraunhofer ISE)

Research in the **Solar Energy - Materials and Technology Physics Group of Andreas Bett** focuses in general on the optimization of photovoltaic devices. This includes to investigate and improve bulk material as well as interface and heterojunction properties. Different materials are under investigation reaching from classical semiconductors like Silicon and III-V compounds, organic semiconductors and mixed in- and organic semiconductors as Perovskites. Dielectric or oxide based layers with high refractive index are investigated to passivate the surfaces of the bulk materials. Experimental procedures to fabricate devices using different tools are one research topic. The experimental work is supported by theory and simulation of the full devices as well as of specific interface behavior. A subgroup lead by Uli Würfel located in the FMF facility focuses on the investigation on organic solar cells and new tandem structures based on different thin film Perovskite materials. In order to develop an understanding of the physical processes involved, e.g. in material aging, but also in module performance the use of luminescence spectroscopy and transient luminescence is under investigation.

A. Bett joined the institute of Physics at the University of Freiburg in April 2020. He is director of the Fraunhofer Institute for Solar Energy System ISE. Therefore, aside his research specific at the University group also other subject areas are available for the students of the university, see description of Fraunhofer ISE.

Research Report

Approaching the highest photovoltaic conversion efficiency

In the field of III-V high efficiency solar cells, among other topics we are working on special photovoltaic (PV) cells for monochromatic laser light conversion, so-called photonic power converters. These devices are used as receivers in optical power transmission systems, where laser light is beamed through free space or optical fiber to power applications wirelessly. For solar cells the maximum efficiency for converting the broadband solar spectrum into electricity is fundamentally limited by hot carrier thermalization losses and low energy photon transmission losses. For laser light with a very narrow photon energy distribution, both these losses can be minimized. By following a thin film approach based on a GaAs cell with back surface reflector directly underneath the epitaxially grown active layer structure, we have developed a micro resonator which exploits Fabry-Perot resonance, see Fig. 2.23. With this cell we have achieved maximal absorptance at a photon energy of 1.445 eV. Hence, for such light (858 nm) thermalization down to the conduction band edge of the absorber (GaAs bandgap 1.424 eV) drops to an energy loss of only 1.5%. At the same time, the back reflector leverages optical confinement for photons generated intrinsically in the absorber by radiative recombination spectrally distributed around the bandgap energy. These photons are trapped inside the cell and, thus, despite weak absorptivity around the

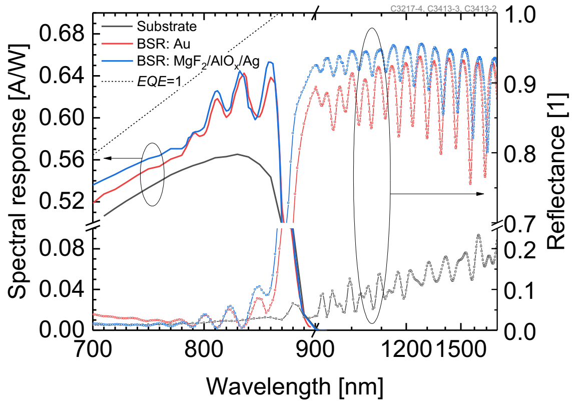


Figure 2.23: Calibrated Spectral Responses at $T = 25°$C and Reflectances of Power Converters with Back-Surface Reflector in comparison with a similar cell on substrate.

Organic solar cells

The research focuses both on better understanding of the factors limiting device performance of organic and perovskite photovoltaics as well as the development of (flexible) cells and modules using materials enabling a cost-effective upscaling. In the reporting period, we have made progress regarding the advanced characterization of charge transfer states at the donor/acceptor interface in bulk-heterojunction organic solar cells (OSC) which play a crucial role in generation and recombination of electrons and holes. The correct determination of their energy is therefore of utmost importance. We have developed an optical model allowing for the calculation of the so-called outcoupling factor. Due to the thin layers, the detected luminescence spectrum can be strongly impacted by the interference pattern. However, when corrected for the wavelength dependent outcoupling, the spectra for devices with e.g. different absorber layer thicknesses do provide reliable information about the real charge transfer (CT) state energy of the specific donor/acceptor combination, see Fig. 2.24. Charge carrier accumulation regions

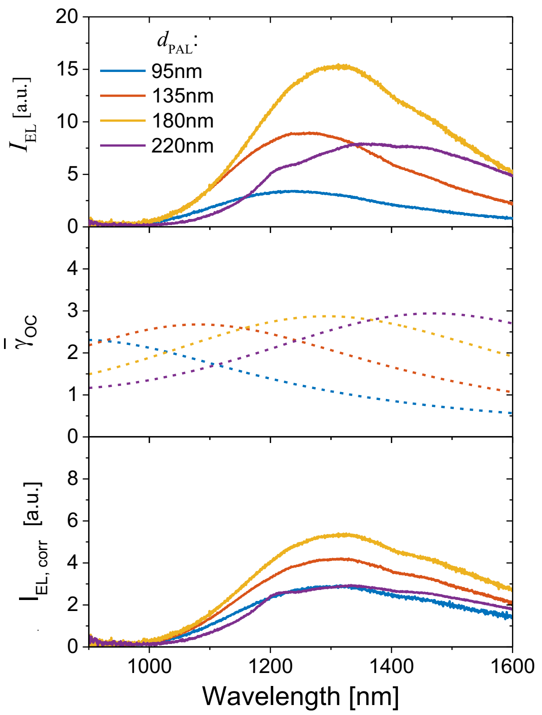


Figure 2.24: EL spectra of P3HT:PC61BM solar cells for different thicknesses dPAL of the photoactive layer for ITO-free devices, the calculated radiant outcoupling factors for the corresponding layer stacks and the spectra for the optical outcoupling.

near the electrodes can have a major impact on the performance of OSC. We carried out two numerical device simulation studies, one on a frequently applied transient measurement technique named TDCF (time-delayed collection field) which is used to probe whether charge carrier generation in OSC is a field-dependent process. We could show that the analysis of experimental TDCF data has shortcomings as it does not account for the strong impact of the above-mentioned accumulation regions, thus underestimating bimolecular recombination. Further, our results proved that the recombination limiting the fill factor in OSC which scales usually linearly with light intensity, is a direct consequence of the large amount of excess dark charge near the contacts. Recently, we improved the record efficiency for OSC with an area of ≥ 1 cm^2 to 15.24%. In this work we provide a detailed optical and electrical loss analysis showing that efficiencies above 18 % would be enabled by the used absorber materials. We further investigated the electro- and photoluminescence (EL and PL) of these record devices and found that the PL intensity does still not allow to derive the internal quasi Fermi level separation in OSC, very much in contrast to all established inorganic PV technologies. Currently, we are setting up a new transient electro-optical measurement with the aim to separate the PL signal of photogenerated excitons from the one of free charge carriers. The preliminary results are very encouraging.

Future Plans

Future activities will focus strongly on the possible separation of the PL signal of photogenerated excitons from the one of free charge carriers in transient electro-optical measurements as preliminary results are very promising. This would help to quantify losses occurring at interfaces between absorber and charge transport layers and generally contribute to a faster and more knowledge-based optimization of OSC. Furthermore, we will target highly efficient large area slot-die coated modules based on alternative Indium-free electrodes developed by our group as well as the development of OSC with high visible transparency.

2.3.7 Nonlinear-Optical Frequency Conversion – Group Kühnemann (Fraunhofer IPM)

Nonlinear-optical frequency conversion is a powerful tool in many areas of optics: Classically, it allows to build (tunable) coherent light sources in wavelength regions without suitable laser materials. Spontaneous parametric downconversion (SPDC), on the other hand, can be used to generate entangled photon pairs which pave the way for novel non-classical measurement schemes. The **research group headed by Frank Kühnemann** works on different implementations of nonlinear-optical frequency conversion, primarily targeting mid-infrared spectroscopy, metrology and trace gas analysis.

Research Report

Nonlinear Interferometers

Nonlinear interferometers rely on the quantum effects observed in the interference phenomena of correlated photons. A typical source of correlated photons is spontaneous parametric down-conversion (SPDC) of pump photons inside a nonlinear-optical crystal. If the pump, signal and idler photons of one SPDC source pass through a second, identical nonlinear crystal, interference can be observed between the two indistinguishable correlated photon sources for both signal and idler photons. Moreover, due to an effect called induced coherence, the visibility and phase of the interference intensity pattern of the signal photons depends on the transmission and phase of all three beams: pump, signal and idler.

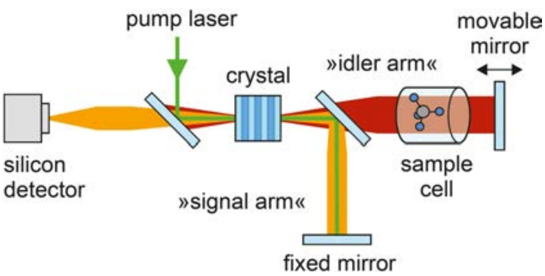


Figure 2.25: The „quantum version" of the Fourier-transform infrared spectrometer. Broadband idler emission between 3.1 and 4.0 μm is achieved by pumping a periodically poled lithium niobate crystal at 785 nm. The idler photons interact with the sample, but the detector records the interferogram generated by the signal photons (wavelength between 975 and 1050 nm). [kue3].

Interferometers using pairs of correlated mid-infrared and near-infrared/visible photons offer interesting measurement concepts for mid-infrared spectroscopy: They allow to "split" the measurement into the interaction of the mid-infrared idler photons with the sample and the recording of the interferogram with the shorter-wavelength signal photons. The use of silicon-based visible or near-infrared detectors promises lower dark noise and higher bandwidth in comparison to infrared detectors, which often require cooling. To retrieve the spectral information, the signal radiation is usually analysed with a grating spectrometer, setting limits for the spectral resolution.
Our group has gone one step further: The potential of the nonlinear Michelson interferometer (see fig. 2.25) is fully exploited by applying the classical concepts of Fourier transform infrared (FTIR) spectroscopy to this quantum optical scheme. As in classical FTIR, the spectral resolution is only limited by the maximum path difference introduced by the mirror movement. We have demonstrated a spectral resolution below 1 cm^{-1} which represents a big step ahead compared to grating-based spectrometers.
With the sample cell in the idler arm of the interferometer, the Fourier transform approach allows high resolution spectroscopy of both, the absorptive and dispersive properties of the sample. We recorded the mid-infrared methane spectrum with resolved ro-vibrational lines and demonstrated a dispersion measurement with an accuracy better than 1 part in 10^{-6} (see fig. 2.26).

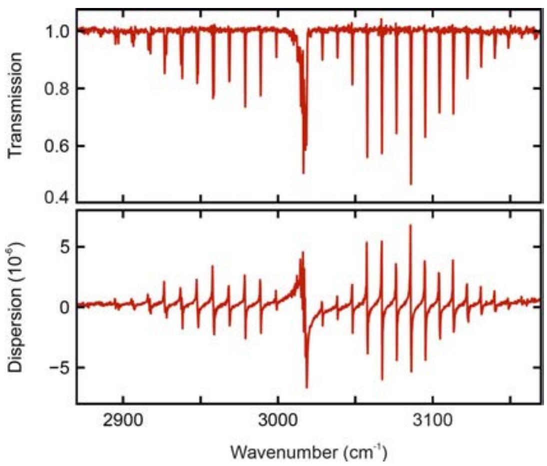


Figure 2.26: Spectrum of the ν_3 band of methane around 3.3 μm, recorded with 1-μm photons. Top: transmission. Bottom: dispersion. [kue3].

Future Plans

Expanding the infrared wavelength range, improving the signal-to-noise ratio and system performance and exploring novel detection schemes will be the next steps in the development of the quantum version of the Fourier-transform infrared spectrometer. Nonlinear interferometers with large spectral separation between signal and idler photons are promising tools for the collection of spectral or image information across different wavelength ranges. As such, they are part of the emerging research field of applied quantum optics. Our group is contributing to the development of this field also by organizing the annual international workshop "Sensing with Quantum Light" together with colleagues from Humboldt University Berlin since 2019.

2.4 Biological Systems

2.4.1 Dynamics in the Life Sciences – Group Timmer

Research Report

Physics has been very successful to quantitatively and predictively describe and understand the inanimate part of nature. The aim of the **Dynamic Processes in the Life Sciences Group of Jens Timmer** is to extend the realm of physics to the animate part of nature, especially cell biology. In cell biology, the gained knowledge is typically presented by so-called *pathway cartoons*, yielding a qualitative, static and descriptive representation. By translating these cartoons into differential equations, the group aims at an quantitative and predictive understanding of the dynamics of the systems. The final goal is to gain understanding by mathematical models that can not be obtained by the plethora of sophisticated experimental techniques and by this pave the way for medical applications. To this aim the group on the one hand develops mathematical methods for modelling and on the other hand, in close collaboration with experimental groups, apply this methods to specific biological and clinical questions.

Development of mathematical methods to model cell biological processes

Typically, the parameters of the systems are not known. Moreover, not all components of the system can be observed and the system exhibits different dynamical time scales. Therefore, the task is to perform parameter estimation in non-linear, partially observed, stiff differential equation based on noisy data. Furthermore, in partially observed differential equation, generically the problem of non-identifiabilities shows up. In the case of *structural* non-identifiabilities this represents a gauge invariance, meaning that changes of one parameter can be completely compensated by changes of one or more other parameters, leading to a manifold in parameter space that results in identical model predictions. In the case of *practical* non-identifiabilities, one typically obtains a unique optimum but confidence intervals based on the profile likelihood are not constrained for small or large values of the parameters. Based on Riemannian geometry, a new method was developed to deal with practical non-identifiabilities [timm1]. Typically, the differences between a healthy and a cancer cell are caused by a few mutations. Mathematically speaking this results in models which are not completely different but only differ in a few parameters which reflect the mutations which typically affecting total concentrations and binding properties of proteins. Thus, the goal is to identify cell-type specific parameters. Therefor, we extended the method of L_1 regularisation to $L_q, 0 < q < 1$ [timm2]. Parameter estimation in non-linear, partially observed, stiff differential equation is numerically challenging due to local optima and premature termination of the optimisation algorithms. Based on the *nudged elastic net* approach, the convergence of the optimisers were improved [timm3]. If not all steps of a reaction cascade can be observed experimentally, a delay is observed between the first and the last observed step, calling for modelling by delay-differential equation. This challenging task can be circumvented by the *linear chain trick*. An open question was who long this chain should be. Based on the profile likelihood, a method was develop to optimally estimate the length based on experimental data [timm4].

Applications

Most of the application were performed in cooperation with Prof. U. Klingmüller, German Cancer Research Center, Heidelberg, and Prof. W. Weber, Faculty of Biology, University Freiburg. The latter collaboration is performed in the frame of Excellence Cluster "Center for Integrative Biological Signalling Systems" (CIBSS). With Prof. Weber, we continued to apply mathematical modelling to optimise optogenetic devices in synthetic biology [timm5]. Additionally, new projects were started to transfer ideas of synthetic biology to design bio-functionalised materials for tasks like signal amplification [timm6] and detection of toxins [timm7]. With Prof. Klingmüller, we continued our long-standing cooperation and analysed the NFκB pathway to quantify the impact of drug-induced liver injury compounds [timm8], resolved the combinatorial complexity of Smad signaling by applying L_1 regularisation [timm9] and analysed interferon signaling [timm10]. To convey a feeling for what modelling can deliver, the last project is described in more detail. Interferon (IFN) is used in the clinics to fight viral infection. It has been observed that a first high dose of IFN lowers the effect of a second dose, while a low first dose enhances the effect of a second dose. To understand this phenomenon, we modelled the JAK/STAT pathway which is the main player in this context including three positive and three negative feedback loops. The pathway cartoon is displayed in fig. 2.27.

It contains 28 species, 60 parameters and 20 observables. Based on 1850 experimental data points, an identifiable model could be established. By analysis of the model, the observed effect could be explained. The expression of the positive and negative feedback mediators react differently to the stimulus. A first low leads to a predominant expression of the positive feedback mediators, while a first high dose to a predominant expression of negative feedback mediators. The model was first developed for a cell line, than adapted for mouse hepatocytes and finally for human hepatocytes. Based on the model, a biomarker for the effectiveness of IFN treatment for individual patients could be identified.

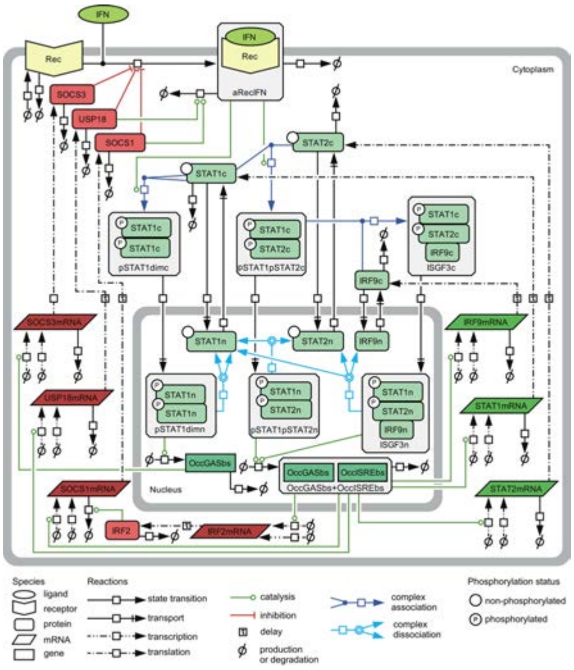


Figure 2.27: Cartoon of the JAK/STAT signalling pathway. The model captures receptor activation and deactivation, the signalling cascade including complex formation, and the induction of positive and negative feedback components.

Future Plans

So far, most projects were focused on intra-cellular signalling. The next step will be to extend this to inter-cellular signalling thereby bridging the scales from the cellular to the tissue level. This is a central goal of the Excellence Cluster CIBSS, and two projects on wound healing with Prof. A. Classen, Faculty for Biology, and early neural differentiation with Prof. W. Driever, Faculty for Biology, have already been initiated.

2.4.2 Bio- and Nano-Photonics – Group Rohrbach (IMTEK)

The **Bio- and Nano-Photonics Group of Alexander Rohrbach** investigates novel techniques for optical microscopy and optical force-based applications, which are used to investigate the physical properties of biological systems based on their nano-mechanics and thermal fluctuations. Advanced optical measurement and manipulation technology developed in our lab enable experiments on the length scale down to a few nanometers and the timescale of a few microseconds. All experiments are supported and compared by mathematical modelling and computer simulations also developed in the group. We are developing laser-based systems for i) particle trapping and tracking, ii) super-resolution microscopy and iii) lightsheet microscopy, which frequently set new benchmarks regarding spatio-temporal resolution and contrast for biological applications. All technologies exploit the highly defined coherent scattering of laser light at single or multiple particles/structures. The systems we investigate and profit from this novel technology can be separated into three classes as well: i) mesoscopic systems, ii) bio-mimetic systems and iii) biological systems.

Research Report

Optical trapping and tracking

We use Fourier-plane interferometric 3D tracking at MHz rates of one or two particles optically, which are trapped or located in maximally focused NIR laser light [rohrb1] [rohrb9] or in time-multiplexed optical tweezers [rohrb2] [rohrb3]. In 2021 we demonstrated that even cell clusters consisting of 10^2 -10^3 cells can be stably rotated in arbitrary directions by applying optical feedback mechanisms for efficient optical trapping by 5-10 point traps. This requires the location of local refractive index changes in the center of cell clusters, which we obtain by the mean photon momentum change from (defocused) scattered laser light [rohrb10] - see Fig. 2.28.

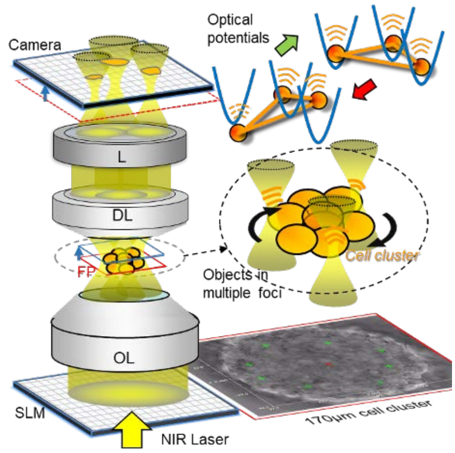


Figure 2.28: Holographic optical tweezers rotate and move large objects non-blindly by a optical feedback mechanism. The light from each laser focus scattered inside inhomogeneous media is analyzed off-focus on a camera through an algorithm. This allows to identify grabbing points of maximized optical forces to apply torques on e.g. cell clusters.

Super-resolution microscopy

Super-resolution microscopy is usually slow in image acquisition, since too many information coding photons have to be collected, thereby restricting imaging applications of dynamic objects. By using a blue collimated laser beam, rotating at typically 100 Hz at highly oblique polar angles around the object (single cell), we recently achieved 150 nm spatial resolution, at 10 ms temporal resolution at unprecedented contrast [rohrb2]. The novel principle of Rotating Coherent Scattering (ROCS) generates interference patterns on the camera, which are spatially incoherent in angular, but spatially coherent in radial direction at high temporal coherence [rohrb5]. ROCS microscopy enables for the first time e.g. realtime imaging and analysis of single viruses binding to cells.

Light-Sheet Microscopy (LSM)

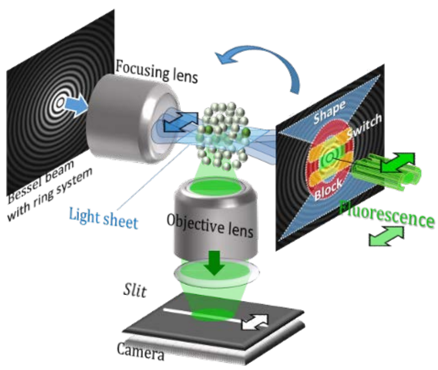


Figure 2.29: The shape-switch-block principle for Light-Sheet microscopy. Holographically shaped fractal Bessel beams switch off fluorophores by stimulated emission by depletion (STED) to achieve increased spatial resolution in combination with photon blocking through a running slit.

LSM) has become the leading technology for imaging 3D objects in the size range of 10^2 - 10^3 μm. Here, the two optical axes for illumination and detection oh that overcomes are oriented in 90○ to each other and allow 3D imaging within unprecedented photon efficiency. In 2010 we introduced Bessel beams (generated by dynamic computer holograms) into the field of LSM, exploiting the self-reconstruction capabilities of such beams [rohrb2]. Our recently presented Shape-Switch-Block principle [rohrb7] increases 3D contrast and resolution by engineering the scanning fluorescence emission distribution through three complementary principles: holographic generation of sectioned Bessel beams to minimize the detection probability far out of focus (blue shade in Fig. 2.29), confocal running slit blocking of fluorescence photons slightly out of focus (red region) and stimulated emission by depletion to switch off central out of focus fluorescent photons (yellow shade in Fig. 2.29).

Future Plans

In the coming years we will concentrate our research even stronger on the superposition and decomposition of different fluctuations modes of particles and cellular structures, i.e. on their short time storage and loss of energy revealing fingerprints about their interactions with the environment. Starting with mesoscopic and biomimetic systems, we will try to identify correlations in motion modes even in biological systems. In particular, we are interested to unravel such concepts for infection diseases, where particulate matter, viruses and bacteria reveal their contact and binding behavior to cell membranes by motions on different temporal and spatial scales.

2.4.3 Computational Neuroscience – Group Rotter (Faculty of Biology)

The **Computational Neuroscience Laboratory of Stefan Rotter** at the Bernstein Center Freiburg comprises a team of theoreticians from mathematics, physics, biology and various engineering sciences. They are interested in the relations between structure, dynamics and function of the neuronal networks of the brain, with a specific focus on the mammalian neocortex.

Research Report

Self-organizing networks and learning

It is a success story of theory-experiment interaction in neuroscience. The idea behind is discussed in every textbook that covers the cellular mechanisms of learning in the brain:

> “When an axon of cell A is near enough to excite a cell B and repeatedly or persistently takes part in firing it, some growth process or metabolic change takes place in one or both cells such that A’s efficiency, as one of the cells firing B, is increased.”

Condensed into a one-liner: “Neurons wire together if they fire together”. This clear-sighted depiction of what may happen in the brain during learning has been formulated by Donald O. Hebb in his book “The Organization of Behavior”, published in 1949. Up to the present day, there have been a great number of experimental reports confirming this general principle. But how exactly are nerve cells doing it? How may a neuron know that its fellow neurons want to associate with it? Which signals are transmitted, and what is the trigger for the “growth process or metabolic change” Hebb conjectures about?

A mechanistic description that clearly delineates cause and effect can only be inferred from experiments in biological neurons. But theory can help designing such experiments. The prevailing interpretation of Hebbian learning assumes that correlation of neuronal activity is the key. This is indeed one possibility how to implement Hebb’s rule: correlation induces growth. And this is how most scientists would conceive associative learning algorithms. But in a biological network, correlation for each and every pair of neurons needs to be measured and represented somewhere. Computer simulations of this setting are straightforward, but it is surprisingly difficult to establish networks that maintain stability while they learn. Something is missing.

We have now described and analyzed a scenario, which corresponds to a more robust implementation of Hebb's rule, also implying less effort [rott12, rott9, rott1]. It is assumed that each neuron takes care of itself by functioning like a thermostat, replacing temperature by activity: If the neuron's activity is too high, the number of its own excitatory synapses is reduced. If the activity is too low, new excitatory synapses are grown. Deletion of contacts and linking new ones into the network is done randomly. The "trick" is to apply the same negative feedback control equally to input and output synapses. This ensures that neurons which are in a similar activity state eventually wire together – without ever assessing their correlations explicitly. In computer simulations, this rule based on homeostatic structural plasticity works extremely well. A number of learning paradigms well-known in psychology, like classical conditioning or associative memory, can be easily implemented in terms of this rule (Fig. 2.30). Experimenters may therefore consider including this possibility in their search for the mechanisms underlying Hebbian plasticity [rott4].

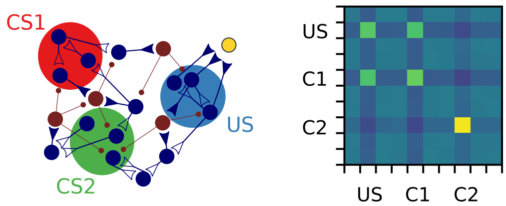


Figure 2.30: Self-organizing networks provide an alternative explanation for learning in biological brains [rott1]. A classical conditioning paradigm (left) leads to the formation of associative memory engrams (right). This kind of dynamic structure formation can be studied theoretically in the context of suitable random graph models.

Interference phenomena in sensory processing

The processing of primary sensory information in brain networks is often based on oscillatory signals, at frequencies imposed by the stimulus. If signals converging from multiple sensors are superimposed, interference phenomena must be expected. We found that such interference may provide an explanation for important phenomena in the auditory and visual systems that are otherwise difficult to understand.

First, we considered orientation selectivity in mammalian vision, which emerges at the interface between thalamus and cortex. Oriented moving gratings are a standard stimulus, frequently used in animal experiments. Such gratings activate the photoreceptors in the retina in an oscillatory fashion. Neurons in the thalamus and in the primary visual cortex receive convergent input from hundreds of photoreceptors. The compound inputs, therefore, are subject to temporal interference. Assuming random sampling of the retina, the amplitude of the resulting oscillation, but not the mean input, carries robust information about the orientation of the stimulus. A nonlinear transformation performed by cortical neurons turns this into a firing rate signal, which shares many properties with biological neurons. This new theory of orientation selectivity is currently being tested for its compatibility with other structural aspects of the early visual system.

Second, we studied spatial hearing in mammals. Azimuth angle is represented by selective responses of certain neurons in the binaural nuclei of the auditory midbrain. Again, interference of oscillatory neuronal inputs coming from sensors in the left and right ear, in combination with nonlinear readouts after processing, provide a consistent explanation for the emergence of spatial tuning in neuronal responses. We will now test the compatibility of this theory with recordings in animals with hearing impairments and implantable hearing aids.

Future Plans

Developing a theory of network self-organization

The self-organization of brain networks has so far mainly been studied in terms of large-scale numerical simulations on high-performance computers. However, recent progress has been made in understanding and quantitatively describing the microscopic processes that underlie network rewiring in biologically relevant scenarios. Appropriate random graph ensembles, in particular the directed configuration model (DCM), may be instrumental for developing a kinetic theory of learning that allows for a more analytic understanding of network growth dynamics and its determinants.

Interference phenomena in recurrent networks

It has been hypothesized in the past that coherent oscillations in different brain areas (hippocampus and neocortex) might also enable cognitive processes, employing rhythms in different frequency ranges. It is not clear, however, how a theory of signal interference can be made compatible with the recurrent architecture of higher-order brain areas. In particular, it needs to be elucidated what is the contribution of graph/network topology to the dynamic signal flow, what is the role of neuronal nonlinearities, and how synaptic plasticity affects the overall operation of such networks.

2.4.4 Medical Physics – Groups Hennig and Bock (Univ. Hospital)

Both the anatomy and the function of organs can be assessed with excellent resolution using novel cross-sectional imaging technologies and advanced image post-processing. In this cross-disciplinary applied research field, Medical Physics is providing new methods at all levels ranging from the development of novel imaging hardware, image acquisition methods to image reconstruction and analysis programs which are often directly applied in a clinical context to improve the detection diseases and the therapy follow-up. In the **Dept. of Radiology - Medical Physics (J. Hennig and M. Bock)** at the University Medical Center Freiburg up to 70 researchers are developing new methods for magnetic resonance imaging (MRI), ultrasound (US) and computed tomography (CT) for applications in basic science and preclinical and clinical studies.

Research Report

In MRI, we develop new hardware such as radio-frequency (RF) and gradient coils (Fig. 2.31), we study new image tracers and their production methods, we implement imaging pulse sequences and describe them theoretically, we program image reconstruction methods (e.g. based on sparse sampling methods), and we provide post-processing algorithms and their implementations to extract clinically relevant parameters from the image data. All these developments help to improve the assessment of patient morphology, function, metabolism, and physiology. Research is carried out at spatial scales ranging from the cellular level (microMR) via tissue samples to small animal pre-clinical imaging and *in vivo* whole body MRI. We have realized methods for applications in basic science, neurology, neuroscience, oncology, as well as to characterize cardiovascular and metabolic diseases. The research is

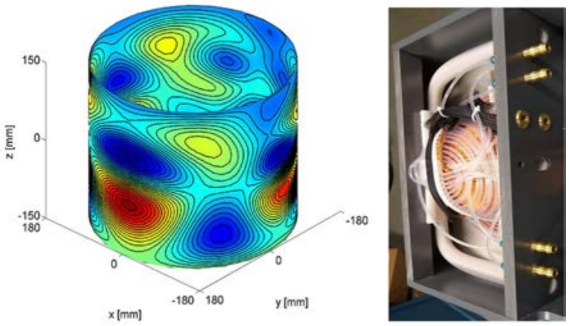


Figure 2.31: Current path layout (left) and gradient coil prototype with cooling system (right) [hennig5].

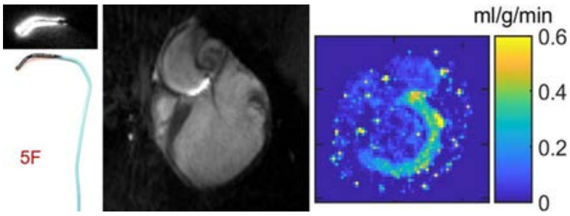


Figure 2.32: Active catheter for myocardial perfusion mapping: the bright MRI signal from an RF coil at the tip of a 5F (1,6 mm) clinical catheter (left) is used to insert the instrument into the coronary artery under MR-guidance (center). After injection of a contrast agent the arterial blood supply (perfusion) in the heart muscle (myocardium) is quantified [bock3].

embedded in a pre-clinical (animal experiments) and clinical environment to translate the results directly into new diagnostic and therapeutic methods.

MRI-guided Interventions

Minimally invasive interventions require image-guidance, which could profit from the excellent soft tissue contrast in MRI. Unfortunately, MR-guided interventions are difficult to perform in closed-bore MRI systems due to the small bore of the MR magnet. To overcome the access limitations we participated in the design of new MRI system hardware with a focus on gradient coil design, and we implemented novel real-time MRI methods with active catheters, which we have used to place stents and measure perfusion in the coronary arteries (Fig. 2.32). To define target regions for interventions, we use artificial intelligence algorithms (convolutional neural networks, CNN) to outline the tumor lesions (Fig. 2.33).

X-nuclear MRI

Metabolic imaging with non-proton X-nuclei can provide tissue functional information such as oxygenation which is important to differentiate lesions in both oncology and cardiology. To assess the

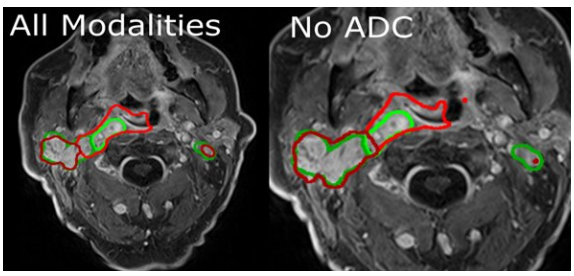


Figure 2.33: AI-based contouring of head&neck tumors with all data (left) and without the diffusion contrast (right) compared to the ground truth (green) [bock4].

rate of oxygen metabolism, we are implementing dynamic ^{17}O-MRI, and we improve the calculation of metabolic rates from the weak MR signal of ^{17}O using pharmaco-kinetic modeling. For oncologic applications we developed ^{13}C hyperpolarization techniques to quantify the metabolism of hyperpolarized pyruvate in tumors using a multi-echo bSSFP pulse sequence that measures pyruvate and its metabolic end product lactate simultaneously. Recently, we started to implement ^{19}F MRI coils and pulse sequences to track fluorine-labeled myeloid cells during their migration into myocardial infarction.

Future Plans

In the future we will combine MRI with new device developments in energy-selective photon counting CT, we will expand our activities in hyperpolarized MRI using fast polarization methods, and we will realize new interventional MRI hard- and software to enable MR-guided percutaneous and intravascular interventions. Research will be carried out in cooperation with members of the Institute of Physics (e.g., Prof. Timmer), clinical partners (e.g., in the SFB 1425) and with industry (e.g., Siemens Healthineers). After the retirement of Prof. Hennig his group will be headed by Prof. Zaisev.

2.5 Important Publications and Conference Talks

Group Bett

Publications

[bett1] M. List, T. Sarkar, P. Perkhun, J. Ackermann, C. Luo, and U. Würfel, "Correct determination of charge transfer state energy from luminescence spectra in organic solar cells", Nat. Comm. **9**, 3631 (2018)
We have developed an optical model allowing for the calculation of the so-called outcoupling factor, thus enabling the correct determination of the luminescence emission spectrum of organic solar cells.

[bett2] U. Würfel and M. Unmüssig, "Apparent Field-Dependence of the Charge Carrier Generation in Organic Solar Cells as a Result of (Bimolecular) Recombination", Sol. RRL **2**, 1800229 (2018)
We use numerical simulation and show that the analysis of experimental TDCF (time-delayed collection field) data has shortcomings as it does not account for the strong impact of the above-mentioned accumulation regions, thus underestimating bimolecular recombination.

[bett3] N. M. Haegel, A. W. Bett *et al.*, "Terawatt-scale photovoltaics: Transform global energy", Science **364**, 836 (2019)
This paper presents the view of an international well-known stakeholder group for the most challenging R&D issues in order to enter in the terawatt scale for photovoltaic manufacturing.

[bett4] U. Würfel, L. Perdigón-Toro, J. Kurpiers, C. M. Wolff, P. Caprioglio, J. J. Rech, J. Zhu, X. Zhan, W. You, S. Shoaee, D. Neher, and M. Stolterfohüt, "Recombination between Photogenerated and Electrode-Induced Charges Dominates the Fill Factor Losses in Optimized Organic Solar Cells", J. Phys. Chem. Lett. **10**, 3473 (2019)
The numerical device simulation study reveals the large impact of charge carrier accumulation regions near the electrodes causing additional bimolecular recombination in time-delayed collection field experiments as well as the fill factor limitation to scale linearly with light intensity.

[bett5] H. Helmers, E. Lopez, O. Höhn, D. Lackner, J. Schön, M. Schauerte, M. Schachtner, F. Dimroth, A. W. Bett, "68,9 % Efficient GaAs-Based Photonic Power Conversion Enabled by Photon Recycling and Optical Resonance", Phys. Status Solidi RRL **15**, 2100113 (2019)
Detailed analysis and experiments including the resonant cavity concept are described to achieve the currently highest efficiency of 68% for photonic power converters.

[bett6] U. Würfel, J. Herterich, M. List, J. Faisst, F. M. Bhuyian, H.-F. Schleiermacher, K. T. Knupfer, ansd B. Zimmermann, "A 1cm2 Organic Solar Cell with 15.2% Certified Efficiency: Detailed Characterization and Identification of Optimization Potential", Sol. RRL **5**, 2000802 (2021)
Report on a world record efficiency for organic solar cells with an aperture area of ≥ 1 cm^2, including a detailed analysis of the optimization potential as well as on the photo- and electroluminescence.

Mandates/Awards

1. Since 2021 Member of the University Council of the University Offenburg

Group Dzubiella

Publications

[dzu1] Xiao Xu, Stefano Angioletti-Uberti, Yan Lu, Joachim Dzubiella, Matthias Ballauff, "Interaction of Proteins with Polyelectrolytes: A comparison between theory and experiment", Langmuir **35**, 5373 (2018)
Feature Article on our studies on polyelectrolyte-protein interactions, comparing theory and experiments, rationalizing the dominant mechanisms behind electrostatic complexation in highly charged (aqueous) biomolecular systems.

[dzu2] Stefano Angioletti-Uberti, Matthias Ballauff, and Joachim Dzubiella, "Competitive adsorption of multiple proteins to nanoparticles: The Vroman effect revisited", Mol. Phys. **116**, 3154 (2018)
Showing the first time the complexity and a variety of possible mechanisms behind the time-dependent formation of protein shells around a nanoparticle, i.e., the structure and dynamics of a nanoparticle protein corona.

[dzu3] Matej Kanduc, Won Kyu Kim, Rafael Roa, and Joachim Dzubiella, "Aqueous Nanoclusters Govern Ion Partitioning in Dense Polymer Membranes", ACS Nano **13**, 11224 (2019)
All-atom computer simulations reveal the complex and unexpected behavior of how salt ions distribute in polymer membranes of high dielectric heterogeneity.

[dzu4] Nicolas Dubouis, Chanbum Park, Michael Deschamps, Soufiane Abdelghani-Idrissi, Matej Kanduc, Annie Colin, Mathieu Salanne, Joachim Dzubiella, Alexis Grimaud, and Benjamin Rotenberg, "Chasing Aqueous Biphasic Systems from simple salts by exploring the LiTFSI/LiCl/H2O phase diagram", ACS Central Science **5**, 640 (2019)
Experiments and all-atom simulations uncover and rationalize the existence of an aqueous biphasic system in a mixture of simple but battery-application-relevant salts in water.

[dzu5] Chanbum Park, Arne Ronneburg, Sebastian Risse, Matthias Ballauff, Matej Kanduc, and Joachim Dzubiella, "Structural and transport properties of Li/S battery electrolytes: role of the polysulfide species", J. Phys. Chem. C **123**, 10167 (2019)
Development of the first force-field for next-generation Li/S battery electrolytes and polysulfides as well as rationalizing of how salts tune polysulfide clustering effects which are unwanted in applications.

[dzu6] Won Kyu Kim, Rafael Roa, Matej Kanduc, and Joachim Dzubiella, "Tuning the permeability of dense membranes by shaping nanoscale potentials", Phys. Rev. Lett. **122**, 108001 (2019)
Coarse-grained simulations reveal how topology and interactions in a membrane delicately control (by massive cancellations between molecular partitioning and mobility) its permeability for molecular transport.

[dzu7] Arturo Moncho-Jorda and Joachim Dzubiella, "Controlling the microstructure and phase behavior of confined soft colloids by active interaction switching", Phys. Rev. Lett. **125**, 078001 (2020)
New phenomenon of non-motile active colloids reported: active interaction switching controls microclustering.

[dzu8] Sam W. Coles, Chanbum Park, Rohit Nikam, Matej Kanduc, Joachim Dzubiella, and Benjamin Rotenberg, "Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations", J. Phys. Chem. B **124**, 1778 (2020)
Large-scale all-atom simulations on solvated, very dense electrolytes reveal correlation length behavior according to theoretical predictions, not experimental conjectures, contributing significantly to a controversial discussion in a hot topic.

[dzu9] Matej Kanduc, Won Kyu Kim, Rafael Roa, and Joachim Dzubiella, "How the shape and chemistry of molecular penetrants control the permeability of responsive hydrogels", ACS Nano **14**, 614 (2021)
All-atom computer simulations reveal the microscopic mechanisms of chemically-specific molecular transport through responsive polymer membranes.

[dzu10] Zhujie Li, Matej Kanduc, Victor Ruiz, and Joachim Dzubiella, "Highly Heterogeneous Polarization and Hydration of Gold Nanoparticles in Aqueous Electrolytes", ACS Nano **15**, 3155 (2021)
Polarizable all-atom computer simulations and electrostatic theory reveal and rationalize the complex heterogeneities of ionic and aqueous solvation of catalytically active, facetted metal nanoparticles.

Conference Talks

1. M. Kanduc, *Transport and solvation of penetrant molecules in a thermoresponsive hydrogel*, at the APS Spring Meeting in Los Angeles, USA, 03/2018.

2. M. Kanduc, *Molecular simulations of applied electrolytes in battery systems : structural and transport behavior*, Invited Talk (Dzubiella, transferred) at "Electrostatics in Concentrated Electrolytes", CECAM Workshop, Lausanne, Switzerland, 04/2018.

3. K. Palczynski, *Coarse Grained Simulations of Polycarbonate: Glass Transition and Material Properties*, Invited Talk (Dzubiella, transferred) at the Covestro (Industry) Workshop: "Modelling Polymers: From Methods to Applications", Leverkusen, 09/2019.
4. J. Dzubiella, *Multiscale Modeling of Nanoreactors*, Invited Talk at the Physical Chemistry Colloquium of the University of Münster, 01/2019.
5. J. Dzubiella, *Binding kinetics in diffusion-influenced bi(o)molecular reactions*, Invited Talk at the Bio/Math Seminar, Institute for Applied Math, UC San Diego, USA, 03/2019.
6. J. Dzubiella, *Statistical mechanics of responsive colloids*, Invited Lecture Series at the University Granada (Erasmus+ Program), Spain, 02/2020.
7. J. Dzubiella, *Competitive sorption of mono- versus divalent ions by highly charged globular macromolecules*, Invited Talk at the Polyelectrolyte workshop "New Challenges in Polyelectrolyte Science", Paris, France, 08/2021.
8. J. Dzubiella, *On the permeability of dense polymer membranes*, Invited Talk at the 84th Annual DPG meeting, Berlin, 09/2021
9. J. Dzubiella, *How the Shape and Chemistry of Molecular Penetrants Control Responsive Hydrogel Permeability*, Invited Talk at the Colloquium of the Institute of Computational Physics (ICP) Stuttgart, 05/2021.

Mandates/Awards

1. 2015-2020: ERC Consolidator Grant (Transferred to Freiburg in 04/2018)
2. Since 10/2017: Advisory Board German Colloid Society
3. Since 04/2018: Head of Organizational Unit CE-GSEM "Simulation of Energy Materials" at Helmholtz-Zentrum Berlin
4. Since 2019: Advisory Board for the NEMO High-Performance Computing Cluster in Freiburg

Group Elsässer

Publications

[elsae1] O. Guillon, C. Elsässer, O. Gutfleisch, J. Janek, S. Korte-Kerzel, D. Raabe, and C. A. Volkert, Manipulation of matter by electric and magnetic fields: Toward novel synthesis and processing routes of inorganic materials, Materials Today 21, 527-536 (2018).
The topic of this review is how electric or magnetic fields can be used on top of conventional processing routes to manufacture materials with better structural or functional properties. The paper describes the scientific fundament of the DFG priority programme 1959 "FieldsMatter". http://www.fieldsmatter.de

[elsae2] J. J. Möller, W. Körner, G. Krugel, D. F. Urban, and C. Elsässer, Compositional optimization of hard-magnetic phases with machine-learning models, Acta Materialia 153, 53-61 (2018).
This paper describes a combination of first-principles high-throughput-screening calculations with machine learning to search for intermetallic multi-component phases with good hard-magnetic key properties.

[elsae3] D. Mutter, D. F. Urban, and C. Elsässer, Computational analysis of composition-structure-property relationships in NZP-type materials for Li-ion batteries, J. Appl. Phys. 125, 215115 (2019).
This paper investigates atomic-scale relationships which are essential for very fast Li-ion conductor compounds which can be used as electrolytes in all-solid-state Li-Ion-battery cells.

[elsae4] F. Lechermann, W. Körner, D. F. Urban, and C. Elsässer, Interplay of charge-transfer and Mott-Hubbard physics approached by an efficient combination of self-interaction correction and dynamical mean-field theory, Phys. Rev. B 100, 115125 (2019).
This work combines two approaches to calculate and analyse properties of transition-metal-oxide compounds with strongly correlated electrons, like pure and Li-doped NiO.

[elsae5] F. Colonna, S. Kühnhold-Pospischil, and C. Elsässer, A density functional theory study on the passivation mechanisms of hydrogenated Si/Al2O3 interfaces, J. Appl. Phys. 127, 035301 (2020).
This work investigates and discusses atomic-scale mechanisms on how interfacial defects causing recombination of electron-hole pairs in solar cells are acting and how they can be passivated.

[elsae6] W. Körner, D. F. Urban, and C. Elsässer, Influence of extended defects on the formation energy, the hyperfine structure, and the zero-field splitting of NV centers in diamond, Phys. Rev. B 103, 085305 (2021).
This work studies how electronic two-level systems of nitrogen-vacancy defect complexes in diamond, which are promising as sensors for quantum magnetometry or as qubits for quantum computing, are affected by nearby extended defects like stacking or twinning faults.

[elsae7] D. F. Urban, O. Ambacher, and C. Elsässer, First-principles calculation of electroacoustic properties of wurtzite (Al,Sc)N, Phys. Rev. B 103, 115204 (2021).
The semiconducting alloy (Sc,Al)N is of high interest in information technology because of its excellent piezo-electric properties. The dependence of the structural parameters and all the components of the elasticity and piezo-electricity tensors on the stoichiometric ratio and compositional arrangement of Al and Sc is calculated from first principles.

[elsae8] J. Gebhardt, W. Wei, and C. Elsässer, Efficient modelling workflow for accurate electronic structures of hybrid perovskites, J. Phys. Chem. C 125, 18597-18603 (2021).
This work describes a computational density-functional-theory workflow to screen hybrid organic-inorganic halide perovskites, whether they have suitable electronic band structures for photovoltaic absorbers.

[elsae9] D. Mutter, R. Schierholz, D. F. Urban, S. A. Heuer, T. Ohlerth, H. Kungl, C. Elsässer, and R.-A. Eichel, Defects and phase formation in non-stoichiometric LaFeO3: a combined theoretical and experimental study, Chem. Mater. 33, 9473-9485 (2021).
The perovskite LaFeO3 is a prototype material for electrodes of high-temperature solid-oxide fuel cells and electrolyzers for hydrogen. Its thermodynamic phase stability and the formation and electronic structure of its atomic defects are studied by density functional theory and experimental materials synthesis and electron microsopy.

[elsae10] T. Michler, C. Elsässer, K. Wackermann, and F. Schweizer, Effect of hydrogen in mixed gases on the mechanical properties of steels – theoretical background and review of test results, MDPI Metals 11, 1847 (2021).
This paper discusses how the effects of pure hydrogen or mixed gases on the mechanical properties of steels (for transport pipes or storage vessels) can measured and analyzed.

Conference Talks

1. C. Elsässer, W. Körner, G. Krugel, J. J. Möller, A. Lehner, and D. F. Urban, “Search for substitutes of hard-magnetic materials containing less critical elements by computational high-throughput screening”, invited lecture, International Workshop on “Future perspectives of novel magnetic materials”, Santorini, Greece, May 2018.

2. W. Körner, D. F. Urban, C. Elsässer, Screening of rare-earth-lean intermetallic 1-11-X, 1-12-X, and 1-13-X compounds for hard-magnetic applications, invited lecture, International Symposium ISAM4-2019, Erlangen, Germany, August 2019.

3. C. Elsässer, W. Körner, D. F. Urban, Screening of rare-earth-lean intermetallic 1-11-X, 1-12-X, and 1-13-X compounds for hard-magnetic applications, invited symposium lecture, International Conference MRM 2019, Yokohama, Japan, December 2019.

4. C. Elsässer, “Materials in contact with hydrogen”, invited online lecture, DVM Conference “Materials Testing”, Berlin, Germany, December 2020.

5. C. Elsässer, “Materials in contact with hydrogen”, special keynote lecture “Hydrogen technologies”, EFDS Conference V2021, Dresden, Germany, October 2021.

6. C. Elsässer, W. Körner, D. F. Urban, Screening of rare-earth-lean intermetallic 1-11-X, 1-12-X, and 1-13-X compounds for hard-magnetic applications, Sanvito-Group Online-Seminar, Trinity College, Dublin, Ireland, October 2021.

Group Kühnemann

Publications

[kue1] Ch. Lindner, S. Wolf, J. Kießling, F. Kühnemann. "Fourier transform infrared spectroscopy with visible light" Optics Express **28** (2020) 4426.

Nonlinear interferometers based on spontaneous parametric downconversion far away from degeneracy allow to perform mid-infrared spectroscopy using silicon detectors. Here we use a Michelson interferometer and demonstrated the Fourier-transform-spectrometer approach to retrieve the spectral information for the first time.

[kue2] Ch. Lindner, S. Wolf, J. Kießling, F. Kühnemann. "Nonlinear interferometers for broadband mid-infrared spectroscopy" Proceedings Volume 11264, Nonlinear Frequency Generation and Conversion: Materials and Devices XIX; 112641D (2020)

We present a nonlinear interferometer for mid-infared spectroscopy. Non-collinear phasematching is used for a broad spectral coverage. The resulting interference conditions are simulated and experimentally analysed to derive design criteria for the spectrometer

[kue3] Ch. Lindner, J. Kunz, S.J. Herr, J. Kießling, S. Wolf, F. Kühnemann. "Nonlinear interferometer for Fourier-transform mid-infrared gas spectroscopy using near-infrared detection", Optics Express **29** (2021) 4035.

The spectral resolution of the Fourier transform nonlinear interferometer is substantially improved to better than 1 cm^{-1}. The methane spectrum around 3000 cm^{-1} is recorded with spectrally resolved rovibrational lines. Dispersion effects in the interferometer require a special solution for the apodization of the spectra..

[kue4] Ch. Lindner, J. Kunz, S.J. Herr, J. Kießling, S. Wolf, F. Kühnemann. "Nonlinear interferometers for Fourier-transform infrared spectroscopy with visible light", Proceedings Volume 11670, Nonlinear Frequency Generation and Conversion: Materials and Devices XX; 1167010 (2021)

Utilizing SPDC with collinear phasematching allows to record interferograms with a single-pixel detector instead of a camera.

[kue5] L. Nitzsche, J. Goldschmidt, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein. "Tunable dual-comb spectrometer for mid-infrared trace gas analysis from 3 to 4.7 μm". Optics Express **29** (2021) 25449.

A mid-infrared trace gas analyzer is presented based on a near-infrared dual-comb system and a widely tunable difference-frequency converter. This allows the coverage of the region between 3 and 4.7 μ m. The EOM-based dual-comb system allows a variation of the line spacing and line number. Spectrometer performance is analyzed in detail for the different operation conditions low allow sensitive trace gas detection.

[kue6] L. Nitzsche, J. Goldschmidt, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein. "A dual-comb spectrometer for trace gas analysis in the mid-infrared ". Proceedings Volume 11670, Nonlinear Frequency Generation and Conversion: Materials and Devices XX; SPIE. paper 1167005 (2021)

Using the EOM based spectrometer and a 7.2-m long-path cell, simultaneous detection of N2O and CO2 is demonstrated.

[kue7] N. Arndt, C. Bolwien, G. Sulz, F. Kühnemann, A. Lambrecht. "Diamond-Coated Silicon ATR Elements for Process Analytics". Sensors **21**, 6442 (2021)

Infrared attenuated total reflection (ATR) spectroscopy is a common laboratory technique for liquids or solid samples. Application in process industr, hoever, requires very robust crystals. The paper presents the use of thin diamond coatings on top of silicon crystals. The impact of the coating properties on signal generation and detection limits is studied in simulation and experiment.

[kue8] V. Vierhub-Lorenz, K. Predehl, S. Wolf, Ch.S. Werner, F. Kühnemann, A. Reiterer. "A multispectral tunnel inspection system for simultaneous moisture and shape detection." Remote Sensing Technologies and Applications in Urban Environments IV. Proc. of SPIE Vol. 11157, paper 111570T (2019).

Laser scanners are an established technique for 3D mapping to collect data for building information modelling (BIM). Using a setup with two near-infrared lasers, moisture detection on surfaces is added as an additional data channel. Up to 2 million data points are collected per second containing distance, intensity and moisture information. This is particularly important for tunnel inspection.

Conference Talks

1. Ch. Lindner, J. Kunz, S.J. Herr, J. Kießling, S. Wolf, F. Kühnemann; "Quantum Fourier-Transform Infrared Spectroscopy". 754 WE Heraeus Seminar "Sensing with Quantum Light", Physikzentrum Bad Honnef; 2021

2. L. Nitzsche, J. Goldschmidt, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein; "Real-Time Data Processing for an Electro-Optic Dual-Comb Spectrometer". Optics and Photonics for Sensing the Environment (OSA); 2021 paper JTu2E.2.

3. J. Goldschmidt, L. Nitzsche, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein; "A Mid-Infrared Dual Comb Spectrometer for the Determination of Stable Isotope Ratios of Carbon Dioxide". Optics and Photonics for Sensing the Environment (OSA); 2021, paper JTu4D.2.

4. Ch. Lindner, J. Kunz, S.J. Herr, J. Kießling, S. Wolf, F. Kühnemann; "Fourier-Transform Infrared Spectroscopy with Near-Infrared Light". Fourier Transform Spectroscopy (OSA), 2021, paper FM2F.4.

5. L. Nitzsche, J. Goldschmidt, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein; "Mid-Infrared Dual-Comb Spectroscopy as sensor: Fast and precise quantification of multiple gases". Sensor and Measurement Science International. (AMA) paper C3.1 (Best paper Award) (2021)

6. L. Nitzsche, J. Goldschmidt, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein;"A Mid-Infrared Dual-Comb Spectrometer for High Sensitivity Multi-Component Trace Gas Detection". Frontiers in Optics (OSA); 2020, paper FW7B.2.

7. S. Wolf, T. Trendle, N. Catalan, J. Kießling, J. Wöllenstein, F. Kühnemann; "Photothermal Common-Path Interferometry for Trace Gas Detection". Laser Applications to Chemical, Security and Environmental Analysis. LACSEA, OSA, 2020, paper LTu3C.3

8. L. Nitzsche, J. Kießling, S. Wolf, F. Kühnemann, J. Wöllenstein; "Ultra-fast gas spectroscopy with a dual-comb spectrometer". Sensor and Measurement Science International (SMSI) 2020-Sensors and Instrumentation (AMA); 2020. paper B4.4

9. Ch. Lindner, S. Wolf, J. Kießling, F. Kühnemann; "Characterization of broadband spontaneous parametric down-conversion in periodically poled materials". The European Conference on Lasers and Electro-Optics (OSA), 2019, paper cd-p-52.

10. S. Wolf, P. Reiser, J. Kießling, F. Kühnemann; "Dynamic Range of an Upconversion Detection Module for MWIR Laser Spectroscopy". The European Conference on Lasers and Electro-Optics (OSA), 2019. paper cd-10-4.

Group Moseler

Publications

[mos1] D. Savio, K. Falk, M. Moseler, "Slipping domains in water-lubricated microsystems for improved load support", Tribo. Int. **120** (2018) 269.
We discuss the use of slipping domains to improve load support in water-lubricated microsystems through a multi-scale approach involving a continuum fluid formulation for a line contact with added slip and classical molecular dynamics estimates of the slip length of water in contact with various surfaces.

[mos2] T. Reichenbach, K. Mondal, M. Jäger, T. Vent-Schmid, D. Himmel, V. Dybbert, A. Bruix, I. Krossing, M. Walter, M. Moseler, "Ab-initio study of CO_2 hydrogenation mechanisms on inverse ZnO/Cu catalysts", J. Catal. **360** (2018) 168.
The different reaction mechanisms of methanol synthesis from CO_2 and H_2 on Cu-supported ZnO catalysts are studied using density functional theory. In contrast to other Cu-supported oxides, the reaction pathway proceeds via the formation of the formate intermediate.

[mos3] G. Moras, A. Klemenz, T. Reichenbach, A. Gola, H. Uetsuka, M. Moseler, L. Pastewka, "Shear-melting of silicon and diamond and the disappearance of the polyamorphic transition under shear", Phys. Rev. Materials **2** (2018) 083601.

Reactive molecular dynamics simulations show the mechanically induced formation of amorphous solids at silicon and diamond sliding interfaces. As a result of different signs of the volume change upon amorphization, pressure enhances amorphization in silicon and suppresses it in diamond.

[mos4] T. Kuwahara, P. A. Romero, S. Makowski, V. Weihnacht, G. Moras, M. Moseler, "Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C", Nature Communications **10** (2019) 151.

We unveil a universal tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs. Atomistic simulations show that unsaturated fatty acids concurrently chemisorb on both surfaces. Sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions releasing passivating groups.

[mos5] T. Reichenbach, M. Walter, M. Moseler, B. Hammer, A. Bruix, "Effects of gas-phase conditions and particle size on the properties of Cu(111)-supported Zn_yO_x particles revealed by global optimisation and ab initio thermodynamics", J. Phys. Chem. C **123** (2019) 30903.

By combining ab initio thermodyanmics with global optimization we find the stable structures of Zn_yO_x nanoparticles on a Cu support under different reaction conditions including catalytic methanol synthesis conditions.

[mos6] T. Reichenbach, L. Mayrhofer, T. Kuwahara, M. Moseler, G. Moras, "Steric effects control dry friction of H- and F-terminated carbon surfaces", ACS Appl. Mater. Interfaces **12** (2020) 8805.

We develop structure-property relationship between surface chemical passivation and friction for H- and F-terminated hard carbon coatings. Our simulation show that the friction of these systems is almost exclusively determined by steric factors.

[mos7] K. Falk, D. Savio, M. Moseler, "Nonempirical free volume viscosity model for alkane lubricants under severe pressures", Phys. Rev. Lett. **124** (2021) 105501.

Viscosities and diffusion coefficients of linear and branched alkanes at pressure < 0.7 GPa and temperature T $\sim$ 500–600 K are calculated from molecular dynamics simulations. Combining Stokes-Einstein, free volume, and random walk concepts results in an accurate viscosity model for the considered P and T.

[mos8] V. R. Salinas Ruiz, T. Kuwahara, J. Galipaud, K. Masenelli-Varlot, M. B. Hassine, C. Héau, M. Stoll, L. Mayrhofer, G. Moras, J. M. Martin, M. Moseler, M.-I. de Barros Bouchet, "Interplay of mechanics and chemistry governs wear of diamond-like carbon coatings interacting with ZDDP-additivated lubricants", Nature Communications **12** (2021) 4550.

Contact-mechanics and quantum-chemical simulations reveal that shear combined with high local contact pressures favour ZDDP fragmentation and the release of sulphur into hard carbon coatings resulting in a decrease of yield stress and wear of the coating.

[mos9] S. von Goeldel, T. Reichenbach, F. König, L. Mayrhofer, G. Moras, G. Jacobs, M. Moseler, "A combined experimental and atomistic investigation of PTFE double transfer film formation and lubrication in rolling point contacts", Tribo. Lett. **69** (2021) 136.

High wear losses of the solid lubricant PTFE impede its applicability in highly loaded rolling point contact. Our combined experimental and theoretical results show that an effective lubrication can be achieved by a constant external resupply of PTFE using the double transfer mechanism.

[mos10] T. Reichenbach, G. Moras, L. Pastewka, M. Moseler, "Solid-phase silicon homoepitaxy via shear-induced amorphization and recrystallization", Phys. Rev. Lett. **127** (2021) 126101.

Reactive molecular dynamics simulations reveal shear-driven amorphization and recrystallization processes at silicon sliding interfaces. Based on their interplay, we propose a novel method to mechanically grow epitaxial silicon nanostructures.

Conference Talks

1. M. Moseler, Friction regimes of water-lubricated diamond surfaces, ACS National Meeting, New Orleans, USA, March 2018.

2. T. Reichenbach, Polar hydrophobicity of fluorinated carbon materials, EMRS Spring Meeting 2018, Strasbourg, France, June 2018.

3. M. Moseler, On the lubrication of hard carbon surfaces: emergence of aromaticity and superlow friction, Beilstein Symposium Molecular Mechanisms in Tribology, Potsdam, Germany, October 2018.

4. M. Moseler, On the in-situ formation of superlubricious layers during boundary lubrication of diamond-like carbon and diamond, Multiscale Materials Modeling 2018, Osaka, Japan, October 2018.

5. M. Moseler, Superlubricity with carbon coatings lubricated by organic friction modifiers, International Conference on Metallurgical Coatings and Thin Films, San Diego, USA, Mai 2019.

6. M. Moseler, Shear driven amorphisation and recrystallization of silicon and diamond, Tribochemistry 2019, Hakodate, Japan, September 2019.

7. M. Moseler, Friction on H- and F-terminated diamond, International Tribology Conference 2019, Sendai, Japan, September 2019.

8. M. Moseler, Mechanochemical friction of supported graphene, CECAM Workshop Molecular Mechanisms of Tribochemistry and Lubrication, Lausanne, Switzerland, January 2020.

9. M. Moseler, Digital twin or digital cartoon: can we master chemical complexity in applied tribology?, CECAM Flagship workshop Constructing Digital Twins in Tribology, Online, October 2021.

10. T. Reichenbach, A combined experimental and atomistic investigation of PTFE double transfer film formation and lubrication in rolling point contacts, European Symposium on Friction, Wear and Wear Protection, Online, November 2021.

Group Reiter

Publications

[reit1] Y. AlShetwi, B. Bessif, M. Sommer, G. Reiter, "Illumination of conjugated polymers reduces nucleation probability and slows down crystal growth rate", Macromolecules **54** (2021) 11478–11485.
Nucleation density and crystal growth rate during crystallization of conjugated polymers are decreased upon illumination with white light. Photon absorption by the polymer is suggested as a possible explanation, leading to chain stiffening, which causes a decrease in the diffusivity of the polymer.

[reit2] W. Chen, B. Bessif, R. Reiter, J. Xu, G. Reiter, "Controlled switching from the growth of mono-lamellar polymer crystals to the formation of stacks of uniquely oriented lamellae", Macromolecules **54** (2021) 8135–8142.
Using a rationally designed two-step crystallization process, we were able to form stacks of lamellar crystals whose morphology can be described as a "pseudo-hollow crystal"

[reit3] Y. AlShetwi, D. Schiefer, M. Sommer, G. Reiter, "Continuous illumination of a conjugated polymer causes strong enhancement of photoluminescence", J. Phys. Chem. B **125** (2021) 5636–5644.
A strong enhancement in the photoluminescence of a conjugated polymer was observed under continuous illumination. It was hypothesized that changes in polymer interactions due to excited electronic states could lead to slow changes in polymer conformations.

[reit4] Z. Guo, S. Yan, G. Reiter, "Formation of stacked three-dimensional polymer 'Single Crystals'", Macromolecules **54** (2021) 4918–4925.
Using the mechanism of self-induced nucleation for isotactic polystyrene, we were able to form 3D single crystals with heights of several micrometers, consisting of hundreds of superposed uniquely oriented lamellar crystals. The presented growth mechanisms can be observed for all crystallizable polymers including block copolymers with a non-crystallizable block.

[reit5] K. Roumpos, S. Fontaine, T. Pfohl, O. Prucker, J. Rühe, G. Reiter, "Measurements of periodically perturbed dewetting force fields and their consequences on the symmetry of the resulting patterns", Scientific Reports **11** (2021) 13149.
The origin of breaking the symmetry for moving circular contact lines of dewetting polymer films suspended on a periodic array of pillars was studied. Elastic restoring forces of deformed pillars locally balance driving capillary forces and broke the circular symmetry of expanding dewetting holes. For the presented system, we succeeded in squaring the circle.

[reit6] A. Das, S. Noack, H. Schlaad, G. Reiter, R Reiter, "Exploring pathways to equilibrate Langmuir polymer films", Langmuir **36** (2020) 8184–8192.
We show that it is practically impossible to obtain fully equilibrated coexisting phases in a Langmuir polymer film, neither under conditions of extremely slow continuous compression nor when allowing for re-organization during long waiting times in the coexistence region.

[reit7] F. Ramezani, J. Baschnagel, G Reiter, "Translating molecular relaxations in non-equilibrated polymer melts into lifting macroscopic loads", Phys. Rev. Materials **4** (2020) 082601.
In creep tests, filaments from films of non-equilibrated polymers show contraction and thereby lifted loads up to a thousand times the weight of the filament over a distance of almost up to 40% of its original length. The molecular origin of such large macroscopic manifestations of deviations from equilibrium in terms of reduced conformational entropy is discussed.

[reit8] S. Chandran, G. Reiter, "Segmental rearrangements relax stresses in non-equilibrated polymer films", ACS Macro Letters **8** (2019) 646.
For preparation-induced residual stresses in polymer films, fast relaxations at temperatures close to or below the glass transition were observed, while at elevated temperatures relaxation times were orders of magnitude longer than the equilibrium "reptation time". These long relaxation times suggest that residual stresses, a consequence of non-equilibrium conformations inherited from preparation, relax via concerted rearrangements of many segments.

[reit9] S. Chandran, J. Baschnagel, D. Cangialosi, K. Fukao, E. Glynos, L. M. C. Janssen, M. Müller, M. Muthukumar, U. Steiner, J. Xu, S. Napolitano, G. Reiter, "Processing pathways decide polymer properties at the molecular level", Macromolecules **52** (2019) 7146–7156.
We emphasize that the search for order parameters, such as topological correlations and heterogeneities, that allow characterizing the processing-induced behavior of polymers requires concerted efforts of theory, simulations, and experiments and provides a deep understanding that can lead to predictable and tunable properties of polymers.

[reit10] M. Kaiser, F. Jug, T. Julou, S. Deshpande, T. Pfohl, O. K. Silander, G. Myers, E. van Nimwegen, "Monitoring single-cell gene regulation under dynamically controllable conditions with integrated microfluidics and software", Nature Communications **9** (2018) 212.
We present here a novel integrated system consisting of a microfluidic chip and associated analysis software that enables long-term quantitative tracking of growth and gene expression in single cells. This chip allows controlled and continuous variation of external conditions and thus direct observation of gene regulatory responses to changing conditions in single cells.

Conference Talks

1. T. Pfohl, Adaptive droplet transport through coupled flow paths, DFG SPP 2171 Workshop, Freiburg, November 2021.
2. B. Bessif, Crystallization of precision polythioethers, Consortium Meeting of the ITN "Photo-Emulsion", Maribor, September 2021.
3. G. Reiter, Entropy in stock in non-equilibrated polymer melts, Macromolecular Colloquium, Freiburg, February 2020.
4. G. Reiter, A nucleation mechanism leading to stacking of correlated lamellar crystals, International Discussion Meeting on Polymer Crystallization, San Sebastian, Spain, October 2019.
5. K. Roumpos, Pattern formation in polymer thin films induced by dewetting and surface forces, Consortium Meeting of ITN "PlaMatSu", Cambridge, September 2019.

6. G. Reiter, Out-of-equilibrium properties of polymers, European Polymer Congress, Heraklion, Greece, June 2019.
7. T. Pfohl, Dynamics of cells in confinement and microflow: From drug testing of unicellular parasites to surface sensing of bacteria, VAAM Conference, Mainz, March 2019.
8. G. Reiter, Time matters - predicting the non-equilibrium behavior of polymer films, Laboratoire Polymàres et Matériaux Avancés - CNRS/Solvay, Lyon, France, November 2018.
9. T. Pfohl, Straightforward microfluidic tools for biology and biophysics, Workshop on "NanoBio Surfaces and Interfaces in Healthcare and Science ", Lausanne, May 2018.
10. T. Pfohl, Microfluidics of cells - from surface sensing of bacteria to drug testing of unicellular parasites, IS2M annual meetings – Microfluidics in Upper Rhine Valley, Mulhouse 2018.

Mandates/Awards

1. 2020: Fellow of the American Physical Society (APS) for "For discoveries of dewetting of thin films driven by residual stresses, cloning of polymer crystals, and control of polymer properties using tunable processing pathways."
2. – 2019: Speaker of the International Research and Training Group (IRTG) Soft Matter Science.
3. – 2019: Member of the Board of Directors of the FMF (Freiburg Materials Research Center).
4. – 2018: Member of the Board of Directors of the FIT (Freiburg Center for Interactive Materials and Bioinspired Technologies).

Group Schilling

Publications

[schill1] H. Meyer, Th. Voigtmann, T. Schilling, "On the dynamics of reaction coordinates in classical, time-dependent, many-body processes", The Journal of Chemical Physics **150**, 174118 (2019)
Using a time-dependent projection operator formalism, we derived an exact coarse-grained evolution equation for systems out of thermal equilibrium and under time-dependent driving, the non-stationary linear Generalized Langevin equation.

[schill2] Fabian Glatzel, Tanja Schilling, "The Interplay between Memory and Potentials of Mean Force: A Discussion on the Structure of Equations of Motion for Coarse Grained Observables", Europhysics Letters, accepted manuscript (2021)
We showed that the frequently used non-linear generalized Langevin equation with a linear memory term and a noise that obeys the 2nd fluctuation-dissipation theorem is neither correct nor a well-controlled approximation. We derived the exact non-stationary, non-linear generalized Langevin equation.

[schill3] H. Meyer, P. Pelagejcev, T. Schilling, "Non-Markovian out-of-equilibrium dynamics: A general numerical procedure to construct time-dependent memory kernels for coarse-grained observables", Europhysics Letters **128**, 40001 (2019)
We introduced a numerical inversion method to construct the memory kernel of the linear generalized Langevin equation from experimentally measured data.

[schill4] Hugues Meyer, Steffen Wolf, Gerhard Stock, Tanja Schilling, "A numerical procedure to evaluate memory effects in non-equilibrium coarse-grained models" Advanced Theory and Simulations 2000197 (2020)
We improved the efficiency of the method introduced in Europhysics Letters **128**, 40001 (2019) and illustrated its use in an analysis of ion dissociation in water. This work was done in collaboration with the Stock group in the context of the research unit FOR 5099

[schill5] C. Widder, T. Schilling, "Generating functions for message-passing on weighted networks: directed bond percolation and SIR epidemics" Physical Review E **104**, 054305 (2021)
We studied the SIR (susceptible, infected, removed/recovered) model on directed graphs with heterogeneous transmission probabilities within the message-passing approximation. We characterizes the percolation transition, predicted cluster size distributions, and suggested vaccination strategies.

[schill6] S. P. Finner, T. Schilling, and P. van der Schoot, "Connectivity, not density, dictates percolation in nematic liquid crystals of slender nanoparticles", Phys. Rev. Lett. **122**, 097801 (2019)
We observed that the cluster size distribution in the nematic phase does not grow monotonically with the particle concentration. Thus the percolation transition shows re-entrant behaviour.

[schill7] F. Coupette, A. Härtel, T. Schilling, "Continuum percolation expressed in terms of density distributions", Physical Review E **101**, 062126 (2020)
We present an approach to derive the connectivity properties of pairwise interacting n-body systems in thermal equilibrium and illustrate how the formalism can be applied to higher-dimensional systems.

[schill8] A. Härtel, D. Richard, T. Speck, "Three-body correlations and conditional forces in suspensions of active hard disks", Physical Review E **97**, 012606 (2018)
We derive an approximate analytic theory for three-body correlations and forces in systems of active Brownian disks and study the dependence of predicted conditional forces on the propulsion speed of self-propelled disks.

[schill9] P. Cats, R. Evans, A. Härtel, R. van Roij, "Primitive Model Electrolytes in the Near and Far Field: Decay Lengths From DFT and Simulations", The Journal of Chemical Physics **154**, 124504 (2021)
We investigate the asymptotic decay lengths of the Restricted Primitive Model for an aqueous electrolyte using classical Density Functional Theory and Molecular Dynamics simulations and conclude that the anomalously large decay lengths found in surface force measurements require an explanation that lies beyond primitive models.

[schill10] F. Coupette, A. A. Lee, A. Härtel, "Screening Lengths in Ionic Fluids", Physical Review Letters **121**, 075501 (2018)
We show using an analytical theory and molecular dynamics simulations that multiple decay lengths can coexist in ionic fluids and provide an explanation for the observed discontinuous change in the structural force across a thin film of ionic liquid-solvent mixtures as the composition is varied.

Conference Talks

Members of the Schilling group obtained invitations to speak at large international conferences in 2020 and 2021, but due to the Covid crisis all events were cancelled. Thus we only report about 2018 and 2019 here.

1. T. Schilling, *Multi-Scale Modeling Far from Thermal Equilibrium*, invited talk at "ETH Materials Day", Zurich, Switzerland, 20th November 2019
2. T. Schilling, *Coarse-Graining Out of Equilibrium*, invited talk at "Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM", Lausanne, Switzerland, 9th-12th September 2019
3. T. Schilling, *Coarse-Graining Out of Equilibrium*, invited talk at "Meco44: 44th Conference of the Middle European Cooperation: Key Challenges in Statistical Physics", Seeon, Germany, 1st-3rd May 2019
4. T. Schilling, *The non-stationary generalized Langevin equation*, keynote lecture at the conference of "The Australian and New Zealand Association of Mathematical Physics", Auckland, New Zealand, Jan. 30th-Feb. 2nd, 2018
5. T. Schilling, *How to go beyond classical nucleation theory by taking it seriously*, invited talk at "Statistical mechanics of interfaces: dynamic phenomena", Berlin, Germany, 4th to 6th October 2018
6. T. Schilling, *Path Sampling Out of Equilibrium*, invited talk at "Adaptive Parallel Strategies for the Exploration of High-Dimensional Spaces with Applications in Particle Simulations and Optimization", Basel, Switzerland, 2nd-4th July 2018
7. H. Meyer, *Non-equilibrium Generalized Langevin Equations* at "StatPhys27 – IUPAP International Conference on Statistical Physics", Buenos Aires, Argentina, 12th July 2019

8. G. Amati, *Memory effects in the Fermi-Pasta-Ulam Model* at "3rd IMA Conference on Nonlinearity and Coherent Structures", Newcastle upon Tyne, UK 10th-12th July 2019

9. A. Härtel, "DFT and electric double layers", Tübinger Density Functional Days, Tübingen, Germany, September 2019

Mandates/Awards

1. Since 10/2021: Dean of Studies

2. Since 10/2021: Member of the "Vorstandsrat der deutschen physikalischen Gesellschaft" (advisory to the Board of Directors of the German Physics Society)

Group Stock

Publications

[stock1] F. Sittel and G. Stock, Identification of Collective Coordinates and Metastable States of Protein Dynamics, J. Chem. Phys. **149** (2018) 150901.
Perspective article on best practices in dimensionality reduction and the definition of biomolecular reaction coordinates and conformational states.

[stock2] P. Hamm and G. Stock, A Nonequilibrium Approach to Allosteric Communication, Phil. Trans. B **373** (2018) 20170187.
A joint experimental/theoretical endeavor that proposes a new view of allosteric transitions.

[stock3] S. Wolf and G. Stock, Targeted molecular dynamics calculations of free energy profiles using a nonequilibrium friction correction, J. Chem. Theory Comput. **14** (2018) 6175.
Development of dissipation-corrected targeted molecular dynamics, which is based on the Jarzynski equality and a Langevin framework. Constraint-biased simulations directly yield both free energies and friction profiles. Time scale analysis of the friction profiles allows to identify microscopic sources of dissipation channels.

[stock4] S. J. Wodak et al., Allostery in its many disguises: From theory to applications, Structure **27** (2019) 566.
Comprehensive review of the current knowledge on allostery and allosteric mechanisms.

[stock5] B. Jankovic, A. Gulzar, C. Zanobini, O. Bozovic, R. Pfister, S. Wolf, G. Stock and P. Hamm, Photocontrolling Protein-Peptide Interactions in the RNase S Complex: From Minimal Perturbation to Unbinding, J. Am. Chem. Soc. **141** (2019) 10702.
Combined experimental/computational study on perturbing protein-ligand interactions with a covalently bound photoswitch, showing that the free energy of ligand binding is quantitatively coupled to the perturbation of the ligand's structure.

[stock6] S. Wolf, B. Lickert, S. Bray and G. Stock, Multisecond ligand dissociation dynamics from atomistic simulations, Nat. Commun. **11** (2020) 2918.
Free energies and friction profiles from dissipation-corrected targeted molecular dynamics serve as inputs for the numerical integration of a Langevin equation. Developing temperature-boosted Langevin simulations, we are able to predict dynamics on time scales far beyond the capability of all-atom MD simulations.

[stock7] O. Bozovic, C. Zanobini, A. Gulzar, B. Jankovic, D. Buhrke, M. Post, S. Wolf, G. Stock and P. Hamm, Real-time observation of ligand-induced allosteric transitions in a PDZ domain, Proc. Natl. Acad. Sci. USA **117** (2020) 26031.
Combined experimental/computational analysis of time-resolved structural changes within a protein during allostery. We show that structurally and dynamically driven allostery are not mutually exclusive but in fact both occur when the protein adapts its free energy landscape to incoming signals.

[stock8] S. Wolf, B. Sohmen, B. Hellenkamp, J. Thurn, G. Stock and T. Hugel, Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations, Chem. Sci. **12** (2021) 3350.
Combined experimental/computational time and spatially resolved analysis of protein structural changes during non-equilibrium relaxation. Structural changes start with small near-ordering changes after ATP hydrolysis and end with large-scale conformational changes of the full protein. The appearing hierarchical length scales of structural changes appear hand in hand with hierarchical time scales.

[stock9] B. Lickert, S. Wolf and G. Stock, Data-driven Langevin modeling of nonequilibrium processes, J. Phys. Chem. B **125** (2021) 8125.
A data-driven Langevin equation is developed that facilitates the modeling of multidimensional nonequilibrium processes.

[stock10] E. Deniz, L. Valiño Borau, J. G. Löffler, K. B. Eberl, A. Gulzar, S. Wolf, P.M. Durkin, R. Kaml, N. Budisa, G. Stock and J. Bredenbeck, Through Bonds or Contacts? Mapping Protein Vibrational Energy Transfer Using Non-canonical Amino Acids, Nat. Commun. **12** (2021) 3284.
Combined experimental/computational study of time-resolved energy transfer after photo excitation through a model protein. Energy is transferred diffusively both along covalent bonds and non-covalent contacts. While backbone energy transfer is faster along short protein sequence distances, side chain contacts form shortcuts at longer distances. Classical simulation-derived rates require a quantum correction of only a factor $\sim$3.

Conference Talks

1. G. Stock, Allosteric Communication Networks, Pacifichem Symposium, Honolulu (online), USA, Dec 2021.
2. G. Stock, Biomolecular Reaction Coordinates, Phys. Chem. Seminar, University of California at Berkeley (online), USA, Nov 2021.
3. G. Stock, Learning Biomolecular Collective Variables, Statistical Physics Seminar, University of Maryland, (online), USA, Sep 2021.
4. G. Stock, Identification of Collective Variables and Metastable States of Protein Dynamics, 57th Symposium on Theoretical Chemistry STC 2021, Universität Würzburg, (online), Sep 2021.
5. G. Stock, Learning the Collective Coordinates of Protein Functional Dynamics, LC Workshop Accelerating the Understanding of Rare Events, Lorentz Center Leiden, (online), Netherlands, Sep 2021.
6. G. Stock, Nonequilibrium Simulation of the Energy Transfer in Proteins, CECAM Flagship Workshop: "Nonequilibrium Dynamical Solvent Effects on Excited States: From Spectroscopy to Photoreactivity (online), Jun 2021.
7. S. Wolf, Accurate Prediction of Absolute Molecular Process Rates on Multisecond Time Scales, APS March Meeting, USA (online), Mar 2021.
8. S. Wolf, Understanding Allosteric Information Transfer Across Time- and Length Scales, 64th Annual Meeting of the Biophysical Society, San Diego (online), USA, Feb 2020
9. G. Stock, Identification of Collective Variables and Metastable States of Protein Dynamics, CECAM Workshop (co-organizer) at Sorbonne Université, Paris, France, Jul 2019
10. S. Wolf, Langevin Modeling of Targeted Molecular Dynamics: A Novel Approach to Calculate, DPG Spring Meeting of the Condensed Matter Section (SKM) together with the EPS, Berlin, Germany, Mar 2018

Mandates/Awards

1. Since 10/2021: Speaker of the DFG Research Unit "Reducing complexity of nonequilibrium systems"

Group Thoss

Publications

[thoss1] D. Weckbecker, P.B. Coto, and M. Thoss, “Molecular transistors controlled through proton transfer”, J. Phys. Chem. Lett. **12** (2021) 413.

The potential of proton transfer reactions as a fundamental mechanism to realize a nanoscale molecular transistor is investigated. Employing density functional theory and the nonequilibrium Green’s function formalism, we identify molecule-graphene nanojunctions, which exhibit high- and low-conducting states depending on the specific location of protons in the molecular bridge and show that an electrostatic gate allows the selection of specific conductance states.

[thoss2] Y. Ke, A. Erpenbeck, U. Peskin, and M. Thoss, “Unraveling current-induced dissociation mechanisms in single-molecule junctions”, J. Chem. Phys. **154** (2021) 234702.

Understanding current-induced bond rupture in single-molecule junctions is both of fundamental interest and a prerequisite for the design of molecular junctions, which are stable at higher-bias voltages. In this work, we analyze the dissociation mechanisms in molecular junctions in a wide range of transport regimes, from off-resonant to resonant, non-adiabatic to adiabatic transport, and weak to strong vibronic coupling.

[thoss3] B.S. Basel, J. Zirzlmeier, C. Hetzer, S.R. Reddy, B.T. Phelan, M.D. Krzyaniak, M.K. Volland, P.B. Coto, R.M. Young, T. Clark, M. Thoss, R.R. Tykwinski, M.R. Wasielewski, D.M. Guldi, “Evidence for charge-transfer mediation in the primary events of singlet fission in a weakly coupled pentacene dimer”, Chem **4** (2018) 1092.

Singlet fission is a photophysical process that converts one singlet excton into two triplet excitons and holds potential to improve the efficiency of solar cells beyond the Shockley and Queisser. In this combined experimental and theoretical study, we analyse the mechanism of intramolecular singlet fission and show that the process is mediated by charge transfer states and involves the formation of an intermediate quintet state.

[thoss4] S.R. Reddy, P.B. Coto, and M. Thoss, “Intramolecular singlet fission: Insights from quantum dynamical simulations”, J. Phys. Chem. Lett. **9** (2018) 5979.

We investigate the dynamics of intramolecular singlet fission in a covalently bonded pentacene dimer using a theoretical approach that combines high-level ab initio multireference perturbation theory methods and quantum dynamical simulations. The results show that the formation of the multiexciton state, corresponding to the first step of the singlet fission process, occurs mainly through a superexchange-like mechanism involving charge transfer states and is facilitated by vibronic coupling.

[thoss5] D. Gelbwaser-Klimovsky, A. Aspuru-Guzik, M. Thoss, U. Peskin, ”High-voltage-assisted mechanical stabilization of single-molecule junctions”, Nano Lett. **18** (2018) 4727.

The realization of efficient nanoscale electronic components depends to a large extent on the ability to mechanically stabilize them in the resonant transport regime. In this work, we focus on single-molecule junctions and demonstrate that their mechanical stability during resonant transport can be enhanced by increasing the bias voltage.

[thoss6] W. Dou, J. Bätge, A. Levy and M. Thoss, ”Universal approach to quantum thermodynamics of strongly coupled systems under nonequlibrium conditions and external driving”, Phys. Rev. B **101** (2020) 184304.

We present an approach based on a density matrix expansion to study thermodynamic properties of a quantum system strongly coupled to two or more baths. For slow external driving of the system, we identify the adiabatic and nonadiabatic contributions to thermodynamic quantities, and show how the first and second laws of thermodynamics are manifested in the strong coupling regime.

[thoss7] S. Wenderoth, H.-P. Breuer, and M. Thoss, ”Non-Markovian effects in the spin-boson model at zero temperature”, Phys. Rev. A **104** (2021) 012213.

We investigate memory effects in the spin-boson model at zero temperature using a recently proposed measure for non-Markovian behavior based on the information exchange between an open system and its environment.

[thoss8] J. Bätge, Y. Ke, C. Kaspar, and M. Thoss, ”Nonequilibrium open quantum systems with multiple bosonic and fermionic environments: A hierarchical equations of motion approach”, Phys. Rev. B **103** (2021) 235413.

We present a hierarchical equations of motion approach, which allows a numerically exact simulation of nonequilibrium transport in general open quantum systems involving multiple macroscopic bosonic and fermionic environments.

[thoss9] J. Okamoto, ”Time-dependent spectral properties of a photoexcited one-dimensional ionic Hubbard model: an exact diagonalization study”, New J. Phys. **21** (2019) 123040.
We study the nonequilibrium spectral signatures of the photo-excited ionic Hubbard model and clarify the interference of multi-photon absorbed states.

[thoss10] G. Homann, J. G. Cosme, J. Okamoto, L. Mathey, ”Higgs mode mediated enhancement of interlayer transport in high-Tc cuprate superconductors”, Phys. Rev. B **103** (2021) 224503.
We propose a new mechanism to control the interlayer transport by optically exciting a plasma mode and the Higss mode in high-Tc superconductors.

Conference Talks

1. M. Thoss, Electron transport in molecular junctions, Symposium on Theoretical Chemistry, Halle, Germany, 2018.
2. M. Thoss, Simulation of nonadiabatic quantum dynamics using multiconfiguration wave-function methods, CECAM-Workshop on Non-adiabatic Quantum Dynamics: From Theory to Applications, Lausanne, Switzerland, 2018.
3. M. Thoss, Quantum Transport in Molecular Junctions, Nano and Quantum Physics Seminar, University of Basel, Switzerland, 2018.
4. M. Thoss, Electron transport in molecular junctions: Theory and application to vibronic phenomena, Penn Conference in Theoretical Chemistry, Philadelphia, USA, 2019.
5. J. Okamoto, Enhanced Josephson coupling in parametrically driven high-Tc superconductors, Plasma 2019 Workshop, Orlando, USA, 2019.
6. M. Thoss, Quantum dynamics in molecular systems: Theory and applications to photoinduced processes, Physikalisches Kolloquium, Universität Rostock, Germany, 2021.
7. M. Thoss, R. Reddy, P. Coto, Quantum dynamical simulation of intramolecular singlet fission, Pacifichem Conference, Honolulu (online), USA, 2021.
8. M. Thoss, Current-induced bond rupture in molecular junctions, International Workshop on Quantum Transport in Nanoscale Molecular Systems, Telluride (online), USA, 2021.
9. J. Okamoto, Numerical time-dependent spectroscopy on the optically excited Mott-Hubbard cluster, Condensed Matter Theory Seminar (online), Charles University, Prague, Czech Republic, 2021.
10. S. Wenderoth, N. Ng, M. Kolodrubetz, E. Rabani, M. Thoss, Dynamics in centrally coupled spin systems, APS-March Meeting (online), 2021

Mandates/Awards

1. Since 10/21 Dean of the Faculty of Mathematics and Physics

Group Timmer

Publications

[timm1] D. Lill, J. Timmer, D. Kaschek, ”Local Riemannian geometry of model manifolds and its implications for practical parameter identifiability”, PLoS ONE **14** (2019) e0217837.
Practical non-identifiable parameters are characterized by unbounded confidence intervals due to a bounded log-likelihood and can not be determined by the local Fisher information matrix. We show that in the frame of local Riemannian geometry, non-vanishing Christoffel symbols can capture the boundedness of the log-likelihood.

[timm2] P. Dolejsch, H. Hass, J. Timmer, "Extensions of L_1 regularization increase detection specificity for cell-type specific parameters in dynamic models", BMC Bioinformatics **20** (2019) 395.
For identifying parsimonious models, typically L_1 regularisation is applied. We investigate L_q regularisation, $0 < q < 1$, and show that this leads to reduced number of false positive results when investigating system-specific parameters.

[timm3] C. Tönsing, J. Timmer, C. Kreutz, "Optimal paths between parameter estimates in nonlinear ODE systems using the nudged elastic band", Frontiers in Physics **7** (2019) 149.
Parameter estimation in non-linear ordinary differential equation often suffers from premature termination of the optimisation algorithm. Using the nudged elastic band algorithm, we propose a method to decide whether two different optimisation results belong to the same local optimum.

[timm4] A. Hauber, R. Engesser, J. Vanlier, J. Timmer, "Estimating chain length for time delays in dynamical systems using profile likelihood", Bioinformatics **7** (2020) 1848.
Numercally challenging modelling by delay differential equation can be converted to ordinary differential equation modelling by the so-called linear chain trick. By identifiability analysis based on the profile likelihood, we propose a method to decide about the length of the chain.

[timm5] R. Ochoa-Fernandez, N.B. Abel, F.-G. Wieland, J. Schlegel, L.A. Koch, B. Miller, R. Engesser, G. Giuriani, S.M. Brandl, J. Timmer, W. Weber, T. Ott, R. Simon, M.D. Zurbriggen, "PULSE: Optogenetic control of gene expression in plants insensitive to ambient light", Nature Methods **17** (2020) 717.
Optogenetics in plants is hampered by the fact that plants needs light to survive. Supported by a mathematical model, we construct an optogenetic device that can be applied under ambient light to control gene expression in plants.

[timm6] H.J. Wagner, R. Engesser, K. Ermes, C. Geraths, J. Timmer, W. Weber, "Synthetic biology-inspired design of signal-amplifying materials systems", Materials Today **22** (2019) 25.
Guided by a mathematical model, we integrate synthetic biology-inspired information-processing circuits into polymer materials. After characterising the building blocks, we predict the amplification of the assembled system including a positive feedback loop.

[timm7] H.J. Wagner, S. Kemmer, R. Engesser, J. Timmer, W. Weber, "Biofunctionalized materials featuring feedforward and feedback circuits exemplified by the detection of Botulinum Toxin A.", Advanced Scienc **6** (2019) 1801320.
Mathematical modelling is applied to characterise and analyse a system of biofunctionalised materials for the detection of toxins. The model comprises positive and negative feedback loops.

[timm8] A. Oppelt, D. Kaschek, S. Huppelschoten, R. Sison-Young, F. Zhang, M. Buck-Wiese, F. Herrmann, S. Malkusch, C.L. Krüger, M. Meub, B. Merkt, L. Zimmermann, A. Schofield, R.P. Jones, H. Malik, M. Schilling, M. Heilemann, B. van de Water, C.E. Goldring, J. Timmer, U. Klingmüller, " Model-based identification of TNFα-induced IKKβ- and IκBα-mediated regulation of NFκB signal transduction as a tool to quantify the impact of Drug-Induced Liver Injury compounds", NPG Systems Biology and Application **4** (2018) 23.
Drug-Induced Liver Injury is a major challenge in drug development. By mathematical modelling, we investigate the influence of the drug diclofenac on the TNFα induced NFκB signalling pathway. The model was developed based on data obtained from a cell line and then adapted to primary human cells.

[timm9] P. Lucarelli, M. Schilling, C. Kreutz, A. Vlasov, M.E. Böhm, N. Iwamoto, B. Steiert, S. Lattermann, M. Wäsch, M. Stepath, M.S. Matter, M. Heikenwälder, K. Hoffmann, D. Deharde, G. Damm, D. Seehofer, M. Muciek, N. Gretz, W.D. Lehmann, J. Timmer, U. Klingmüller, "Resolving the combinatorial complexity of Smad protein complex formation and the link to gene expression",Cell Systems **6** (2018) 75.
Smad signalling is characterised by trimer formation of Smad molecules leading to a hugh complexity of possible models. We apply L_1 regularisation to identify the three relevant Smad complexes in human hepatoma cell lines and primary hepatocytes and linked these complexes to gene expression.

[timm10] F. Kok, M. Rosenblatt, M. Teusel, T. Nizharadze, V.G. Magalhaes, C. Dächert, T. Maiwald, A. Vlasov, M. Wäsch, S. Tyufekchieva, K. Hoffmann, G. Damm, D. Seehofer, T. Boettler, M. Binder, J. Timmer, M. Schilling, U. Klingmüller, "Disentangling molecular mechanisms regulating sensitization of interferon alpha signal transduction", Molecular Systems Biology **16** (2020) e8955.
Interferon is clinically used to fight viral infection. Repeated application leads to a desensitisation of the signaling

system. By mathematical modelling we revealed the molecular mechanism of this process and identified a biomarker to predict the effectiveness of the treatment patient-individually.

Conference Talks

1. Ch. Tönsing, Profile likelihood based analyses of infectious disease models, Spring Meeting, Deutsche Physikalische Gesellschaft, Berlin, March 2018
2. D. Lill, dMod - A development library for dynamic modeling in R, Integrative pathway modeling in systems biology and systems medicine, Bernried, October 2018
3. S. Kemmer, Growth factor signaling in breast cancer - A dynamic model of the MAPK pathway, Signal transduction in organells, cells and organisms - GBM Young Scientists Meeting 2019, Günzburg, April 2019
4. S. Kemmer, Model-based predictions of drug responses in breast cancer, From Cells to Hospitals - Linking Systems Biology and Precision Medicine, Mai 2019
5. S. Kemmer, Model-based analysis of ligand- and drug-controlled growth regulation in breast cancer, Integrative pathway modeling in systems biology and systems medicine, Berlin, November 2019
6. A. Hauber, In vivo Analysis of Cell-Autonomous Oscillations in Thalamic Stem Cells, Tri-Regional Stem Cell and Developmental Biology Meeting, online, October 2020
7. D. Lill, Efficient simulation of clinical target isoboles applied to drug combinations for malaria, American Conference on Pharmacometrics, online, November 2020
8. J. Timmer, A multi-scale model to improve anemia treatment in cancer patients, Solvay Workshop on 'Physics of living systems: from molecules to cells to whole organisms, online, December 2020
9. J. Timmer, Mathematical modelling to optimise the design in synthetical biology, Engineered Living Materials, online, Mai 2021
10. J. Hermes, A non-parametric model-based approach for the estimation of the reproduction number R, Robert Koch-Institute, online, August 2021

Mandates/Awards

1. since 10/05 Member of Board of Directors of the Freiburg Center for Data Analysis and Modelling
2. 5/12 - 5/20 Executive Director Freiburg Center for Systems Biology
3. 10/16 - 9/19 Dean of Studies
4. Since 1/19 Member of the Steering Board of the Excellence Cluster "Center for Integrative Biological Signalling Studies"

Group Waldmann

Publications

[waldm1] A. B. Lysenko, O. A. Bondar, G. A. Senchyk, E. B. Rusanov, M. Srebro-Hooper, J. Hooper, K. Prsa, K. W. Kramer, S. Decurtins, O. Waldmann, S. X. Liu, "On the Border between Low-Nuclearity and One-Dimensional Solids: A Unique Interplay of 1,2,4-Triazolyl-Based $Cu_5^{II}(OH)_2$ Clusters and Mo^{VI}-Oxide Matrix", Inorg. Chem. **10** (2018) 6076-6083.
The ferromagnetic interactions in a molecule with a chain-like arrangement of five magnetic centers were elucidated in terms of electronic energies.

[waldm2] K. Prsa, O. Waldmann, ”Inelastic Neutron Scattering Intensities of Ferromagnetic Cluster Spin Waves”, Inorganics **6** (2018), 1-25.

In this review the results of spin wave theory when applied to ferromagnetic clusters of small nuclearity, so called ferromagnetic cluster spin wave theory, are compiled and extended to a consistent description for energies and wave functions.

[waldm3] K. Prsa, O. Waldmann, ”Ferromagnetic Cluster Spin Wave Theory: Concepts and Applications to Magnetic Molecules”, Eur. J. Inorg. Chem. (2019) 1128–1141.

In this article, which was selected as cover feature, ferromagnetic cluster spin wave theory was applied to the calculation of spectroscopic intensities such as observed in inelastic neutron spectroscopy, and shown that it is possible to directly observe magnetic wave functions experimentally.

[waldm4] S. Nekuruh, J. Nehrkorn, K. Prsa, J. Dreiser, A. M. Ako, C. E. Anson, T. Unruh, A. K. Powell, O. Waldmann, ”Multimodeling Approach to Ferromagnetic Spin-Wave Excitations in the High-Spin Cluster Mn18Sr Observed by Inelastic Neutron Scattering”, Inorg. Chem. **58** (2019) 1125611268.

Experimental inelastic neutron scattering data on the Mn18Sr magnetic cluster, which is comprised of 18 magnetic manganese centers, were presented and in a tour-de-force analysis the magnetic interactions determined.

[waldm5] C. Wessler, B. Roessli1, K. W. Krämer, B. Delley, O. Waldmann, L. Keller, D. Cheptiakov, H. B. Braun, M. Kenzelmann, ”Observation of plaquette fluctuations in the spin-1/2 honeycomb lattice”, npj Quantum Materials **5** 85 (2020).

For the first time the plaquette fluctuations in a magnetic spin-1/2 honeycomb lattice were experimentally identified, and confirmed by combining simulations for extended and small magnetic clusters of appropriate structure.

Group Hennig

Publications

[hennig1] Weiller C, Reisert M, Peto I, Hennig J, Makris N, Petrides M, Rijntjes M, Egger K. ”The ventral pathway of the human brain: A continuous association tract system”, NeuroImage 234: 117977

The brain hemispheres can be divided into an upper dorsal and a lower ventral system. To study the ventral connections, we used cutting-edge in vivo global tractography on high-resolution diffusion tensor imaging (DTI) data.

[hennig2] Wang F, Hennig J, LeVan P. ”Time-Domain Principal Component Reconstruction (TPCR): A More Efficient and Stable Iterative Reconstruction Framework for Non-Cartesian Functional MRI”, Magnetic Resonance in Medicine 84(3): 1321–35 (2020)

In this work we increase the reconstruction efficiency and stability of iterative reconstruction for non-Cartesian fMRI when using high undersampling rates and/or in the presence of strong off-resonance effects.

[hennig3] Tuovinen T, Kananen J, Rajna Z, Lieslehto J, Korhonen V, Rytty R, Mattila H, Huotari N, Raitamaa L, Helakari H, Elseoud AA, Krüger J, LeVan P, Tervonen O, Hennig J, Remes AM, Nedergaard M, Kiviniemi V. ”The variability of functional MRI brain signal increases in Alzheimer’s disease at cardiorespiratory frequencies”, Scientific Reports 9;10(1):21559 (2020)

With fast BOLD scans we showed that the elevated BOLD signal variability in Alzheimer’s disease arises mainly from cardiovascular brain pulsations.

[hennig4] Schmidt AB, Wörner J, Pravdivtsev A, Knecht S, Scherer H, Weber S, Hennig J, von Elverfeldt D, Hövener JB. ”Lifetime of Parahydrogen in Aqueous Solutions and Human Blood”, Chemphyschem 20(19):2408-2412 (2019)

In this work we report longitudinal relaxation times and lifetimes of pH2 in methanol and water, with or without O2 , NaCl, rhodium-catalyst or human blood. Furthermore, we present a relaxation model for more precise theoretical predictions of the H2 spin state in PHIP experiments.

[hennig5] Littin S, Jia F, Layton KJ, Kroboth S, Yu H, Hennig J, Zaitsev M. ”Development and implementation of an 84-channel matrix gradient coil”, Magn Reson Med 79(2):1181-1191 (2018)

In this work the design, implementation, integration, and characterization of a customized coil system is described that allows for generating spatial encoding magnetic fields (SEMs) in a highly-flexible fashion.

[hennig6] LeVan P, Akin B, Hennig J. ”Fast imaging for mapping dynamic networks”, Neuroimage 180(Pt B):547-558 (2018)
The development of highly accelerated fMRI acquisition techniques has led to novel possibilities to monitor cerebral activity non-invasively and with unprecedented temporal resolutions. High sampling rates improve the measurement of physiological noise, yielding an exceptional sensitivity for the detection of periods of transient connectivity at time scales of a few tens of seconds.

[hennig7] Hennig J, Kiviniemi V, Riemenschneider B, Barghoorn A, Akin B, Wang F, LeVan P. ”15 Years MR-encephalography”,MAGMA 34(1):85-108 (2021)
This review article gives an account of the development of the MR-encephalography (MREG) method, which started as a mere ’Gedankenexperiment’ in 2005 and gradually developed into a method for ultrafast measurement of physiological activities in the brain.

[hennig8] Harloff A, Mirzaee H, Lodemann T, Hagenlocher P, Wehrum T, Stuplich J, Hennemuth A, Hennig J, Grundmann S, Vach W. ”Determination of aortic stiffness using 4D flow cardiovascular magnetic resonance - a population-based study”, J Cardiovasc Magn Reson. 20(1):43 (2018)
Increased aortic stiffness is an independent predictor of cardiovascular disease. Here, we selectively measure aortic stiffness using a novel imaging method and to provide reference values from a population-based study.

[hennig9] Braig M, Menza M, Leupold J, LeVan P, Feng L, Ko CW, von Zur Mühlen C, Krafft AJ, Hennig J, von Elverfeldt D. ”Analysis of accelerated 4D flow MRI in the murine aorta by radial acquisition and compressed sensing reconstruction”, NMR Biomed 33(11):e4394 (2020)
Preclinical 4D flow MRI is challenging due to the limited number of available receive channels. Here, a 3D radial retrospectively triggered phase contrast sequence was developed with parallel imaging and compressed sensing reconstruction.

[hennig10] Barghoorn A, Riemenschneider B, Hennig J, LeVan P. ”Improving the sensitivity of spin-echo fMRI at 3T by highly accelerated acquisitions”, Magn Reson Med 86(1):245-257 (2021)
Spin-echo fMRI can be highly advantageous compared to gradient-echo fMRI with respect to field-inhomogeneity artifacts. Here we present a SE implementation to improve the sensitivity of SE-fMRI while profiting from a reduction of susceptibility-induced signal dropout.

Group Bock

Publications

[bock1] Fischer J, Özen AC, Ilbey S, Traser L, Echternach M, Richter B, Bock M. ”Sub- millisecond 2D MRI of the vocal fold oscillation using single-point imaging with rapid encoding”, MAGMA (2021) (epub ahead of print)
So far, the slow spatial encoding of MRI did not allow to image rapid physiologic motion such as the vocal fold oscillation. In this work a new fast acquisition method is presented to visualize the 2D motion of the human vocal folds with sub-ms resolution.

[bock2] Reiss S, Özen AC, Lottner T, Dlaikan-Campos N, Düring K, Massmann A, Bock M. ”Artifact quantification of venous stents in the MRI environment: Differences between braided and laser-cut designs.”, Phys Med 88:1-8 (2021)
MRI artifacts in braided venous stents differ from that of conventional laser-cut stents. In this work we described their B_0- and B_1-dependency and suggested methods for optimal stent designs.

[bock3] Stephan S, Reiss S, Lottner T, Özen AC, Bock M. ”Catheter-based Arterial Input Function Determination for Myocardial Perfusion Measurements”, Z Med Phys 31(1):65-72 (2021)
In MR-guided vascular interventions active catheters with tracking coils are used for device localisation. In this work we use the coils in transmit mode to quantify perfusion without the use of contrast agents.

[bock4] Bielak L, Wiedenmann N, Berlin A, Nicolay NH, Gunashekar DD, Hägele L, Lottner T, Grosu AL, Bock M. "Convolutional neural networks for head and neck tumor segmentation on 7-channel multiparametric MRI: a leave-one-out analysis", Radiat Oncol 15(1):181 (2020)
CNNs can be used for automatic segmentation of tumor lesions. In this work we investigate the influence of 7 MRI input channels of a CNN with respect to their performance in head&neck cancer.

[bock5] Özen AC, Silemek B, Lottner T, Atalar E, Bock M. "MR safety watchdog for active catheters: Wireless impedance control with real-time feedback.", Magn Reson Med 84(2):1048-1060 (2020)
Active catheters can heat up during MRI due to coupling with the E-fields of the body coil. Here, we dynamically minimize radiofrequency (RF)-induced heating through an automatic change of the termination impedance.

[bock6] Bielak L, Wiedenmann N, Nicolay NH, Lottner T, Fischer J, Bunea H, Grosu AL, Bock M. "Automatic Tumor Segmentation With a Convolutional Neural Network in Multiparametric MRI: Influence of Distortion Correction", Tomography 5(3):292-299 (2019)
We investigate the difference in CNN segmentation performance of geometrically distorted and distortion-corrected diffusion-weighted MRI data in patients with head and neck tumors.

[bock7] Reichert A, Bock M, Reiss S, Overduin CG, Fütterer JJ, Krafft AJ. "Simultaneous slice excitation for accelerated passive marker tracking via phase-only cross correlation (POCC) in MR-guided needle interventions", MAGMA 31(6):781-788 (2018)
Passive tracking of needles is accelerated using highly undersampled radial acquisitions and reconstructions with prior knowledge to determine the position of interventional devices.

[bock8] Kurzhunov D, Borowiak R, Reisert M, Özen AC, Bock M. "Direct estimation of ^{17}O MR images (DIESIS) for quantification of oxygen metabolism in the human brain with partial volume correction", Magn Reson Med 80(6):2717-2725 (2018)
Low-resolution ^{17}O MRI measurements of the cerebral rate of oxygen consumption require partial volume correction. Here, we propose a method withou image reconstruction to directly extract metabolic rates from the measurement data.

[bock9] von zur Mühlen C, Reiss S, Krafft AJ, Besch L, Menza M, Zehender M, Heidt T, Maier A, Pfannebecker T, Zirlik A, Reinöhl J, Stachon P, Hilgendorf I, Wolf D, Diehl P, Wengenmayer T, Ahrens I, Bode C, Bock M. "Coronary magnetic resonance imaging after routine implantation of bioresorbable vascular scaffolds allows non-invasive evaluation of vascular patency", PLoS One 25;13(1):e0191413 (2018)
BVS do not cause shielding artefacts in MRI - here, we show for the first time that vascular patency can be assessed non-invasively in BVS patients using advanced MRI protocols.

[bock10] Dadakova T, Krafft AJ, Özen AC, Bock M. "Optimization of acoustic radiation force imaging: Influence of timing parameters on sensitivity", Magn Reson Med 79(2):981-986 (2018)
In MR-guided ARFI the phase change induced by motion encoding gradients (MEGs) is measured to assess tissue displacement. Here, timing parameters such as the MEG duration and the offset time between ultrasound (US) and MEG are otpimized to increase the sensitivity of the ARFI experiment.

Conference Talks

1. M. Bock, Devices and Imaging Methods for MR-Guided Intravascular Interventions, ISMRM Interventional MR Study Group Virtual Meeting, 2020
2. M. Bock, Die Zukunft der MRT. MHH Hannover, 2019
3. M. Bock, MRI beyond protons: Oxygen-17 MRI and MRS to study oxygen and glucose metabolism, Seminar "Bildgebende Verfahren der Neurowissenschaften" Uni Jena, 2018
4. M. Bock, Novel MR Imaging Techniques and Their Implications for iMRI, Interventional MRI Symposium, Boston/MA, 2018
5. M. Bock, Technische Grundlagen neuer MR Kontraste: Multikern MR und CEST, Deutscher Röntgenkongress, 2018

Mandates/Awards

1. 2018: Fellow of the International Society for Magnetic Resonance in Medicine (ISMRM)

2. Since 2018: Associate Editor of the *Zeitschrift für Medizinische Physik*

Group Rohrbach

Publications

[rohrb1] H. Kermani and A. Rohrbach, "Orientation-control of two plasmonically-coupled nanoparticles in an optical trap", ACS Photonics, **11**, 4660-4667 (2018).
We measure how two 80 nm silver NPs form a dimer inside an optical trap and orient along the electric field of the trapping laser, allowing to rotate them stably in the horizontal plane.

[rohrb2] M. D. Koch and A. Rohrbach, "Label-free imaging and bending analysis of microtubules by ROCS microscopy and optical trapping", Biophys J, **9**, 168 - 177 (2018).
Using ROCS microscopy we observe 25 nm thin microtubules, fluctuating in solution over ¿ 1000 images. Held by an oscillating twin trap, we measure their complex viscoelastic response.

[rohrb3] J. Roth, M. D. Koch, and A. Rohrbach, "Dynamics of a molecular protein chain motor driving helical bacteria under stress", Biophys J, **114**, 1955 - 1969 (2018).
We measure and manipulate the initiation of kinks, their propagation velocities, and the time between two kinks for a single deforming bacteria trapped in an optical line potential.

[rohrb4] F. Jünger and A. Rohrbach, "Strong cytoskeleton activity on millisecond timescales during particle binding and uptake revealed by ROCS microscopy", Cytoskeleton, **75**, 410–424, (2018).
We demonstrate how strong cytoskeleton activity becomes visible on millisecond timescales upon particle binding using 100 Hz ROCS microscopy.

[rohrb5] D. Ruh, J. Mutschler, M. Michelbach, and A. Rohrbach, "Superior contrast and resolution by image formation in rotating coherent scattering (ROCS) microscopy", Optica, **5**, 1371-1381 (2018).
We find that cross-correlations of elementary waves emitted in a distance of several μm to each other positively contribute to ROCS image formation and do not distort image formation.

[rohrb6] T. Meinert and A. Rohrbach, "Light-sheet microscopy with length-adaptive Bessel beams", Biomedical Optics Express, **10**, 670-681 (2019).
We show that scanned Bessel beams enable object adapted tailoring of the light-sheet defined by its beam length and position, thereby increasing contrast and reducing bleaching.

[rohrb7] L. Koebele and A Rohrbach, "A Shape-switch-block principle for confocal light-sheet microscopy with sectioned Bessel beams and stimulated emission depletion", Communication Physics, (2020).
We increase resolution and contrast in light-sheet microscopy by making the effective light-sheet thinner through the combination of phase shaping, fluorophores-switching, and dynamic blocking of fluorescence.

[rohrb8] J. Roth, J. Mehl, and A. Rohrbach, "Fast TIRF-SIM imaging of dynamic, low-fluorescent biological samples", Biomedical optics express, **11**, 4008 - 4026 (2020).
We present a novel TIR-fluorescence structured illumination microscope (TIRF-SIM), which generates images at 110 nm spatial and 8 Hz temporal resolution, and apply it to dim, moving samples.

[rohrb9] A. Rohrbach, T. Meyer, E. H. K. Stelzer, and H. Kress, "Measuring Stepwise Binding of Thermally Fluctuating Particles to Cell Membranes without Fluorescence", Biophys. J. **118** (2020).
We show by experiments and simulations that it is possible to detect single binding events of a coated bead, held in an optical trap near the cell membrane of a macrophage.

[rohrb10] B. Landenberger and A. Rohrbach, ”Towards non-blind optical tweezing by finding 3D refractive index changes through off-focus interferometric tracking”, Nature Communications, **12**, 6922, (2021).
We localize and track regions with increased refractive index using several holographic optical traps with a single camera in an off-focus position, allowing to rotate cell clusters in arbitrary directions.

Group Rotter

Publications

[rott1] J. Gallinaro, N. Gašparović, S. Rotter, ”Homeostatic structural plasticity leads to the formation of memory engrams through synaptic rewiring in recurrent networks”, PLOS Computational Biology (2022) in press.
A new theory describes how structure formation, associative memory and learning is achieved by constrained network remodeling based on random self-organization.

[rott2] P. Pfaffelhuber, S. Rotter, J. Stiefel, ”Mean-field limits for non-linear Hawkes processes with excitation and inhibition”, arXiv **[math.PR]** (2021) 2102.01052
Mathematical analysis of a multivariate stochastic point process that corresponds to spiking neuronal networks.

[rott3] S. Spreizer, J. Senk, S. Rotter, M Diesmann, B. Weyers, ”NEST Desktop, an Educational Application for Neuroscience”, eNeuro **8(6)** (2021) ENEURO.0274-21.2021.
A graphical user interface to numerical simulations and rapid prototyping in computational network modeling. The client-server architecture allows to use HPC-enabled backends.

[rott4] H. Lu, J.V. Gallinaro, C. Normann, S. Rotter, I. Yalçın, ”Time Course of Homeostatic Structural Plasticity in Response to Optogenetic Stimulation in Mouse Anterior Cingulate Cortex”, Cerebral Cortex (2021) bhab281.
Experimental work demonstrating experimental phenomena consistent with the theory of homeostatic structural plasticity.

[rott5] M.M. Nejad, S. Rotter, R. Schmidt, ”Basal ganglia and cortical control of thalamic rebound spikes”, European Journal of Neuroscience **54** (2021) 4295–4313.
Analyzing the role of higher-order neuronal correlations in brain networks for movement initiation.

[rott6] M. Kordovan, S. Rotter, ”Spike Train Cumulants for Linear-Nonlinear Poisson Cascade Models”, arXiv **[q-bio.NC]** (2020) 2001.05057.
Analysis of higher-order moments in nonlinear network activity using loop integrals.

[rott7] F. Lagzi, F.M. Atay, S. Rotter, ”Bifurcation analysis of the dynamics of interacting subnetworks of a spiking network”, Scientific Reports **9(1)** (2019) 11397.
Numerical 3-dimensional bifurcation analysis of nonlinear network dynamics based on Lotka-Volterra equations.

[rott8] B. Merkt, F. Schüßler, S. Rotter, ”Propagation of orientation selectivity in a spiking network model of layered primary visual cortex”, PLOS Computational Biology **15(7)** (2019) e1007080.
Coarse-grained analysis of the activity of a large-scale multilayer network model of primary visual cortex.

[rott9] H. Lu, J. Gallinaro, S. Rotter, ”Network remodeling induced by transcranial brain stimulation: A computational model of tDCS-triggered cell assembly formation”, Network Neuroscience **3(4)** (2019) 924-943.
Weak transcranial electric fields can reliably induce homeostatic network remodeling.

[rott10] A.P. Buccino, M. Kordovan, T.V. Bækø Ness, B. Merkt, P.D. Häfliger, M. Fyhn, G. Cauwenberghs, S. Rotter, G.T. Einevoll, ”Combining biophysical modeling and deep learning for multi-electrode array neuron localization and classification”, Journal of Neurophysiology **120** (2018) 1212-1232.
Compressed sensing methods applied to extracellular electric fields recorded with novel high-resolution probes.

[rott11] C. Lennartz, J. Schiefer, S. Rotter, J. Hennig, P. LeVan, ”Sparse Estimation of Resting-State Effective Connectivity from fMRI Cross-Spectra”, Frontiers in Neuroscience **12** (2018) 287.
Successful application of a new method for network inference at very low sampling rates.

[rott12] J.V. Gallinaro, S. Rotter, ”Associative properties of structural plasticity based on firing rate homeostasis in recurrent neuronal networks”, Scientific Reports **8** (2018) 3754.
Robust associative learning can be obtained from self-organized network remodeling.

[rott13] J. Schiefer, A. Niederbühl, V. Pernice, C. Lennartz, P. LeVan, J. Hennig, S. Rotter, ”From Correlation to Causation: Estimation of Effective Connectivity from Continuous Brain Signals based on Zero-Lag Covariance”, PLOS Computational Biology **14(3)** (2019) e1006056.
A new algorithm to infer the connectivity of large networks from measured zero-lag correlations using $L1$ regularization.

Mandates/Awards

1. since 2009 Founding Member and Managing Director of the Bernstein Center Freiburg
2. since 2012 Principal Investigator in the Cluster of Excellence BrainLinks-BrainTools, 2015–2020 member of its Executive Board
3. since 2017 Member of the Steering Committee of the Bernstein Network Computational Neuroscience
4. 2015–2019 Member of the Executive Committee of the German Neuroscience Society (GNS) and Spokesperson of the Section Computational Neuroscience
5. since 2013 appointed representative in the User Committee for large-scale IT infrastructures in the State of Baden-Württemberg (bwHPC, bwData), since 2020 elected spokesperson of the User Committee

2.6 Bachelor, Master and PhD Theses

Group Bett

Master Theses

1. Adrian Callies, ”Erstellung und Validierung eines optischen Modells des Schicht-Struktur-Systems ’MorphoColor’ für die Anwendung in farbigen Solarmodulen”, 2021
2. Jared Faißt, ”Spectral and Time Resolved Luminescence Spectroscopy on Organic Solar Cells”, 2021
3. Georgios Loukeris, ”Characterization of Passivated Perovskite Solar Cells”, 2021
4. Moritz Spannenkrebs, ”Determination of the Energy Yield and nominal Power Output of Flat Multi-Junction PV-Modules”, 2021
5. Wiebke Wirtz, ”Proof of principle for contactless current-voltage measurements on silicon solar cells”, 2021
6. Adrian Callies, ”Erstellung und Validierung eines Modells zur optischen Simulation von Morpho inspirierten Schicht-Struktur-Kombinationen für die Anwendung in farbigen PV-Modulen”, 2021
7. Michel Erlemann, ”Elektrische Defektcharaketrisierung und Methodenvergleich zur Anwendung an hochreinem Silizium”, 2021
8. Nik Poppe, ”Simulation of Transient Luminescence and Photovoltage of Pervoskite Solar Cells”, 2021

Bachelor Theses

1. Liel Bühler, ”Optimierung von reaktiv gesputterten, dünnen Dielektrikschichten für die Anwendung in O2-Sensoren”, 2021

Group Dzubiella

PhD Theses

The following PhD theses were completed in the reporting period 2018-2021. Dzubiella moved from Berlin to Freiburg in April 2018. Due to his ongoing association with the Helmholtz-Zentrum Berlin and the Humboldt-Universität zu Berlin some of the students finished their PhD in Berlin while supervised from Freiburg.

1. Richard Gregor Weiss, The role of water in the kinetics of hydrophobic molecular recognition using stochastic modeling and molecular simulations, 2018.
2. Xiao Xu, Molecular modeling of the complexation of proteins with strong anionic polyelectrolytes, 2018.
3. Rohit Nikam, Highly charged dendritic polyelectrolytes: Competitive ion binding and charge renormalization, 2020.
4. Chanbum Park, Structure, dynamics, and phase behavior of concentrated electrolytes for applications in energy storage devices, 2020.
5. Mila Miletic, Computational study of structure formation and dynamic properties of organic molecules at hybrid inorganic/organic interfaces, 2021.

Master Theses

1. Florian Gutsche, Battery modelling using Poisson-Nernst-Planck equations with applications to electrochemical impedance spectroscopy, 2018.
2. Rang Noh, Simulation of embossing conditions in a variothermal roll-to-roll hot-embossing system, 2020.

3. Simon Gramatte, Computational study of structure and dynamics of polycarbonate nanodroplets: glass or liquid?, 2020.

4. Rolf Schimmer, Catalytic feedback control in core-shell nanoreactors, 2021.

5. Polina Gaindrik, Active responsive colloids with differently thermostatted degrees of freedom, 2021.

6. Nils Göth, Modeling of active responsive colloids driven by an internal dichotomous noise, 2021.

Bachelor Theses

1. Lennard Holschuh, Bestimmung der Skalengesetze des Konformitätsverhaltens eines BAB-Blockcopolymers mithilfe der Monte-Carlo Simulation, 2021.

Group Elsässer

PhD Theses

1. Cong Tao, "Atomistic modeling of grain boundaries in SrTiO3 and their effects on oxygen vacancies", submitted 2021.

Master Theses

1. Daniel Pfalzgraf, "Deriving macroscopic diffusivity from a microscopic master-equation approach", 2021.

Bachelor Theses

1. Daniel Pfalzgraf, "Theoretical investigation of the diffusion of Lithium ions in a solid-state electrolyte material at the atomic scale", 2019.

2. Johanna Waltenspiel, "Calculation of mechanical properties of metal-metal interfaces at the atomic scale", 2019.

3. Patrick Sell, "Investigation of ordering processes in ferromagnetic phases on the atomic scale", 2021.

Group Kühnemann

Master Theses

1. V. Vierhub-Lorenz, "Schnelle bildgebende Oberflächenfeuchtemessung mit Nahinfrarot-Lasern", 2018

2. P. Reiser,"Nichtlinear-Optischer Hochkonverter für die Laserspektroskopie im Mittleren Infrarot", 2018.

3. E.-M. Butscher, "Chromatische Oberflächenanalyse mit Fresnel-Zonenplatten", 2019

4. J. Kunz, "Breitbandige Fourier-Transform-Infrarot-Spektroskopie mit nichtlinearen Interferometern", 2020.

5. N. Arndt, "ATR-Spektroskopie unter Verwendung einer nanokristallinen Diamant-Deckschicht", 2020

6. S. Unmüßig, "Elastokalorische Materialien: Experimentelle Charakterisierung und Beschreibung mit einem phänomenologischen Materialmodell", 2021

Bachelor Theses

1. T. Wipf, "Optische Simulation und experimentelle Erprobung eines ATR-Messsystems mit hohlzylinderförmiger Geometrie", 2018

2. J. Kunz, "Hochempfindliche Absorptionsmessungen an einem neuen Material für Faraday-Isolatoren", 2018.

Group Moseler

PhD Theses

1. T. Reichenbach, ”Atomistic Insights into Dry Friction and Shear-Induced Nonequilibrium Phase Transitions in Silicon and Carbon Materials”, 2021.

Master Theses

1. N. Lemcke, ”Activation volumes of mechanochemical reactions in amorphous materials”, 2020.

Group Reiter

PhD Theses

1. F. M. Keheze, Optical studies on indicators of order and disorder in films and crytals of a bulky substituted polythiophene, 2018.
   `https://freidok.uni-freiburg.de/data/15324`
2. P. Pudel, Formation of periodically modulated polymer crystals, 2018.
3. S. K. Majumber, Growth kinetics of stacks of lamellar crystals in polymer thin films, 2018.
   `https://freidok.uni-freiburg.de/data/164292`
4. F. Ramezani, Adapted creep test for the study of non-equilibrated thin polymer films, 2019.
   `https://freidok.uni-freiburg.de/data/151904`
5. A. Das, Controlling phase transitions in Langmuir polymer films, 2020.
   `https://freidok.uni-freiburg.de/data/167266`
6. T. Wu, Formation of large polymer crystals from metastable solutions, 2020.
   `https://freidok.uni-freiburg.de/data/167415`
7. K. Roumpos, Tuning topography and patterns of thin polymer films on structured substrates, 2021.
   `https://freidok.uni-freiburg.de/data/194127`
8. E. Khechine, Morphological transitions in Langmuir films of a diblock copolymer from polyethylene glycol and poly-L-lactide, 2021.
   `https://freidok.uni-freiburg.de/data/222609`

Master Theses

1. S. Kraus, Structure formation of core/interlayer/shell nanoparticles in Langmuir monolayers, 2018.
2. A. Probst, Untersuchung des Phasenverhaltens von Methoxy-Polyethylenglykol in quasi-zweidimensionalen Langmuir-Filmen, 2019.
3. M. Fink, Morphology and behaviour of methoxy-poly(ethylene glycol)-poly(lactic acid)copolymer films at the air-water interface, 2020.
4. S. Saikumar, Probing viscoelastic properties of ultra-low molecular weight polystyrene and its blend films”, 2021.
5. W. Chen, Formation of ‘pseudo-hollow polymer crystals’ via controlled initiation and growth of vertical stacks of correlated lamellae”, 2021.

Group Schilling

PhD Theses

1. Arshia Atashpendar, Geometric percolation and electrical conductivity in suspensions of conductive nanoparticles, 2021
   https://freidok.uni-freiburg.de/data/176060
2. Graziano Amati, Coarse-graining analysis of the Fermi-Pasta-Ulam model, 2020
   https://freidok.uni-freiburg.de/data/167294
3. Hugues Meyer, Generalized Langevin equations and memory effects in non-equilibrium statistical physics, 2020
   https://freidok.uni-freiburg.de/data/220023

Master Theses

1. Wilkin Wöhler, Nucleation and crystallization of the metastable hard sphere fluid, 2021
2. Moritz Schäffler, Memory effects of non-equilibrium processes in a polymer melt, 2021
3. Philipp Elsässer, Phase behaviour of chiral liquid crystals, 2021
4. Fabian Glatzel, Thermodynamic Study of Supercapacitors, 2020.
5. Moritz Bültmann, Computing The Interfacial Tension Of Hard Spheres, 2019
6. Philipp Pelagejcev, Simulation study of non-Markovian effects in crystal nucleation, 2019
7. Fabian Coupette, Structure and Screening in Ionic Solutions: An analytical approach, 2018.
8. Motoya Suzuka, Monte Carlo Simulation of Binary Helical Yukawa Rods , 2018

Bachelor Theses

1. Christoph Widder, Message-Passing und erzeugende Funktionen für Perkolation auf gerichteten Netzwerken, 2021
2. Fabian Joseph, Monte Carlo Simulationen von Ionischen Flüssigkeiten (Monte Carlo simulations of ionic fluids), 2020.
3. Viktor Tänzel, Monte Carlo simulations of smectic liquid crystalline fibrils, 2020
4. Malte Henes, Numerical Study of Different Versions of the FPU Model, 2020
5. Marlene Heinrich, The random walker in confinement, 2020
6. Tim Ingenbrand, Percolation and Charge Transport in Suspensions of Platelets, 2019
7. Nadja Helmer, Computer Simulation Study of Chiral Liquid Crystal Membranes, 2019
8. Nils Göth, Membranen aus kolloidalen, chiralen Teilchen, 2019
9. Marleen Leveringhaus, Simulation of a Water Model, 2019.

Group Stock

Habilitations

1. Steffen Wolf, Nonequilibrium Dynamics of Living Soft Matter on Atomic Scales, 2021.

PhD Theses

1. Florian Sittel, The Secret Life of Proteins: Exploring moleular dynamics through statistics, 2018.
2. Matthias Ernst, Finding Reaction Coordinates for Protein Folding and Functional Motion, 2018.
3. Adnan Gulzar, Energy and Signal Transport in Photoswitched Proteins, 2020.
4. Luis Valiño Borau, Master equation modelling of energy transport in biomolecules, 2020.
5. Benjamin Lickert, Data-based Langevin modeling of biomolecular systems, 2021.

Master-Theses

1. Simon Bray, Approaches to analyzing protein-ligand dissociation with targeted molecular dynamics, 2018.
2. Anna Weber, Markov State Modeling of an Allosteric Transition, 2019.
3. Andre Cieluch, Langevin Modeling of solvated sodium chloride, 2019.
4. Georg Diez, Markov Modeling of Nonequilibrium Biomolecular Data, 2020.
5. Miriam Jäger, Nonequilibrium Molecular Dynamics Simulations of Ion Channels, 2020.
6. Nadja Helmer, Energy Transport in Proteins, 2021.

Bachelor-Theses

1. Anna Weber, Comparison of Network Models for the Analysis of Protein Dynamics, 2018.
2. Sophia Ohnemus, Photoswitchable PDZ2 Domain, 2018.
3. Moritz Schäffler, Targeted Molecular Dynamics Simulations of the Unbinding of a S-Peptide from RNase, 2018.
4. Daniel Bartle, Sampling and Equilibration of Biomolecular Simulations, 2019.
5. Lennart Koenig, VAMPnets Analysis of the Structural Dynamics of a Peptide Helix, 2020.
6. Tim Uttenweiler, Validation and Coarse Graining of Biomolecular Markov State Models, 2020.

Group Thoss

PhD Theses

1. C. Schinabeck, ”Hierarchical quantum master equation approaches to nonequilibrium charge transport through single-molecule junctions”, 2019.
2. A. Erpenbeck, ”Electron transport through single-molecule junctions in the presence of external driving and electronic-nuclear interactions”, 2019.
3. C. Hofmeister, ”Feldinduzierter Protonentransfer zur Kontrolle der elektrischen Leitfähigkeit eines Einzelmolekülkontakts”, 2019.
4. V. Prucker, ”Theory and simulation of electron transfer processes at molecule-metal interfaces”, 2019.

5. D. Weckbecker, ”Electronic transport in graphene-based nanostructures”, 2019.

Master Theses

1. C. Hertlein, ”Extension of the hierarchical quantum master equation approach to low temperatures and realistic band structures”, 2018.
2. K. Chan, ”Heat current and thermoelectric effect analysis through single molecule junctions”, 2019.
3. S. Stumper, ”Numerical studies of static and dynamical properties of the one-dimensional extended Bose-Hubbard model”, 2019.
4. R. Smorka, ”Dynamics in quantum-classical hybrid spin models”, 2020.
5. S. Mirmohammadi, ”Theoretical study of photoinduced phase transitions in the extended Peierls-Hubbard model”, 2021
6. R. Fischer-Süßlin, ”Nonequilibrium heat and charge transport through single-molecule junctions”, 2021.

Bachelor Theses

1. R. Smorka, ”Transport through inhomogeneous charge orderings in the Falicov-Kimball model”, 2019.
2. D. Mazibrada, ”Non-Markovian effects in the XXZ-Heisenberg spin chain”, 2020.

Group Timmer

PhD Theses

1. Marcus Rosenblatt. From Steady States to Dynamics - Methods for Mechanistic Modeling of Biological Systems with Applications to Interferon α Signaling. February 2021
2. Christian Tönsing. Quantitative Modeling of Human Diseases - Methods and Applications, March 2020

Master Theses

1. Jacques Hermes. Modeling the SARS-CoV-2 Pandemic Using the Augmented Kalman smooter Method, August 2021
2. Theodor Haug. Testing for Interactions in Predator-Prey Time Series, April 2021
3. Yasaman Heshmatzadeh. Application and Calibration of the Bayesian Force Inference Method on the Wing Disc Epithelial Tissue of Drosophila, June 2020
4. Tim Litwin. Optimal Experimental Design Based on Two-Dimensional Likelihood Profiles, December 2019
5. Franz-Georg Wieland. Bayesian parameter estimation in systems biology: Markov chain Monte Carlo sampling of biochemical networks, December 2018
6. Adrain Lukas Hauber. Estimating Time Delays in Dynamical Systems Using Profile Likelihood, November 2018

Bachelor Theses

1. Frederike Dörr. Control Coefficient profiles: Development of a method for uncertainty analysis of control coefficients of metabolic staedy-state networks, August 2021
2. Philipp Alekos Tudor. Improving Parameter Estimation by Duplicating the Model Equations, July 2018
3. Pascal Dolejsch. Adapted Lasso Methods for Ordinary Differential Equation Systems with Applications to Dynamic Models of Signal Transduction, July 2018

4. Robin Thomm. Untersuchung der Konfidenzintervalle bei der Parameterschätzung in PK/PD Modellen, January 2018

Group Waldmann

PhD Theses

1. Siyavash Nekuruh Motlagh, Untersuchung der Niedrigenergie-Zustände in Heisenberg-Spin-Clustern mittels inelastischer Neutronenstreuung, 2018
   `https://freidok.uni-freiburg.de/data/15773`

Master Theses

1. Leo De Souza, High-Frequency AC Susceptometer for Studying Lanthanide-Based Single-Molecule Magnets, 2018
2. Hetti Jayawardena, Efficient Medium Scale Simulation of Magnetism in Single Molecule Magnets, 2020
3. ShaoqiChen, Exploration of the Ability of Neural Networks for Interpreting Magnetic Susceptibility of Single Molecule Magnets, 2020
4. Ruolin Li, Applying Point Charge Model to Single Molecule Magnets, 2021
5. Yuanlin Xu, Analysis and interpretation of experimental magnetization of Mn2Ln2 Single Molecule Magnets, 2021

Bachelor Theses

1. Kaleb Strahringer, Anwendung des Angular Overlap Models auf Lanthanoid-basierte Einzelmolekülmagnete, 2021

Group Hennig

PhD Theses

1. M. Dacko, "Methodological Improvements of the Mescher-Garwood (MEGA) J-editing Sequence in Conjunction with adiabatic pulses", 2021
2. A. B. Schmidt, "Liquid-State Nuclear hyperpolarization without a polarizer - Synthesis Amid the magnet Bore allows a dramatically enhanced Nuclear Alignment", 2020
3. P. Rovedo, "1H and 15N hyperpolarization using SABRE - Experimental approaches and hardware designs for continuous and batch hyperpolarization", 2020
4. B. Riemenschneider, "Highly Accelerated fMRI using non-cartesian trajectories: Enhanced data acquisition and enabling real-time reconstruction", 2020
5. C. Lennartz, "Inference of sparse cerebral connectivity from high temporal resolution fMRI data", 2020
6. S. Berner, "Parahydrogen Hyperpolarized Metabolites and Spin Dynamics at High Magnetic Field", 2020
7. S. Knecht, "On the interplay of spin dynamics and chemical kinetics in the nuclear spin hyperpolarization technique Signal Amplification by Reversible Exchange (SABRE): a simulation and experimental NMR study", 2019

Master Theses

1. N. Molochidis, ”Optimization of signal quality in preclinical EEG-fMRI”, 2021
2. V. Ivantaev, ”Effect of macroscopic motion on intermolecular hyperpolarization transfer”, 2021
3. M. Zimmermann, ”Implementation and Characterization of a SAMBADENA-Polarizer in a Preclinical 9.4 Tesla MRI”, 2018

Group Bock

PhD Theses

1. A. Reichert, ”Beschleunigte Instrumentenverfolgung in der Magnetresonanztomographie durch simultane Schichtanregung und radiale Akquisition”, 2021
2. S. Reiss, ”Endovaskuläre Stents in der Magnetresonanztomographie: Untersuchung der Hochfrequenzanregung im Kontext der Patientensicherheit und Bildgebungsartefakte”, 2020

Master Theses

1. K. Waescher, ”Intra-Arterielle Spin Markierung mit einer Katheterspule zur Perfusionsquantifizierung im Myokard”, 2021
2. L. Haegele, ”Neuronale Netze zur Tumorsegmentierung in der Multikontrast-Magnetresonanztomographie: Physikalische Modellierung und Klinische Anwendung”, 2020
3. J. O. Prima, ”Radiofrequency Resonator (RF coil) Design for Functional ^{17}O-MRI of Kidney Transplant”, 2020
4. Y. Taege, ”Optimized Acquisition and Reconstruction in Functional ^{17}O-MRI”, 2019
5. S. Stephan, ”Katheter-basierte Messung der arteriellen Inputfunktion”, 2019
6. F. Bayer, ”Modelling Magnetization Transfer in Binary Spin-Bath Systems”, 2019

Bachelor Theses

1. F. Spreter, ”Sende- und Empfangsspule für Fluor-19 MRT bei 3 Tesla”, 2021
2. T. Rachel, ”Parameteroptimierung für die simultane Messung der T2-Relaxation und des Diffusionskoeffizienten in radialen, unterabgetasteten Spin-Echo-Sequenzen”, 2021
3. L. V. Haas, ”Kombination von elektro-optischen E-Feldmessungen und MR-Thermometrie zur Beurteilung der HF-Anregung von intravaskulären Stents in der MRT”, 2020
4. P. Bronner, ”Elektrooptische Messung von Transferfunktionen für Instrumente der interventionellen MRT”, 2020

Group Rohrbach

PhD Theses

1. Tobias Meinert: Optimierungsstrategien zur computerholographischen Beleuchtung und zur Abbildung streuender Objekte in der Lichtscheibenmikroskopie mit Bessel-Strahlen, 2018.
2. Hamideh Kermani: Optical trapping of metallic nanoparticles and evaluation of relevant parameters, 2018

3. Julian Roth: Super-resolution structured illumination microscopy of MreB dynamics and cell wall synthesis in B. subtilis, 2019.
4. Rebecca Michiels: Investigation of filopodia dynamics in macrophage cells by photonic force microscopy, 2019.

Master Theses

1. Johanna Mehl: MreB Dynamics and Cellwall Synthesis in Bacillus subtilis investigated by Structured Illumination Microscopy, 2018.
2. Julius Mutschler: Untersuchungen zur Mikroskopie mit rotierend kohärenter Streuung (ROCS) von Laserlicht, 2018.
3. Moritz Michelbach: Bildgebungskonzepte zur Mikroskopie mit rotierender, kohärenter Streuung (ROCS) von Laserlicht, 2018.
4. Shantanu Kiran Paranjape: Holographic generation of lattice-like illumination beams for light-sheet microscopy, 2019.
5. Franziska Moos: Investigation of the bacterial cell wall synthesis with super-resolution microscopy and optical tweezers, 2020.
6. Umar Rafique: Investigating Angular Correlations in Rotating Coherent Scattering (ROCS) Image Formation, 2021.
7. Kexin Lyu: Monitoring Particle Binding and Uptake into Macrophages with Brightfield and DIC Microscopy Techniques, 2021.
8. Victor Chuman: Contrast and specificity by absorption markers in ROCS microscopy, 2021.

Bachelor Theses

1. Robert Schütze: Digitale Mikrospiegelarrays zur holographischen Erzeugung von Bessel-Strahlen für adaptive Lichtscheibenmikroskopie, 2019.

Group Rotter

Bachelor Theses (submitted to the Institute of Physics)

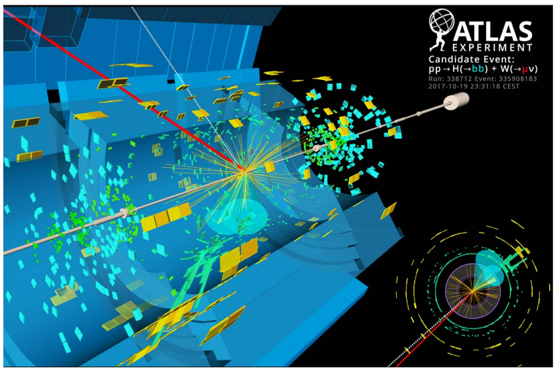
1. Dennis Weitze, “Synaptic Correlations and Volume Conduction in Simulated ECoG Signals”, 2019

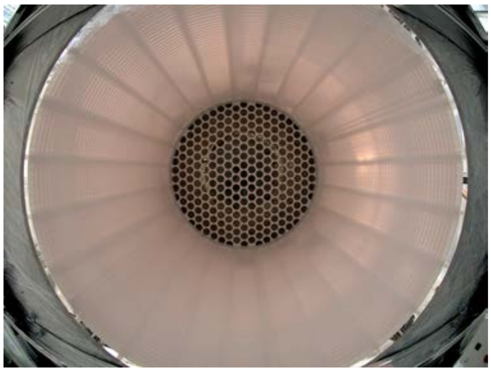
Master Theses (submitted to the Institute of Physics)

1. Lukas Friedrich, “Computational model of ocular dominance in a recurrent network with homeostatic structural plasticity”, 2019.
2. Moritz Spreter, “Homeostatic structural plasticity in the developement of feature specific connectivity and tonotopy”, 2020

Chapter 3

Particles, Fields and Cosmos





- **Experimental Particle Physics**
  Prof. B. Heinemann (IoP and DESY)

- **Experimental Particle Physics**
  Prof. G. Herten
  apl. Prof. U. Landgraf

- **Experimental Particle Physics**
  Prof. K. Jakobs
  Hon.-Prof. P. Jenni
  Emmy-Noether Group
  S. Argyropoulos

- **Experimental Particle Physics**
  Prof. M. Schumacher

- **Experimental Astroparticle Physics**
  Prof. M. Schumann
  apl. Prof. H. Fischer

- **Theory of Particle Physics and Quantum Field Theory**
  Prof. S. Dittmaier

- **Quantum Fields and Particle Phenomenology**
  Prof. H. Ita

- **Elementary Particle Phenomenology**
  Prof. J. van der Bij

- **Theoretical Astroparticle Physics**
  JProf.S. Vogl

Chapter caption: View of a candidate event for the production of a Higgs boson decaying to pair of b-quarks in association with a W boson decaying to a muon and the corresponding neutrino (left). View inside the field cage of the Time Projection Chamber of the XENONnT dark matter detector (right).

3.1 Overview

The research activities in the area **Particles, Fields and Cosmos** strive to understand the spectrum and properties of observed and hypothetical elementary particles, the laws which govern their interactions, symmetries and structures at the fundamental level, and the development of the universe. Progress on these research lines will contribute to unravel the big open questions, such as the nature of dark matter, the origin of the baryon asymmetry of the universe and the hierarchy of mass scales. To this end the analysis of the data collected in today's leading-edge experiments, precise predictions in the Standard Model (SM) of particle physics and its extensions as well as developments of new detector and computing technologies for future experiments, are performed in the area's nine research groups.

The activities of the four groups in experimental particle physics led by **B. Heinemann, G. Herten, K. Jakobs** and **M. Schumacher** focus on the participation in the ATLAS experiment operated at the European Centre for Particle Physics CERN in Geneva / Switzerland. **P. Jenni** (spokesperson of the ATLAS collaboration from 1995 to 2009) works as a Honorary Professor at our institute and **S. Argyropoulos** joined as leader of an Emmy Noether Group in October 2020. Both are associated with the group of K. Jakobs. During the term of K. Jakobs' spokespersonship of the ATLAS Collaboration from March 2017 to February 2021, **C. Weiser** acted as his substitute for teaching, research and academic administration. All groups are involved in leading roles in the investigation of the Higgs boson and in precise measurements of other SM processes (di-boson and top-quark production). An additional focus is the search for new physics, in particular for candidates of dark matter, supersymmetric particles and for the violation of fundamental symmetries. The groups also contribute significantly to the operation of the experiment, in particular in the SemiConductor Tracker (SCT, group Jakobs with permanent staff **U. Parzefall**) and the muon spectrometer (group Herten, with permanent staff **U. Landgraf** and **S. Zimmermann**) and to the development of new reconstruction algorithms and simulation tools. Another major contribution is made via the operation of the WLCG-Grid computing infrastructure (group Schumacher, with new permanent staff member **M. Böhler** since April 2020).

During the shutdown of the LHC in the years 2019 to 2021 the Phase-I upgrade took place, during which the construction of the *New Small Wheel* muon detector was finalized and successfully installed in the cavern. This international effort has been coordinated by S. Zimmermann as project leader since 2013. The upgrade of the LHC to the High Luminosity phase (HL-LHC) requires significant efforts for the Phase-II upgrade of the ATLAS experiment in both the detector and the computing areas. The groups are involved in upgrade activities for the new inner tracking detector, the muon spectrometer and the computing models and infrastructures. After successful completion of the R&D phase during the reporting period, the activities have meanwhile moved towards the detector construction, targeting installation in Long Shutdown 3 starting in 2028.

All activities are performed within the international ATLAS Collaboration and, at the national level, in the *BMBF-Forschungschwerpunkt / Collaborative Research Focus* FSP-T02-ATLAS of the German Ministry for Education and Research (BMBF), a collaboration of 14 German universities, the Deutsches Elektronen Synchrotron (DESY) and the Max-Planck-Institute for Physics in Munich (MPP). Data analysis, detector operation, computing infrastructure operation and Phase-I upgrade are funded by BMBF within the ErUM-Pro programme in the FSP-T02 ATLAS. Two specific analysis projects are funded by the German Israeli Foundation for Scientific Research and Development (GIF): group Jakobs with the Tel Aviv University (2015-2017) and group Schumacher with the Weizmann Institute of Science (2021-2023). The Phase-II upgrade activities (groups Herten and Jakobs) are funded by BMBF via the Research Infrastructure Programme *(Forschungsinfrastruktur (FIS))* in the project *Upgrade of the ATLAS Experiment for the HL-LHC*. Since 2021 the computing activities are funded seperately via the BMBF ErUM-Data programme in the *Collaborative Research Compound (CRC) Federated Computing for the ATLAS- and CMS-Experiments at the LHC in Run-3 (Comp4Run3)*. More generic R&D for novel detector technologies is performed in the international RD50 *Radiation hard semiconductor devices for very high luminosity colliders* (K. Jakobs, U. Parzefall) and RD51 *Development of micro-pattern gas detector technologies* (G. Herten, U. Landgraf, S. Zimmermann) collaborations. The Jakobs group is also involved in research projects on the application of semiconductor detectors in other areas, e.g. medical diagnosis or radiation surveillance, which are carried out in collaboration with the *Freiburg Material Research Centre (FMF)*. The generic R&D activities in the area of federated HPC and HTC computing are performed and funded by BMBF in the ErUM-Data programme within the national CRCs IDT-UM *Innovative Digital Technologies for the Investigation of Universe and Matter* (2018-2021) and FIDIUM *Federated Digital*

Infrastructures for the Investigation of Universe and Matter (since 2021) (M. Schumacher, M. Böhler), where 13 German university groups from astroparticle physics, hadron and nuclear physics and particle physics cooperate.

The experimental astroparticle physics group led by **M. Schumann** participates in the XENON experiments directly searching for dark matter at the Gran Sasso Laboratory (LNGS) in Assergi/Italy and in the proposed DARWIN project. The detectors are low-background dual-phase time projection chambers (TPCs) filled with cryogenic liquid xenon (LXe). In the reporting period, the XENON1T experiment, which still sets the most stringent constraints on WIMP dark matter over a wide WIMP mass range, was upgraded to XENONnT with a 5.9 t active LXe target. XENONnT completed its first science run end of 2021; the data is currently being analysed. The groups main responsibilities are TPC design/construction, data acquisition and analysis. In addition, the group develops low-background methods and conducts R&D towards DARWIN, a low-background astroparticle physics observatory with a neutrino-dominated background. A unique detector test platform for DARWIN is under commissioning in Freiburg. Recently the group joined the SHiP project, proposed to be installed at the SPS at CERN; Freiburg contributes to R&D on mechanics, electronics and detector performance for the Surround Background Tagger (SBT), a large-area liquid scintillator-based veto detector. The permanent lecturer **H. Fischer** leads the group's contributions to the CAST (axion search) and COMPASS (hadron physics) experiments, also located at CERN. The main contributions are the KWISP sub-detector, detector operation and analysis for CAST and DAQ/electronics and analysis for COMPASS.

The XENON/DARWIN dark matter activities are funded by BMBF within the ErUM-Pro programme via the CRCs *CRESST-XENON* (until 2020) and *CRESST-XENON-DARWIN* (since 2020), with five and six participating universities, respectively. R&D towards DARWIN is also supported by the European Research Council (ERC) consolidator grant *ULTIMATE* and by the Major Instrumentation Programme grant *DARWIN Demonstrator* funded by DFG and SIBW. The COMPASS activities and the R&D on highly-segmented detectors, e.g., usable in the SHIP experiment, are also funded by BMBF via the ErUM-Pro CRCs *COMPASS* (five university groups) and *R&D Detectors (HIGH-D)* (14 university groups). Work on an advanced construction facility for ultra-low radioactive materials at LNGS is also supported by BMBF.

The experimental activities are accompanied by strong activities in the theory groups led by **S. Dittmaier** and **H. Ita**. From 2014–2019 the theory groups were complemented by the junior group of **F. Febres Cordero**, funded by a Sofja Kovalevskaja Award of the Alexander von Humboldt foundation. Together, the theory activities 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. 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 for the physics of Higgs and electroweak gauge bosons and developed corresponding Monte Carlo programs used in analyses by the LHC experiments. Technically, both traditional Feynman-diagram-based methods as well as modern unitarity-based techniques for many-particle processes are further developed at the "next-to-leading-order" (NLO) and "next-to-next-to-leading-order" (NNLO) levels and applied in cutting-edge calculations where existing techniques are not sufficient. Besides the activities directly related to LHC physics, also more fundamental aspects of quantum field theory are analysed, such as the structure of infrared singularities, the calculation of loop scattering amplitudes, or the renormalization of quantum field theories. The theory group is integrated in important international working groups such as the *LHC Higgs Cross Section Working Group* and the *LHC Electroweak Working Group*.

The **van der Bij** / **Steinwachs** group studies aspects of quantum gravity, the origin of the universe and the uniqueness of fundamental laws.

The theoretical research was strengthened at the interface between particle physics and cosmology by the appointment of **S. Vogl** as Juniorprofessor for theoretical astroparticle physics in November 2020. His group investigates the phenomenology of physics beyond the Standard Model that is required to address some of the great puzzles of modern cosmology. A particular focus is on dark matter. The group analyzes the production of dark matter in the early Universe and works on improved methods to compute the relic density. These studies are combined with detailed analyses of the associated experimental signatures within concrete UV-complete models and a simplified model framework.

The theoretical particle physics groups receive BMBF funding via the FSP-T02 ATLAS project. The Dittmaier group receives additional DFG funding for several research projects from the Research Grants

Programme.

The experimental and theoretical particle physics groups are involved in the Helmholtz Alliance (HGF) *Physics at the Terascale* (since 2007), a national research network comprising 18 universities, two Helmholtz Centres (DESY, KIT) and the MPP, which provides additional opportunities for education in schools and workshops and exchange fora beyond the borders of experimental collaborations. All groups from the research field “Particle, Fields and Cosmos” have been involved in the successful applications for a new mass storage in the *bwSFS* framework (Baden Württemberg Storage for Science) and the HPC cluster *NEMO-2*. Both IT-infrastructures are heavily utilized by the nine research groups. All groups are participants in the consortium *PUNCH4NFDI* (43 partners from particle, astroparticle, nuclear and hadron physics and astronomy) in the framework of DFG-funded *National Research Data Infrastructure program (NFDI)*.

The application for the continuation of the DFG-funded Research Training Group (RTG) 2044 *Mass and Symmetries after the Discovery of the Higgs particle at the LHC* for the second funding period (9/2019 – 2/2024) was successful. Hence the excellent education and research environment for all doctoral researchers in the research area will be maintained. The RTG allows fostering an even closer collaboration between theory and experiment as well as between particle and astroparticle physics. The principle investigators and associated members in the new funding period are S. Argyropoulos, S. Dittmaier (deputy spokesperson), H. Fischer, B. Heinemann, G. Herten, H. Ita, K. Jakobs, A. Knue, M. Schumacher (spokesperson), M. Schumann, S. Vogl, C. Weiser, and S. Zimmermann (until 11/2020). The program continues to attract PhD candidates from other universities to carry out their doctoral research in Freiburg. The topics covered within the RTG span the entire range of research activities in theory, data analysis, and detector R&D in particle and astroparticle physics.

Particle physicists from Freiburg have a high visibility in the national and international research communities. S. Dittmaier acts as Theory Convener of the LHC Electroweak Working Group since 2017 and was member of the Theory Advisory Committee of the LHC Higgs Cross Section Working Group from 2016 to 2019 and of the BMBF Advisory and Evaluation Panel from 2014 to 2021. B. Heinemann has been member of the Particle Physics Preparation Group for the European Strategy of Particle Physics from 2018 to 2020 and member of the CERN Scientific Policy Committee from 2017 to 2023; she was recently appointed as Director for Particle Physics research at DESY, with the mandate starting in February 2022. G. Herten was member of the International Advisory Board of the Future Circular Collider (FCC) Project at CERN from 2017 to 2021. K. Jakobs was spokesperson of the ATLAS Collaboration from 2017 to 2021 and is chairperson of the European Committee for Future Accelerators (ECFA) since 2021. M. Schumacher is member of the GridKa (German WLCG Tier-1 centre) Overview Board since 2011, spokesperson of the BMBF-funded CRC ”Comp4Run3” since 2021 and deputy chair of the German committee for Particle Physics (KET) since 2021. M. Schumann is co-spokesperson of the DARWIN collaboration since 2017 and has been member of the APPEC Dark Matter Committee from 2019 to 2021.Many other mandates are listed in Section 3.3.

The changes in professorships are reported in section 1.1.4 and the promotion of four junior researchers to permanent positions at other universities in section 1.1.5. S. Zimmermann (permanent staff member in group Herten) tragically deceased in November 2020.

Future developments and plans

Prof. Ita accepted an offer by the University of Zurich and the Paul Scherrer Institut in Switzerland in November 2021 and Prof. Herten and apl. Prof. Landgraf (permanent staff member in group Herten) will retire in September 2023. To expand the research portfolio, the successor of Prof. Herten is expected to investigate flavour aspects in the quark and/or lepton sector or in studying properties of neutrinos. The successor of Prof. Ita is foreseen to work on particle physics phenomenology, covering precision physics at colliders up to new physics beyond the Standard Model. These appointments will lead to a broadening of the research activities in the area of particle and astroparticle physics, and hence will further increase the attractiveness of Freiburg. All professors will participate as principal investigators in the application for a Cluster of Excellence in the context of the DFG-funded excellence strategy initiative together with the University of Heidelberg and the Karlsruhe Institute of Technology. A first sketch of the application is currently under internal review at the three participating universities. An application for a new DFG Research Training Group (RTG) will be submitted after the successors of Profs. Herten and Ita will have been identified. The proposal will be centered around updated core research activities incorporating the activities of the new professors. The future activities of the individual groups are presented in the following sections.

3.2 Research Groups

3.2.1 Theory of Particle Physics and Quantum Field Theory – Group Dittmaier

The **Theoretical Particle Physics Group of Stefan Dittmaier** is concerned with particle phenomenology at the LHC and potential future colliders and perturbative quantum field theory (QFT), which is the most important work horse in particle theory for collider physics. In detail, major areas of research are

1. Higgs physics of the Standard Model and its extensions,
2. electroweak precision physics,
3. concepts, techniques, and tools for perturbative QFT.

In the following we highlight some typical research projects from those areas and indicate possible future directions.

Research Report

1. Higgs physics of the Standard Model and its extensions

In the previous years, several of the precision calculations performed in the group of Prof. Dittmaier for the production and decays of Higgs bosons have been generalized from the Standard Model (SM) to models with extended Higgs sectors such as a Higgs Singlet Extension of the SM (SESM) or the Two-Higgs-Doublet Model (THDM) (see, e.g., Refs. [ditt9, ditt10]). In particular, this is the case for the Monte Carlo programs PROPHECY4F and HAWK, which provide predictions for the four-body decays $\mathrm{H} \to \mathrm{WW/ZZ} \to 4$ fermions and for Higgs production via vector-boson fusion or Higgs-strahlung, respectively, at the next-to-leading-order (NLO) level. PROPHECY4F and HAWK are both used in LHC data analyses.

Although the machinery of perturbative QFT applies to most SM extensions, in many cases some subtle issues arise. An important example of this kind concerns the theoretically and phenomenologically sound renormalization of mixing angles in extended Higgs sectors. Ref. [ditt9] lists and discusses the most desirable features of a "good" renormalization scheme:

- *gauge independence,* so that renormalized observables become gauge-independent functions of the renormalized mixing angles;
- *symmetry with respect to the mixing degrees of freedom,* so that no participating degree of freedom is distinguished over the others;
- *perturbative stability,* so that no higher-order corrections get artificially large;
- *regular behaviour in the limit of mass degeneracy of mixing fields and for extreme mixing angles,* guaranteeing the applicability of the scheme in the full parameter space.

Moreover, Ref. [ditt9] proposes new renormalization schemes based on combinations of observables *(on-shell schemes)* or symmetry requirements such as rigid or background-field gauge invariance and compares their properties to previous approaches based on $\overline{\mathrm{MS}}$ schemes. Figure 3.1 shows some exemplary predictions from PROPHECY4F and HAWK for decay

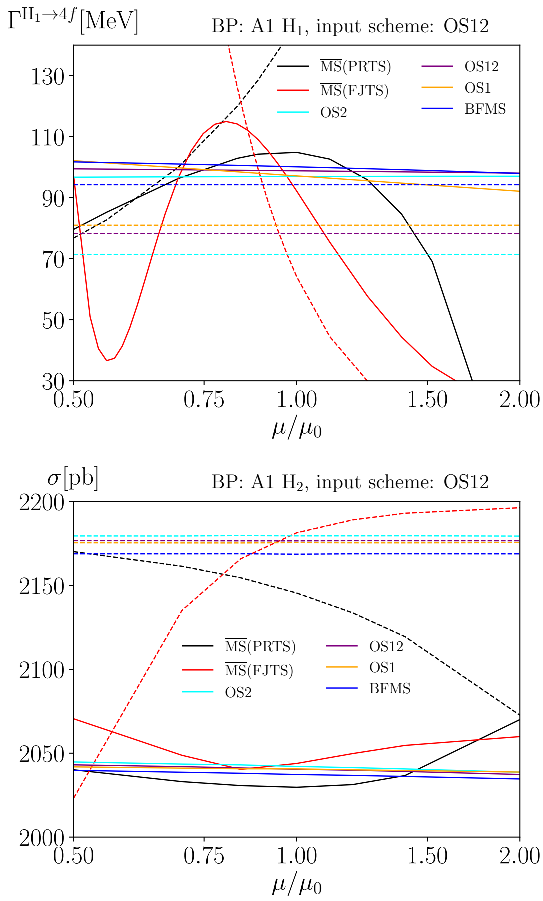


Figure 3.1: Scale dependence of the decay width $\Gamma^{\mathrm{H}_1\to 4f}$ of the heavy Higgs boson H_1 (upper plot) and cross section σ for light-Higgs-boson (H_2) production via vector-boson fusion for the THDM scenarios A1 in different renormalization schemes. "$\overline{\mathrm{MS}}$(PRTS/FJTS)" refers to different tadpole treatments in $\overline{\mathrm{MS}}$ renormalization, "OS" to on-shell schemes, and "BFMS" to a scheme based on background-field gauge invariance. LO results are shown as dashed, NLO as full lines. (For more details, see Ref. [ditt9].)

and production of the two CP-even Higgs bosons of the THDM as functions of the (unphysical) renormalization scale μ (see Ref. [ditt9] for details on the input procedure and the model scenario). The results illustrate the typical stabilization in the transition from leading-order (LO) to NLO predictions, both in the μ dependence and in the spread between different renormalization schemes, but also show that the earlier $\overline{\mathrm{MS}}$ schemes suffer from stability problems.

2. Electroweak precision physics

Most of our present-day knowledge about electroweak interaction results from precision studies of the weak gauge bosons W and Z at particle colliders. In the previous years, the first successful analyses of the scattering of electroweak gauge bosons and of triple gauge-boson production at the LHC mark another milestone in the area of electroweak physics. Both classes of processes have a great sensitivity to physics beyond the SM in the sector of gauge interactions and serve as windows to the mechanism of electroweak symmetry breaking complementary to studies of Higgs bosons. The corresponding theory predictions comprise complete NLO calculations for $2 \to 6$ particle scattering processes which are at the frontier of current capabilities.

Following its long tradition of precision calculations for electroweak gauge-boson production processes, the AG Dittmaier in recent years provided NLO predictions for WZ scattering [ditt8], which is observed in complex processes like $\mathrm{pp} \to \mu^+\mu^-\mathrm{e}^+\nu_\mathrm{e}\mathrm{jj}+X$ at the LHC, and for WWW production [ditt5], as for instance observed in $\mathrm{pp} \to \mu^+\mu^+\mathrm{e}^- + 3\nu + X$ at the LHC. Figure 3.2 illustrates the complexity of the contributing Feynman diagrams. Figure 3.3 shows a typical NLO prediction for a differential cross section, demonstrating the importance of the corrections, which can reach the size of some 10%. Including the corrections clearly reduces the scale uncertainty of the prediction, which is indicated by the bands underneath the LO (blue) and NLO (black) predictions.

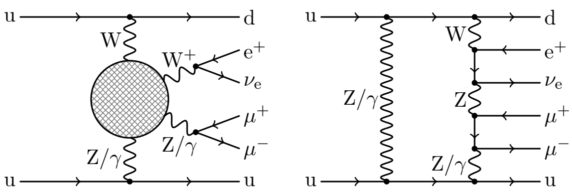


Figure 3.2: Structural LO diagram for WZ scattering in the uu channel (left), with the blob representing all tree diagrams for the $\mathrm{WZ}/\gamma \to \mathrm{WZ}/\gamma$ subprocesses, and exemplary one-loop diagram of the $\mathcal{O}(\alpha^7)$ NLO electroweak corrections (right) for the process $\mathrm{pp} \to \mu^+\mu^-\mathrm{e}^+\nu_\mathrm{e}\mathrm{jj}+X$.

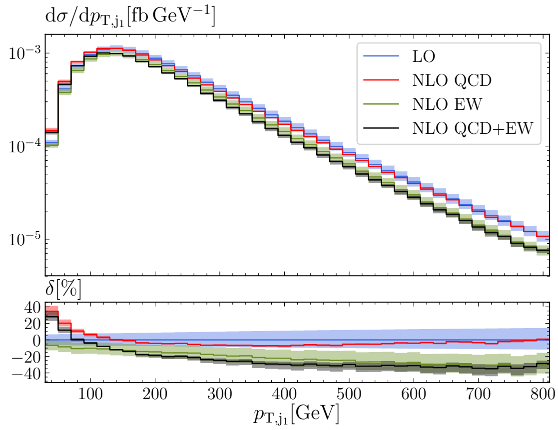


Figure 3.3: Transverse-momentum distribution of the hardest jet in $\mathrm{pp} \to \mu^+\mu^-\mathrm{e}^+\nu_\mathrm{e}\mathrm{jj}+X$ at the LHC with CM energy 13 TeV. Upper panel: LO contributions of order $\mathcal{O}(\alpha^6)$, the two NLO predictions [$\mathcal{O}(\alpha^7)$ (NLO EW) and $\mathcal{O}(\alpha_s\alpha^6)$ (NLO QCD)] as well as their sum. Lower panel: relative NLO corrections δ with respect to the LO in percent. (Taken from Ref. [ditt8].)

3. Concepts, techniques, and tools for perturbative QFT

The above examples show typical results of "NLO multi-leg calculations" with internal resonances, which are only possible due to the tremendous progress in the perturbative evaluation of QFT made in the last decades, a process to which the AG Dittmaier made substantial contributions (see, e.g., the review [ditt4]). Several advances were driven by postdocs of the group, such as the development of the amplitude generator OpenLoops [ditt7] (P. Maierhöfer) and the precision Monte Carlo programs Bonsay [ditt5, ditt8] (C.Schwan) and MoCaNLO [ditt8] (M. Pellen, senior postdoc of RTG2044).

Each higher level reached in accuracy (either by a higher loop order or higher particle multiplicities) and each step beyond the SM potentially bears new aspects or issues that need a higher level of understanding of QFT. The renormalization issues with Higgs mixing angles [ditt9] discussed above are an example of this kind that concerns SM extensions. The mentioned NLO calculation for the WZ scattering process $\mathrm{pp} \to \mu^+\mu^-\mathrm{e}^+\nu_\mathrm{e}\mathrm{jj}+X$ provides another within the SM, where the high multiplicity brought in a new effect. This NLO calculation revealed a singularity resulting from the electroweak splitting $\gamma^* \to q\bar{q}$ in the limit of collinear (quark-induced) jets, an effect that cannot be described perturbatively. In Ref. [ditt6] this problem was solved by introducing a non-perturbative *photon-to-jet conversion function* that is related to the experimentally determined hadronic vacuum polarization via dispersion relations. As a final example where the shift to higher orders touches upon subtle QFT issues, we mention the issue of electric charge renormalization to all perturbative orders, which was worked out in Ref. [ditt2].

In recent years, the research focus in the AG Dittmaier gradually went beyond the NLO level. For instance, P. Maierhöfer and collaborators developed the multi-loop integral reduction program KIRA [ditt3], which is one of the leading tools in the field. KIRA is used in the group in current two-loop calculations.

Future Plans

Owing to the great potential of Higgs and electroweak precision physics at the LHC and possible future e^+e^- colliders, the main research lines, as described above, will be continued in the near and medium-term future. Of course, specific directions will be adapted to developments in the field and to new experimental directions:

- Current and planned precision calculations for processes with electroweak gauge bosons and Higgs bosons aim at next-to-next-to-leading order electroweak and mixed strong–electroweak corrections relevant for the phenomenology at the LHC and potential future e^+e^- colliders. Investments in programs like KIRA will certainly pay off in those projects.
- In the area of physics beyond the SM, the focus will further shift to models with different portals to dark matter and/or heavy neutrinos, to address the known phenomena that are unexplained by the SM most directly. In particular, we will study the constraints of electroweak precision observables on such models.
- To further boost the new developments, we have started to work on Effective Field Theories (EFTs), a direction that is mainly driven by M. Stahlhofen in the AG Dittmaier. In the SM, variants such as *Soft–Collinear EFT* offer new possibilities to address higher-order effects both in the strong and electroweak interactions. Beyond the SM, heavy-particle effects can be described by higher-dimensional EFT operators, an ansatz that is also supported by current and future experimental analyses. Recently, in Ref. [ditt1] we have proposed a method to integrate out heavy fields directly in the path integral, which goes beyond other variants proposed in the literature in various respects (e.g. renormalization) and offer manifold future applications.

3.2.2 Experimental Particle Physics – Group Heinemann

The **Experimental Particle Physics Group of Beate Heinemann** is concerned with the study of the interactions between electroweak gauge bosons at the LHC. Heinemann has a joint appointment with DESY and here only her activities that directly involve the junior group members in Freiburg are described.

The interactions between electroweak gauge bosons is precisely predicted in the Standard Model but might be altered if there are new phenomena beyond the Standard Model. The most prominent example is that the cross section for pair production of longitudinally polarized $W^\pm$ bosons at pp colliders increases faster than the total pp cross section, and thus would violate unitarity at $\sqrt{\hat{s}} \approx 1.4$ TeV if there were no new physics mechanisms to prevent this. The study of both triple and quartic couplings between the gauge boson is an important part of the exploration of the electroweak energy scale, in addition to the precision measurements of the Higgs boson. The results are often interpreted in the context of effective field theories.

Research Report

W^+W^- Cross Section

We are contributing to the differential cross section measurements of W^+W^- production, in close collaboration with DESY. The analysis is carried out for the case where one of the W-boson decays to $e^\pm\nu_e$ and the other to $\mu^\mp\nu$. The two largest and most challenging backgrounds are $t\bar{t}$ production and dijet or W+jet events where the jet was misidentified as an isolated lepton, and we have made important contributions to both of them. For the $t\bar{t}$ background we developed a new method that is using directly the data and has a small sensitivity to the theoretical modeling of $t\bar{t}$ production. The background due to misidentified jets (mostly hadrons decaying leptonically) was also measured carefully by members from our group. We have already published cross sections for $W^\pm W^\mp$ production in association with one jet with the full Run-2 dataset [hein1], and are now working on the inclusive measurement and the measurements with zero and two jets. Fig. 3.4 shows the cross section as a function of the transverse momentum of the jet compared to several Monte Carlo generators. Preliminary studies show that we will significantly improve the precision compared to the previous measurement based on 35 fb^{-1}.

$W^{\pm}W^{\pm}$ Cross Section

The production of two W bosons with the same electro charge occurs primarily via electroweak processes, where two W bosons from the two protons interact via an echange of a neutral boson or a quartic interaction. The cross section for QCD processes is strongly suppressed, making it one of the best channels to study quartic interactions. Previously, with the 2015+2016 data, the process $W^{\pm}W^{\pm}+2$ jets with $W \rightarrow \ell\nu$ ($\ell = e, \mu$) was observed and the inclusive cross section was determined with a precision of about 20% [hein2]. The measurement of the full Run-2 data will include differential cross section measurements and improve the precision. We have played a leading role here and determined all important backgrounds (fake leptons, charge misidentification and WZ events), the event selection, the unfolding and the final fit including all systematic uncertainties. This analysis is at present in the internal review of the ATLAS collaboration. In addition, we are working on determining the cross section for longitudinally polarized $W^{\pm}$ bosons, based on a deep neural network.

Technical Contributions to ATLAS

The group of Heinemann has also contributed to the operation of ATLAS and the construction of the New Small Wheel. Two PhD students (Solomon and Fernandez Pretel) did their qualification task on projects for the New Small Wheel working with the group of Herten. Kuprash made major contributions to the trigger: leading the event data model (EDM) group 2019-2022 and the release and validation group 2016-2018. The EDM group was crucial for the preparation for the software for Run 3 as it needed to substantially reduce the size of trigger objects on the AOD to reduce the overall data size.

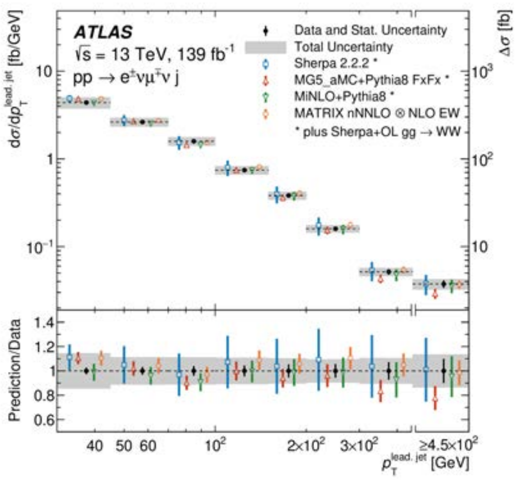


Figure 3.4: The $W^{\pm}W^{\pm}+1$ jet cross section as function of the jet transverse momentum. The data are compared to four different Monte Carlo generators [hein1]

Future Plans

In the future, at ATLAS we plan to analyse the $W^{\pm}W^{\mp}$ data in view of possible contributions from axion-like particles that couple to W bosons. A first analysis was carried out [hein3] based on published data and we will optimize the analysis to maximize the sensitivity. For the $W^{\pm}W^{\pm}$ analysis we plan to measure the cross section for $W^{\pm}W^{\pm}$ production via double-parton scattering. In addition, with the Run-3 data we will again measure the cross section for electroweak production of $W^{\pm}W^{\pm}+2$ jets, extract the longitudinally polarized component, and combine the result with the Run-2 data.

In addition, Heinemann started a new experimental activity at DESY called "Laser Und XFEL Experiment" (LUXE) [hein5]. The electron beam of the European XFEL will be brought in collision with low-energy photons from a very high-intensity laser to study QED in the non-perturbative regime and to search for axion-like particles [hein6]. It is planned that students from Freiburg will also be involved in this activity, in particular the search for axion-like particles.

3.2.3 Experimental Particle Physics – Group Herten

The **Experimental Particle Physics Group of Gregor Herten** has about 20 members with the four senior scientists, Gregor Herten, Andrea Knue, Ulrich Landgraf, Stephanie Zimmermann († November 2020). The research activities in the past four years were concentrated on the muon chamber upgrade and the data analysis of the ATLAS experiment.

By 2018, a large amount of data had been recorded with the LHC at the proton-proton center-of-mass energy of 13 TeV. The year 2019 marked the beginning of the long shutdown, during which major upgrade projects of the detector were undertaken. The largest of these projects, the muon New Small Wheels (NSW), involved key contributions from the working group. Fig. 3.5 shows the moment of construction of both wheels when the left wheel was just completed. The long-time project leader of the NSW (S. Zimmermann) was a member of our working group. By the end of the 2021, the required detector components were completed and both NSWs were installed into the ATLAS cavern. Therefore the NSW will be available for data taking in 2022. That achievement has been a great and rewarding success after a long period of intense R&D and construction effort.

Another focus of the activities was on data analysis. Several analysis were performed with the full data set of 139 fb^{-1} at a proton-proton center-of-mass energy of 13 TeV. In the search for supersymmetry, an important analysis based on events with jets and missing energy was successfully completed and published. The exclusion ranges of the SUSY parameters could be significantly extended [hert2, hert7]. Another focus in the analysis was the measurement of the properties of the top quark [hert3, hert4] and the coupling of the top quark to the Higgs boson in $t\bar{t}H(H \to b\bar{b})$ events [hert1, hert5, hert6]. In addition, the group was able to significantly improve the detection of heavy flavour decays using new machine learning (DNN) methods. This offers many opportunities in future ATLAS data analyses with the hope to improve previous results significantly.

Research Report

Myon detector and New Small Wheel

One of the main activitiy of the working group was in the area of the ATLAS muon detector and in particular the completion of the NSW. The excellent technical and personal capabilities of the machine shop in the Physics Institute were a crucial asset for us in this work. Many components for the NSW were developed in Freiburg, manufactured in the workshops, and installed and commissioned at CERN. Due to severe technical difficulties delays occurred in the start of the Micromegas (MM) chamber production. However, after an intensive R&D effort of the NSW teams, a solution was found so that production could start, advance quickly and the installation of the NSW could be completed in time for the LHC Run-3, starting in 2022.

Figure 3.5: Both New Small Wheels during the construction phase.

Cooling system and alignment

In addition to the already mentioned contributions, our group took over the responsibility for the cooling system of the NSW. Cooling the electronics of the new Micromegas and sTGC muon chambers presents a particular challenge. Several thousand metal cooling plates had to be machined in Freiburg with high precision to connect to all electronic front-end chips over the whole area of the wheels. Since the NSW is only poorly accessible, the cooling must function very reliably. To avoid leaks of cooling liquids, the system is operated with less than 1 bar pressure. Because of the large static pressure difference due to the height of the NSW (8 m), the available pressure range for operation is very limited. All work was successfully completed by the time the wheels were installed in the ATLAS cavern, so that all cooling channels are now functioning as planned and the NSW can be operated.

A precise muon alignment system is crucial for achieving the ultimate muon momentum resolution. Already for the existing ATLAS detector the precise alignment bars for the endcap were fabricated and measured by our group. In this work we profit from the very large 3D-coordinate measurement machine (CMM) in our group. For the NSW 32 alignment bars were fabricated and measured. The alignment bars were mounted on the structures of the NSW at CERN. This involved ensuring that all muon chambers were properly detected by the cameras mounted on the bars. Overall, the construction of the alignment project was very successful and was completed on time.

Data Control System (DCS) and Database
Due to the long experience in the field of the detector control system (DCS), our working group continued this activity for the MDT subdetector of the muon system and for the NSW. For Run-3, starting in 2022, the DCS system had to be modified and partially redesigned because of the newly installed NSW detectors. The overall schedule was met, so that the system can now be deployed and verified with the first measurements with LHC beams. Everything will be operational as planned for the start of Run-3 in 2022.

Members of the working group have developed a database system with which the production parameters of NSW chambers are documented, tracked and statistically analyzed. The parameters are essential to create appropriate calibration and correction data during data collection and in the data analysis.

Software development
Muon performance work took place in a wide variety of areas of the NSW and, in particular, the Micromegas software. The simulation of the MMs was improved and adapted to real detector conditions.

Processing capacity is a limiting factor for the performance of the ATLAS experiment software infrastructure. In order to improve processing throughput, the ATLAS software framework is currently being converted to a multi-threaded architecture that takes advantage of parallel processing. Our group has contributed to this effort by updating and rewriting several modules of the ATLAS software package for the muon spectrometer.

Data Analysis

Search for supersymmetric particles
Previous successful work in inclusive searches for supersymmetric particles ('0-lepton analysis') was continued with the full data set. This analysis is sensitive to a wide range of parameters in SUSY models. In particular, in 'Natural SUSY' scenarios, gluinos are expected to be relatively light and should be observable in Run-2 of the LHC. The new analysis using the full data set was completed and published [hert2]. Although no evidence for the existence of supersymmetric particles could be found, the obtained exclusion limits of SUSY parameters are very important. They allow to exclude many models with SUSY particles in the range of 1 TeV, which were preferred from a theoretical point of view before the start of the LHC.

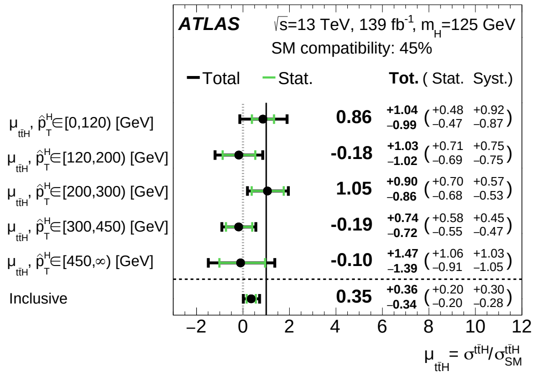


Figure 3.6: The signal strength in $t\bar{t}H(b\bar{b})$ in the 1-lepton channel for intervals in the Higgs p_T and for an inclusive measurement [hert1].

Measurement of Higgs boson production in $\mathbf{t\bar{t}H(H \to b\bar{b})}$
A precise measurement of the Yukawa coupling of the top quark is an important test of the Standard Model (SM). If the Yukawa coupling deviates significantly from the expected value (about 0.997), this would be an indication of physics beyond the SM. A direct measurement is only possible in events where the Higgs boson is produced together with one or two top quarks (tH and ttH production). However, the production rate of ttH events is kinematically suppressed due to the high mass of the t-quark. Therefore, the most common decay of the Higgs boson, into a $b\bar{b}$-pair, is used in the analysis. The disadvantage of this channel is the very large background due to the production of $t\bar{t}b\bar{b}$ events. Since the signal and background have the same signature in the detector, it is not easy to distinguish between both processes. The focus of the analysis was on the measurement of the inclusive effective cross section and the simplified effective cross section measurements. The analysis was successfully completed with the entire data set and published [hert1]. The result of the signal strength measurement is shown in Fig. 3.6.

Precise measurement of the top-quark mass
The entire Run-2 data set is used to measure the top quark mass more precisely than in our previous publication [hert3]. Machine learning techniques are important tools to obtain a purer reconstruction of the top quark mass. Another focus was on studies

of the simulation uncertainties, which could be reduced successfully. The limiting factor for the total uncertainty is currently on jet energy scale uncertainties, so the main focus of the analysis is on reducing these uncertainties.

Improvement of the heavy-flavour tagger

For many data analyses, the efficient selection of heavy quarks, b and c, is essential to suppress the background of lighter quarks. This is important for all analyses involving top quarks, since a b-quark is almost always emitted in the decay of the top quark. For the selection of b-quark jets one uses the fact that these quarks are relatively long-lived. The b-quark selection programs (b-taggers) are elaborate and complex. As part of a PhD thesis, studies were carried out in the research group to increase the efficiency of the existing b-tagger. Machine learning methods (Deep Neural Network DNN) were used for this purpose. With these methods and other advancements, a significant improvement was achieved; the suppression of jets of light quarks was improved by a factor of 2 with the new tagger. Within the ATLAS collaboration, the new tagger will be used for many analyses in the future, which is expected to lead to many more accurate measurements. The PhD student, whio dis this work, received the 2021 ATLAS thesis award.

Future Plans

Due to retirement of G. Herten and U. Landgraf in September 2023 the working group will officially end its activities at that time. External funding is available to complete all PhD theses and research responsibilities in ATLAS until the end of June 2024. On this time scale we plan, together with the NSW community, to publish several articles about the R&D activities, the lessons learned during construction and the performance of the NSW in the upcoming data taking. Our results and experience will be very valuable for other groups who plan to construct a similar muon detector in the future.

In the data analysis the main goal is to complete and publish the analyses on top quark and Higgs boson physics. The ongoing four PhD theses related to data analysis should be completed by June 2024.

3.2.4 Quantum Fields and Particle Phenomenology – Group Ita

The **Theoretical Particle Physics Group of Harald Ita** is concerned with precision predictions for hadron-collider experiments at the high-energy regime which will match the precision of the upcoming measurements at the LHC. Most recently the group has extended its research towards gravitational-wave astronomy. The central ambition of this research is to provide predictions for compact binary systems for LIGO and its follow-up observatories.

The research is focused on scattering amplitudes, which allow to obtain transition probabilities of particle collisions at hadron colliders, as well as for compact massive objects, such as astrophysical black holes. During the last five years the group could contribute and often lead a number of developments:

1. Advance the state of the art in perturbative QCD by providing new scattering amplitudes with increased precision and multiplicity of the final-states particles,
2. contribute predictions of relativistic effects for compact binary systems,
3. develop a new numerical approach in perturbative quantum field theory (QFT), which exploits the physical properties of scattering processes in conjunction with concepts in number theory and computational algebraic geometry.

The research is founded in QFT with strong links to high-energy particle physics, formal field theory, as well as general relativity.

Research Report

Amplitude methods

In principle QFT gives a clear prescription for computing scattering amplitudes in a perturbative expansion in coupling constants; depending on the expansion order and particle content sums of Feynman diagrams have to be integrated over kinematic variables. The diagrams' closed loops determine the expansion order and the required integration steps. In practice the computation of scattering amplitudes is hugely complex due to the large number of Feynman diagrams, the multi-dimensional integration and challenging efficiency demands in Monte-Carlo integration for cross-section computation. In order to meet these demands compact analytic forms of scattering amplitudes are crucial. Unfortunately obtaining analytic expressions through algebraic algorithms is often forbiddingly challenging, even with large scale computational facilities. During the last years we have developed a new computational paradigm in perturbative QFT to address these challenges. We use numerical algorithms to first obtain numerical values of the amplitudes and, in a second step, 'reconstruct' analytic expressions from sufficient numerical samples. Both steps are done in number fields that exclude rounding errors, namely finite fields (integers modulo a prime number). The amplitude computations are often referred to as the 'numerical unitarity method', which exploits the amplitudes' unitarity properties to reduce limiting combinatoric complexity of textbook approaches.

In a series of papers we have constructed the numerical unitarity method suitable for Standard Model particles and interactions [ita1, ita2], and have developed strategies to reconstruct the amplitudes analytic forms. This work is implemented in the C++ program 'Caravel' [ita6] for multi-loop computations in field theory.
We have developed a similar approach for the computation of Feynman integrals. This relies on deriving differential equations for the integrals, which reduce the number of integration variables, and identifying crucial components, that can be computed numerically [ita5]. Furthermore the first-order partial differential equations are reduced to one-dimensional systems, which are straight forward to integrate.

The state of the art in amplitude computation is arguably defined by our most recent computation of the $W+2$-jet scattering amplitudes. A representative diagram is displayed in Fig. 3.7. The amplitudes are

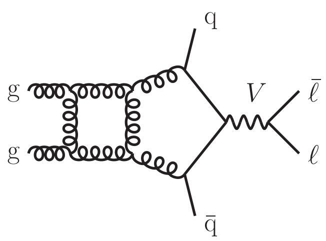


Figure 3.7: Example diagram of two loop contribution to $pp \to W+2-$jet process.

published in analytic form and are written in terms of six kinematic variables. The reconstruction of the analytic form uses several 100k numerical evaluations. We could demonstrate that mathematical properties of the functions will allow to reduce the number of evaluations further. We also demonstrated that the reconstruction of the analytic forms can be trivially parallelised and is well suited for high-performance computing facilities such as the local NEMO cluster. Based on these observations we anticipate that percent-level predictions for two-to-three processes will become broadly available in the coming years. The newly obtainable QCD amplitudes are a central contribution to such predictions. In order to reach this goal we have to increase the state from six to nine parameters, i.e. two final-state masses and a mass parameters for top-quark contributions. Some of the variables may be treated as numerical constants making this an achievable challenge.

Amplitudes for LHC phenomenology

We have obtained a new class of multi-particle predictions for hadron colliders with two-loop scattering amplitudes for three-jet production [ita9], three photon production and first results for $W+2$-jet production [ita10]. In Fig. 3.8 we demonstrate that the stable numerical evaluation of the three-jet amplitudes by comparing to a reference computation. In order

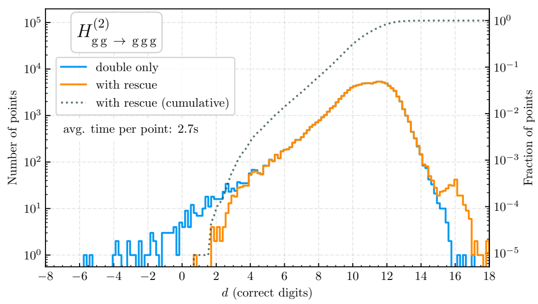


Figure 3.8: Numerical stability and evaluation time for the two-loop $pp \to 3$-jet amplitudes over phase space.

to gauge the complexity of these results, one can refer to the timeline of progress: the related two-to-two four-parton amplitudes appeared 20 years ago, and depend on two kinematic variables. The recent two-to-three particle processes depend on up to six kinematic variables. The phenomenological impact of these results are percent-level predictions matching upcoming measurements of the ATLAS and CMS experiments. The physics potential of multi-particle predictions is to access new production processes and the interactions' kinematic dependence. Such measurements will advance the high-energy understanding of the Standard Model and increase the experiments' reach in indirect new-physics searches.

Predictions for gravitational binary systems

In 2016 gravitational waves were directly observed by LIGO and associated to black-hole merger events. In the coming decade the precision and reach of the observations will drastically increase with the planned Einstein Telescope, the Cosmic Explorer and the space-borne LISA mission. Precise theory predictions are required for the discovery of gravitational-wave signals in strain-data, and play an important role for the characterization of sources.

The coalescence processes of compact binary systems is partially accessible in perturbative field theory based on the Einstein-Hilbert action. A diagrammatic representative of gravitational-wave exchange of two black holes is depicted in Fig. 3.9. In particular the initial inspiral takes place in the

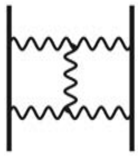


Figure 3.9: Feynman diagram contributing G^3 post-Minkowskian corrections to the binary black-hole potential. The straight lines represent black holes, wavy lines represent gravitational-wave exchange.

weak field regime, such that its dynamics can be obtained from the classical limit of scattering amplitudes. This approach provides perturbative corrections in the Newton constant G, the so called post-Minkowskian corrections. This field theory approach advances the field in two ways: 1) new methods from field-theory computations in particle physics can be exploited. 2) the conventional post-Newtonian approach is a simultaneous expansion in the Newton coupling and orbital velocity. The post-Minkowskian approximation resums velocity corrections and yields relativistic predictions advancing the predictions for excentric orbits and extreme mass-ratio systems.
Overall perturbative predictions for the inspiral phase complement predictions in numerical relativity, which are computationally expensive when sampled over large phase spaces.

We could already contribute to the perturbative field-theory approach to compact binary systems. We have demonstrated that our numerical field-theory method is effective for the computation of gravity amplitudes, by completing the two-loop four graviton-scattering amplitudes [ita4], which originally allowed Goroff, Sagnotti and van de Ven to demonstrate that Einstein gravity diverges in the ultraviolet. In Ref. [ita3] we obtained the classical scattering angle in high-energy binary systems, which contributed to validating the field-theory approach. The transfer of methods from QCD to gravity was later substantiated in Feynman-integral calculus [ita7]. Finally, we could contribute to the state-of-the-art computation of the order G^4 corrections to the conservative binary black-hole potential [ita8].

3.2.5 Experimental Particle Physics – Group Jakobs

The main activity of the **Experimental Particle Physics Group of Karl Jakobs** is the investigation of proton-proton collisions at the highest energies in the ATLAS experiment at the LHC. The group has been involved in all aspects of the experiment, starting from the conceptual design, the detector construction and commissioning, detector operation, studies of the detector performance, physics analysis and in the detector upgrade programme towards the High-Luminosity phase of the LHC (HL-LHC). In addition, research and development activities on silicon-based tracking detectors are carried out. The major areas of research during the past years (2018 – 2021) are:

1. Analysis of the ATLAS Run-2 data (Higgs boson physics, searches for supersymmetric particles, Standard Model (SM) processes);
2. Detector performance studies (e and τ identification, b-tagging);
3. Operation of the ATLAS detector with focus on the SemiConductor Tracker (SCT);
4. Construction of the new ATLAS Inner Tracking (ITk) detector for HL-LHC;
5. Research and development (R&D) on silicon detectors.

Research Report

Higgs boson physics

The focus in Higgs boson physics in Run 2 moved towards improving the measurements of Higgs boson parameters and establishing couplings to fermions. In 2018 the ATLAS Collaboration presented the observation of both the associated ttH production as well as the observation of $H \to b\bar{b}$ decays. This constituted a major achievement; together with the previously observed $H \to \tau\tau$ decays the couplings to fermions were unambiguously demonstrated. The large Run-2 dataset, corresponding to an integrated luminosity of 139 fb^{-1}, was used to carry out important differential cross-section measurements based on the Simplified Template Cross Section (STXS) approach.

Our group participated in the $H \to \tau\tau$, $H \to b\bar{b}$ and $H \to WW^*$ studies and contributed significantly to the above-mentioned observations. Given our broad involvement, we were also well positioned to contribute to the determination of the Higgs boson coupling parameters via the combination of measurements.

For $H \to WW^*$, both the gluon fusion and the vector boson fusion production modes were investigated. A major contribution of our group was the development, implementation and validation of the statistical model to extract the final results as well as the evaluation of systematic uncertainties. Results based on data collected in 2015 and 2016 were published [jak1]. The studies were continued to include the full Run-2 dataset and measurements of cross sections were performed in 11 STXS bins. Preliminary results, normalised to the SM predictions, are shown in Fig. 3.10. In this analysis also the observation of the vector boson fusion mode in this decay channel was demonstrated for the first time.

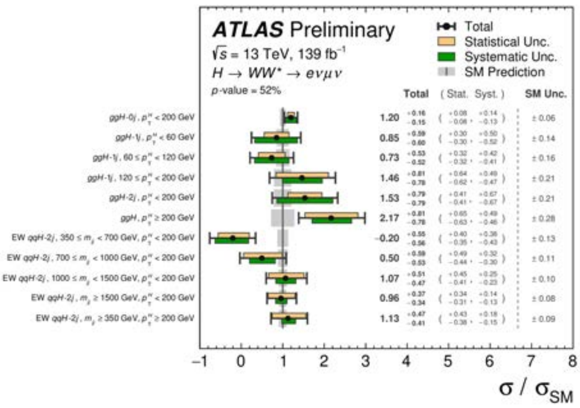


Figure 3.10: Best-fit values and uncertainties for the $H \to WW^*$ cross sections measured in the STXS categories, normalised to the corresponding SM predictions.

After the observation of the $H \to b\bar{b}$ decay mode in 2018 the focus in this channel moved to the measurement of STXS cross sections for different bins of transverse momentum. Based on the full Run-2 dataset the observation of the $H \to b\bar{b}$ decay in the ZH (WH) process with a significance of 5.3 (4.0) standard deviations was published [jak2]. Our group continued to play a leading role with focus on the determination of systematic uncertainties, where new methods were developed, as well as on the validation of the statistical model and on the extraction of the final results.

Studies of $H \to \tau\tau$ decays were continued by ATLAS in order to determine the Yukawa coupling with the best possible precision as well as to study other important aspects like e.g. CP properties (see Section (3.2.7), Group Schumacher). The studies focused mainly on the precise measurement of vector boson fusion mode with contributions of gluon fusion at large transverse momenta [jak3]. Our group contributed substantially to these studies. Major responsibilities were the optimisation of the event selection based on multivariate methods as well as the final signal extraction.

In the combination of the various Higgs boson measurements, a leading role was taken in the combination effort based on data collected from 2015 to 2017 [jak4]. The publication of results using the complete Run-2 dataset is in preparation; preliminary results on extracted coupling modifiers are shown in Fig. 3.11 (assuming only SM contributions to Higgs boson decays and loop processes). The measurements impressively confirm the relations between particle mass and coupling strength, as expected for the SM Higgs boson.

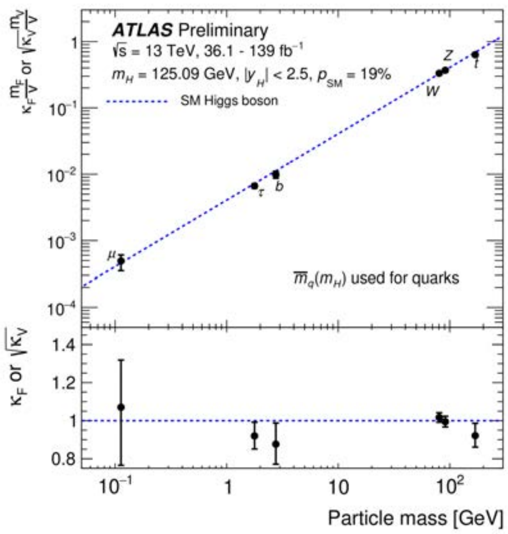


Figure 3.11: Reduced coupling-strength modifiers for fermions and weak gauge bosons as a function of their masses. The SM prediction is shown as a dotted line.

Searches for Physics Beyond the Standard Model

Our group contributed significantly to the search for supersymmetric partners of the top quark. Two analyses were carried out, one considering final states with missing transverse energy and one lepton and the other one considering final states with missing transverse energy and multiple jets. Including the full Run-2 dataset, no significant excesses over the SM background expectation were found and the SUSY parameter space could be further constrained. In Fig. 3.12 the excluded regions are shown for various decay scenarios for the fully hadronic analysis [jak5]. In the scenario where $m_{\tilde{t}} > m_t + m_{\tilde{\chi}_0^1}$, top squark masses are excluded in the range 400-1250 GeV for $\tilde{\chi}_0^1$ masses below 200 GeV at 95% confidence level.

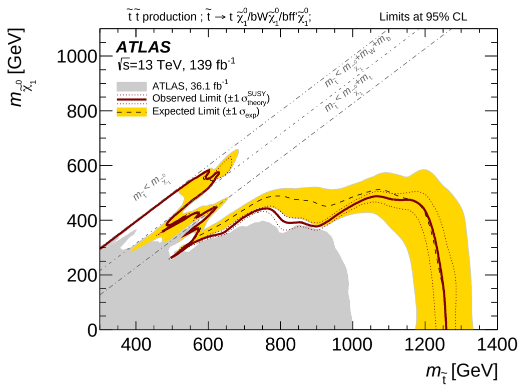


Figure 3.12: Observed (red solid line) and expected (black dashed line) exclusion contours at 95% CL as a function of the $\tilde{\chi}_0^1$ versus stop masses.

Results based on the analyses with one charged lepton were extracted under co-leadership of a member of our group [jak6]. In comparison to previous analyses the gain in sensitivity – in addition to the larger dataset – is due to the exploitation of new observables and the application of recursive neural networks developed in our group. In this analysis also additional signal regions are designed specifically to search for spin-0 mediators that are produced in association with a pair of top quarks and decay into a pair of dark-matter particles.

Our group also participated in a leading role in the combination of searches for new physics, and their impact on constraining dark-matter models and the parameter space of minimal supersymmetric extensions of the Standard Model.

Measurement of WW production

The production of like-sign $W^{\pm}W^{\pm}$ pairs is a key signature for the investigation of the electroweak scattering of two vector bosons and thereby of the study of electroweak symmetry breaking. Our group made key contributions to the 6.5σ observation of this important process in Run 2 [jak7]. We achieved a significant reduction and better understanding of important backgrounds (WZ production, fake leptons and background resulting from mis-measured electric charges).

Detector performance

We participated in a visible way to improvements of the reconstruction of final state signatures. The contributions focused on the reconstruction and identification of electrons, tau leptons and on the identification of b-quark jets (B tagging). In addition, we continued to work on improvements of the ATLAS fast calorimeter simulation which was initiated in our group. These contributions are essential for improved physics analyses that rely on an efficient reconstruction of particle signatures and a precise knowledge of reconstruction and identification efficiencies.

Detector operation

Our group has participated in the design and construction of the SemiConductor Tracker (SCT) and thereby carries responsibility for its operation. During Run 2, scientists from Freiburg were involved in the detector operation. One of them took the role as SCT Run Coordinator and led important studies on the radiation damage of silicon sensors as a function of the integrated luminosity collected. In addition, the evolution of other important detector parameters, like depletion voltage, efficiency and noise were studied [jak8]. Further contributions were made to the alignment of the inner tracking detector.

Upgrade of the ATLAS Tracking Detector (ITk)

In the framework of the BMBF programme *Forschungsinfrastruktur ATLAS* for the upgrade of the LHC experiments for HL-LHC, groups from Germany (HU Berlin, DESY, Dortmund and Freiburg) have committed to construct one complete endcap of the new silicon strip tracker [jak9]. Freiburg has major responsibilities in the development, test and procurement of electronic components (hybrids, power boards), in the test and assembly of modules and in the mounting onto larger petal structures. During the past years the design of the electronics components has been completed and the relevant ATLAS reviews (Final Design and Production Readiness) have been successfully passed. First prototype series of sensors and electronics components have been produced and the first complete, electrically functional petal with modules of all endcap geometry types has been built in Freiburg (see Fig. 3.13). Overall the work on this ambitious project is well advanced, although due to the massive impacts of the Corona pandemic, delays have been accrued. They are, however, in line with those accumulated by other groups and we are confident that the recently updated CERN schedule will allow us to deliver the ITk on time for installation in Long Shutdown 3 (LS3).

R&D on silicon detectors

Towards establishing the concept of the ITk detector, our group has contributed substantially, within the RD50 Collaboration, to the development of more radiation hard silicon detectors [jak10]. At present

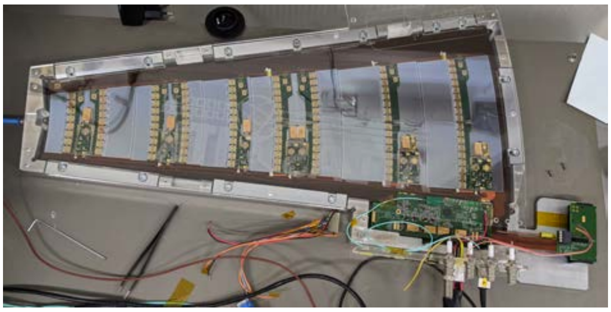


Figure 3.13: Test of the first electrical petal of ATLAS (built in Freiburg) in our clean room.

our R&D activities are concentrated on CMOS sensors and detectors for fast timing for future colliders. CMOS sensors are investigated for pixel and strip configurations, with a view of integrating front-end electronics. In the fast timing domain we investigate the application of 3D-detectors as an alternative to Low Gain Avalanche Detectors.

Future Plans

The focus over the next years will lie on the full exploitation of the physics potential of the ATLAS experiment with data collected at the slightly increased LHC energy of 13.6 TeV and on the completion of the ITk. We plan to continue the detailed investigation of the Higgs boson in the $H \to WW$ and $H \to \tau\tau$ decays, with improved measurements and interpretations in Effective Field Theories. Capitalizing on our experience, we plan to extend our activities to search for di-Higgs production in the $HH \to b\bar{b}\ \tau\tau$ decay mode. This channel is expected to contribute substantially to the sensitivity of the combined Run-2 and Run-3 data on HH production and thereby in constraining the Higgs boson self coupling. In the search for extensions of the SM, more emphasis will be given to the exploration of Dark Matter scenarios. In addition, we plan to get engaged in physics studies for future e^+e^- and hadron colliders.

A large fraction of the group, with the support of the Electronic and Mechanical Workshops of the Institute, will be fully occupied with ITk module building and testing. High priority will be given to this activity as its successful completion is vital for the future physics programme of ATLAS.

In the detector R&D area, we plan to continue our work on the investigation of the application of silicon detectors for fast timing and of integrated CMOS sensors for strip-like tracking detectors (large pixels or short strips) for future colliders.

3.2.6 Emmy Noether Group – Group Argyropoulos

The **Emmy Noether Group of Spyridon Argyropoulos** focuses on searches for new physics using Higgs boson signatures, aiming to shed light on the unresolved problems at the interface of particle physics and cosmology: dark matter (DM), dark energy (DE) and the generation of the matter-antimatter asymmetry ("baryogenesis").

The group was established in October 2020, employing a postdoctoral (Dr. T. Moskalets) and two doctoral researchers (R. Küsters, I. Kalaitzidou) and it is hosted by the AG Jakobs.

Research Report

Electroweak baryogenesis

Electroweak baryogenesis models reproduce the observed matter-antimatter asymmetry via the dynamics of the electroweak symmetry breaking. This requires the introduction of two Higgs doublets that give rise to five Higgs bosons: A (CP-odd), H, h (heavy, light CP-even) and H^+, H^-.

A necessary condition for electroweak baryogenesis is a large mass splitting $m_A - m_H \gtrsim 250$ GeV, which renders $A \to ZH$ the dominant decay mode. The H boson decays almost exclusively either to a pair of top or bottom quarks depending on whether m_H is above or below the top-pair production threshold.

The group has initiated two new searches in the $A \to Z(\ell^+\ell^-)H(t\bar{t})$ and $A \to Z(\nu\bar{\nu})H(b\bar{b})$ channels, in order to cover the whole m_H range. Searches in these final states have not been performed so far at collider experiments, therefore these analyses will cover a previously unexplored parameter region, complementing the existing results from other final states. A publication is expected in 2023.

Dark Matter

It it known that particles that could serve as DM candidates should have small interaction rates with SM particles. A possibility that has started being explored relatively recently at the LHC is for DM particles to interact with SM particles exclusively via the exchange of Higgs bosons.

Our group has led the search for DM in the final state with a SM Higgs boson decaying to b-quarks and missing transverse energy (known as "mono-Higgs"), which provides the tightest constraints in a large region of parameter space. The search has been published in [arg2] constraining models with vector and pseudoscalar mediators.

A combination of the aforementioned search with other final states is under way, with preliminary results published in [arg4] and a publication expected in 2022.

An invited review article compiling the DM constraints from the LHC searches and comparing to direct detection experiments for a series of DM models has been published in [arg3], with our collaborating partner Dr U. Haisch (MPI Munich).

Event generators and flavour tagging

The group is also participating in studies targeting the improvement of the performance of the ATLAS detector and event generators.

In the area of flavour tagging, we are investigating the impact of fake tracks on the b-tagging algorithms and developing new techniques to identify b-jets without relying on tracking information (an effort initiated by AG Jakobs). These are particularly important for the identification of high-momentum b-jets that arise in the $A \to ZH$ search and also highly displaced b-jets that arise in models with exotic Higgs decays and DE [arg3].

In the area of event generators, the group is working on the parametrisation of theory uncertainties with modern Machine Learning methods (a project initiated by AG Jakobs) and on the improvement of the modelling of the processes involving heavy-flavour hadrons.

The above studies are expected to lead to two publications in 2023.

Future Plans

The second funding period of the Emmy Noether group (2023-2026) will coincide with the Run 3 data-taking period. The aim of the group during this period will be to put direct and indirect constraints on dark sector models using the available data.

Direct constraints on DM will be placed by an extension of the previous mono-Higgs search [arg2]. An interpretation of this search in the context of DE models, where missing energy is expected to arise from DE candidate particles, is also planned in collaboration with Prof. Dr. C. Burrage (Nottingham).

Indirect constraints on DM/DE models will be placed using measurements of the production of the SM Higgs boson in association with a Z-boson decaying to neutrinos [arg1]. These are expected to provide model-independent limits on dark sector models, thus complementing the constraints from the direct searches.

3.2.7 Experimental Particle Physics – Group Schumacher

The **Experimental Particle Physics Group of Markus Schumacher** focuses (a) on the investigation of the discovered Higgs boson and the mechanism of electroweak symmetry breaking and searches for violation of fundamental symmetries based on data collected by the ATLAS experiment at the LHC and (b) on the advancement of models and tools for distributed HPC and HTC computing and data management on heterogeneous compute resources.

The major activities in the area of data analysis are:

- Higgs-boson cross section measurements in the $H \to \tau\tau$ decay mode
- Searches for CP violation (CPV) in Higgs-boson production via vector boson fusion (VBF)
- Searches for lepton flavour violating (LFV) Higgs-boson decays
- Searches for Higgs-boson pair production in the $HH \to bb\tau\tau$ final state

Our group also successfully continued and extended their efforts to the determination of the efficiency for trigger signatures arising from hadronically decaying τ-leptons, to the modelling of backgrounds with τ-leptons via the so-called embedding method and the measurement of the integrated luminosity.

The major activities in the area of R&D for federated computing are:

- Integration of the HPC cluster NEMO as opportunistic resource in the ATLAS compute workflow
- Development of a smart caching prototype
- Advancement of the *HammerCloud* monitoring framework

In addition to these R&D activities our group has operated the local ATLAS-Tier-2 grid-center *ATLAS-BFG* in the context of the Worldwide LHC computing Grid (WLCG) with very high reliability and availability and contributes in a significant way to the successful operation of the whole cloud of Tier-2 centers around the Tier-1 center GridKa via performance evaluations and monitoring efforts. The activities in this area are headed by the new permanent faculty member Michael Böhler. This position was realized following the recommendations of the SAB in the last evaluation.

Research Report

Data analysis at the ATLAS Experiment

During Run-2 of the LHC (2015-2018) the data set collected by the ATLAS experiment has increased significantly. The analysis of this data allows to perform measurements of cross sections and parameters with unprecedented precision and to set most stringent limits on phenomena of new physics. Our group has contributed in leading or major role to the following measurements and searches:

Higgs-boson measurements in the $H \to \tau\tau$ decay

With the analysis of the data from 2015 and 2016 (1/4 of the full Run-2 data set) the observation of the decay mode $H \to \tau\tau$ with a significance of 6.4 σ could be established [schumach1]. The full Run-2 data set allowed to measure the global strength as $\mu = \sigma/\sigma_{SM} = 0.93^{+0.13}_{-0.12}$ [schumach4] and to measure cross sections in the different production modes and in specific phase space regions called Simplified Template Cross Sections (STXS) (see Fig. 3.14) [schumach2]. So far no deviation from the predictions in the SM have been observed. Our group contributed to many aspects of the analysis (e.g. optimization of event selection and of the definition of the event categories). Our group is responsible for the advancement of the statistical model, the extraction of the results and their interpretation. The results have been included in the combination of all decay modes [schumach3, schumach4, schumach5]. Our group was responsible for the inclusion of the results from $H \to \tau\tau$ decay and their validation.

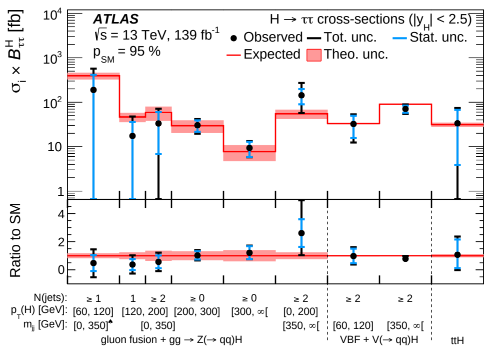


Figure 3.14: Measurement of STXS cross sections.

Search for CPV in VBF Higgs-boson production

CPV is a necessary ingredient to explain the observed baryon asymmetry of the universe. New sources of CPV beyond the SM e.g. in the Higgs sector are needed in order to explain the observed magnitude. A test of CP invariance in VBF Higgs boson production exploiting the $H \to \tau\tau$ decay using the data from 2015 and 2016 has been performed using the method of Optimal Observables. The analysis was led by our group. The investigation of two out of three final states and the overall combination and statistical interpretation were conducted by us. No hints for new CP-violation were observed (see Fig. 3.15) and the most stringent limits on a CP-violating parameter in the context of an effective field theory (EFT) were derived [schumach6].

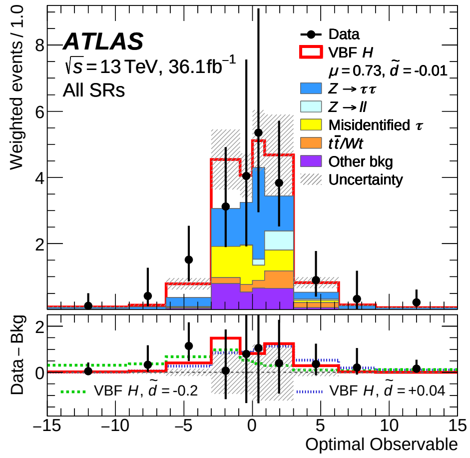


Figure 3.15: Distribution of the optimal CP-odd observable. No hints for CPV are observed

Search for LFV in Higgs-boson decays

LFV was observed in the form of neutrino-oscillations in the neutral lepton sector. LFV in the charged lepton sector is predicted in many extensions of the SM and can be searched for e.g. in Higgs-boson decays $H \to \tau e(\tau\mu)$. The analysis based on the first quarter of the Run-2 data is published [schumach7]. Our group contributed to several aspects of the analysis. For the search in the $e\mu 2\nu$ final state based on the full Run-2 data the data-driven symmetry method for the estimation of the major backgrounds has been advanced and applied. The complete analysis is done by our group in collaboration with the group of Dr. Shikma Bressler from the Weizmann Institute of Science (WIS). Recently the results have been unblinded.

Search for Higgs-boson pair production

The measurement of the cross section of Higgs-boson pair production allows to directly constrain the Higgs-boson triple self-coupling and to reconstruct the shape of the Higgs potential. The search is performed for the first time in the final state originating from $HH \to bb\tau\tau \to bbee(e\mu,\mu\mu)4\nu$. The full search for non-resonant inclusive production is performed by our group. The estimated sensitivity yields a limit corresponding to 10 times the SM prediction and hence will significantly contribute to the overall combination for HH searches at the ATLAS experiment.

Federated HPC and HTC computing

The data rates and volumes at the High Luminosity (HL) LHC pose huge challenges on the computing models and infrastructures. In order to meet these requirements significant changes in the compute model are foreseen e.g. opportunistic usage of HPC clusters and the concentration of the mass storage at a few sites, which is part of the so-called data-lake model. The realization of these new concepts require major R&D efforts and their benchmarking. As a test bed for most developments the HPC cluster NEMO hosted at the compute center in Freiburg is used.

<u>Integration of NEMO in the ATLAS workflow</u>
In order to integrate NEMO as an opportunistic resource in the ATLAS compute workflow the whole ATLAS-specific software stack and services have to be provided via virtualization and an interface called "meta scheduler" had to be deployed. This technology has been developed, implemented and successfully validated by our group [schumach8]. Further on, a sophisticated monitoring tool was developed, which allows to analyze performance data and to optimize operational parameters [schumach9].

<u>Development of a smart caching prototype</u>
In the data-lake model smaller sites as Freiburg will provide no mass storage to the WLCG. In order to allow efficient analysis of remotely stored data at the Freiburg Tier-2 site a smart caching solution for temporary storage of files had to be deployed, so that users do not observe any major difference between locally and remotely stored data sets. The prototype setup was benchmarked with a typical user analysis. For remote sites in Germany no significant difference has been observed, while for sites which are far away like TRIUMF some overhead can be observed (see Fig. 3.16), which can be minimised by the caching setup.

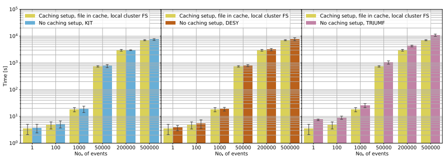


Figure 3.16: Comparison of analysis time for remotely stored files and locally stored files.

<u>Advancement of the *HammerCloud* framework</u>
The *HammerCloud* (HC) monitoring and benchmarking framework is used for evaluating the performance of all WLCG (CMS and) ATLAS sites and guarantees a certain site quality by auto-excluding faulty sites. The framework was continuously adapted to various changes in the compute model. To optimize the performance the *job shaping tool* was developed and validated, which allows to speed up the auto-exclusion and recovery decisions made by the HC framework [schumach10] .

Future Plans

Data analysis at the ATLAS experiment

The recorded data set will at least double during the upcoming Run-3 of the LHC (2022-2025). This will allow to continue and extend the above mentioned research activities with higher statistical sensitivity, but also with novel analysis methods e.g. based on new methods of machine learning for classification, regression, anomaly detection and unfolding. The test of CP invariance in the Higgs sector will be extended to probe also the effective coupling to gluons and the coupling to τ-leptons. New likelihood models will be developed and the interpretation will be extended to more EFT operators. The search for LFV will be extended also to other hypothetical gauge and Higgs bosons and will use newly developed methods for anomaly detection in close cooperation with the group of S. Bressler at WIS. A new project is the measurement of the anomalous magnetic and electric dipole moments of the τ-lepton in ultra-peripheral lead collisions. This will be conducted by Valerie Lang (junior temporary staff), who received independent funding for this project via the BW Eliteprogramm for Postdocs. New applications for funding in the framework of the BMBF action plan ErUM-Pro and in the new Nexus program of GIF are foreseen.

Federated HPC and HTC computing

The activities to develop models for HPC and HTC computing on federated resources will be extended in order to solve the challenges at the HL-LHC. The main focus will be on the development of "AUDITOR: <u>A</u>ccoU<u>n</u>ting <u>D</u>ata handl<u>I</u>ng <u>T</u>oolbox for <u>O</u>pportunistic <u>R</u>esources", which will be of uttermost importance to use HPC resources such as provided by the newly installed National High Performance Computing Centers (NHR) in an opportunistic and transparent way. Smaller projects concern the advancement of smart caching solutions within the data-lake model and the optimization of the whole workflow with respect to efficiency and sustainability. New applications for funding in the framework of the BMBF action plan ErUM-Data are foreseen.

Further ideas

It is foreseen to extend the research activities by joining another collaboration e.g. the LUXE experiment planned at DESY and to contribute to their efforts to search for light scalar dark matter candidates and axion-like particles.

3.2.8 Experimental Astroparticle Physics – Group Schumann

The **Experimental Astroparticle Physics Group** of **Marc Schumann** focuses on the detection of new particles from the "dark sector" of the Universe with low-background detectors. Neither the particle(s) that makes up the galactic dark matter nor other dark particles (dark photons/scalars, axions/ALPs, heavy neutral leptons, dark mediators etc.) have been detected yet, despite the plethora of theories predicting such particles and the many experiments searching for them [schumann1].

The group (which includes the activities of Prof. Fischer, Sect. 3.2.9) is involved in several projects exploring the dark Universe: The main activity is the direct detection of dark matter in the form of WIMPs (weakly interacting massive particles) in dual-phase time projection chambers (TPCs) filled with cryogenic liquid xenon (LXe). The XENONnT experiment, currently running at the Italian LNGS underground laboratory, is one of the most sensitive detectors thanks to its ultra low-background. Its predecessor XENON1T still sets the most stringent constraints for most WIMP masses and interaction models. In addition, the group is one of the leading institutions in the R&D activities towards DARWIN, a LXe TPC capable to explore the entire accessible WIMP parameter space before the background is dominated by irreducible neutrino interactions.

The group has recently joined the SHiP experiment which is proposed to be installed at a new beam-dump facility at CERN. Once more, the instrument's background needs to be minimal to detect decays of hidden sector particles created in the dump. The new SHiP activities ideally extend and complement the group's expertise and replace the discontinued CAST activities at CERN (see Sect. 3.2.9).

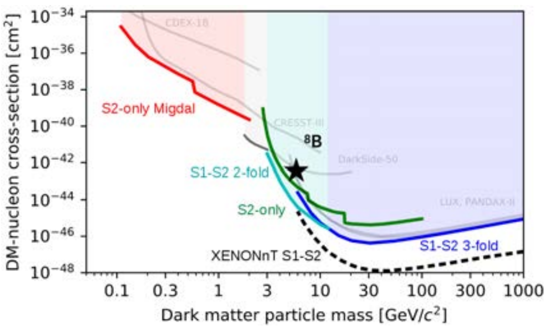


Figure 3.17: The XENON1T constraints on spin-independent WIMP-nucleon interactions are the most stringent for most WIMP masses >180 MeV/c^2. The projected XENONnT sensitivity is shown by the dashed line.

Research Report

XENON: Dark Matter Search at LNGS

The activities comprised operating and analyzing XENON1T, a dual-phase TPC with a 2.0 t active LXe target, and the construction and installation of its upgrade XENONnT (5.9 t target), followed by commissioning and the first science run.

XENON1T observed no signal in a 1 t×yr exposure and placed some of the most stringent constraints on WIMP-nucleon interactions. The results for spin-independent interactions are summarized in Fig. 3.17: the analysis based on the simultaneous detection of light (S1) and charge signals (S2) in the TPC, with a threshold defined by a 3-fold PMT coincidence requirement for the S1 signal, led to the most stringent limits for WIMP masses $m_\chi \geq$ 6 GeV/c^2 (blue) [schumann10]. This is the most important result from XENON1T; the analysis was coordinated by a Freiburg PostDoc. Lowering the threshold by reducing the PMT coincidence level increased the background but excluded new parameter space at lower m_χ (cyan). An analysis using only the charge signal ("S2 only", green) reduced the threshold even more and placed limits down to $m_\chi = 3$ GeV/c^2 [schumann7]. Interpreting this data with the Migdal effect, a predicted but not yet observed phenomenon which is expected to enhance the signal, pushes the best limits from XENON1T down to $m_\chi > 180$ MeV/c^2.

Two more results from XENON1T gained lots of attention and demonstrate the impressive potential of LXe TPCs to detect ultra-rare processes: (i) XENON1T observed the two neutrino double electron capture process of ^{124}Xe. This rare 2nd order weak decay has a half-life of $T_{1/2} = 1.8 \times 10^22$ yr – the largest one ever measured directly [schumann9]. (ii) The low-energy electronic recoil background spectrum (i.e., from particles scattering off the atomic electrons) shows a $> 3\sigma$ excess of events above the background model. This excess could be caused by novel backgrounds (e.g., ^{3}H) or by new physics such as solar axions, ALPs or a large neutrino magnetic moment [schumann3].

The origin of the excess will be clarified by **XENONnT** which was constructed during this reporting period. Freiburg coordinated the TPC working group and focused on the large TPC field cage and the optimization of its electric fields. Many TPC components were produced in Freiburg's workshops. The team coordinated the disassembly of XENON1T at LNGS and participated in the installation of XENONnT (Fig. 3.18). Freiburg is also responsible for the data acquisition (DAQ) system of XENONnT, a triggerless system based on the successful sys-

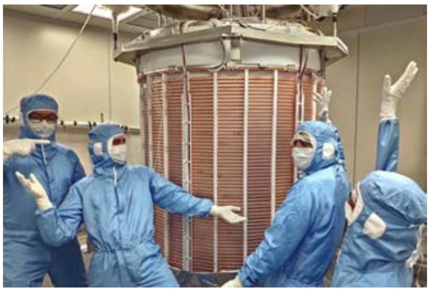


Figure 3.18: Members of the astroparticle physics group after successfully transporting the XENONnT TPC to its final location in the water shield at LNGS.

tem delivered for XENON1T [schumann8], and coordinated the Monte Carlo simulation efforts: based on measured radioactivity contributions and a detailed detector model, the sensitivity of XENONnT to detect WIMP dark matter was predicted [schumann2]. With a planned exposure of 20 t×yr XENONnT will be about 30× more sensitive than the XENON1T result (see Fig. 3.17).

DARWIN: The low-background LXe observatory

DARWIN will be a LXe detector with a background dominated by irreducible neutrino interactions. This implies that the background from ^{222}Rn, dominating current detectors, has to be reduced significantly. With a proposed target mass of 40 t, the cylindrical DARWIN TPC will be ~2.6 m in size, imposing severe challenges for detector construction, e.g., for the electrodes required to establish the fields in the TPC.

Figure 3.19: The new LXe detector test platform in the astroparticle physics laboratory in Freiburg.

The group conducts R&D to identify solutions to some of the most relevant challenges for DARWIN. In the last year, **PANCAKE** has been set up in the laboratory in Freiburg (see Fig. 3.19), a worldwide unique detector test platform to operate flat detector components up to 2.7 m diameter in a shallow LXe environment; prime examples for such components are DARWIN's TPC electrodes. PANCAKE is currently under commissioning and will be first used to examine improved electrodes for XENONnT. In addition, the small-scale LXe test platform XeBra is used to investigate novel ways to build LXe TPCs addressing the above-mentioned challenges of ^{222}Rn reduction and stability of large-scale TPC electrodes.

The Freiburg team was also leading DARWIN's "Science and Sensitivity" working group. Using detailed Monte Carlo simulations, a background model for the DARWIN baseline design was established to study the sensitivity to new science channels: DARWIN will be able to measure low-energy solar pp-neutrinos with unprecedented precision and will be able to compete in the search for the neutrinoless double beta decay of ^{136}Xe, even without expensive isotopic enrichment [schumann5].

Low-background Techniques

Rare-event detectors require low-background materials and components. Two important methods to identify such materials are γ-spectrometry and the measurement of Rn-emanation. Freiburg's low-background **γ-spectrometer GeMSE** is installed underground in the Swiss Vue-des-Alpes laboratory. Apart from the participation in material selection campaigns (GeMSE measured most of the new XENONnT PMTs) the facility has a dedicated meteorite program in collaboration with geologists: the detection of short-lived isotopes in meteorites allows for terrestrial age dating [schumann6]. Over the last years GeMSE was upgraded to ease remote operation and to improve analysis; the background level was reduced. A **Rn-emanation chamber** was successfully built and set up in Freiburg. It collects the ^{222}Rn atoms (daughters from the ^{238}U chain) emanated from all material surfaces and measures their concentration via α-spectroscopy. It is now used for routine measurements.

SHiP: A Beam Dump Experiment CERN

SHiP aims at detecting hidden sector (HS) particles produced by interactions of an intense beam of 400 GeV protons in a massive beam dump at CERN. Depending on the specific model the HS particles are expected to decay into standard model particles ($\ell\pi$, ℓK, $\ell\ell(\nu)$, $\pi\pi$, $\gamma\gamma$,) in a ~50 m long decay volume. Energy, production/decay vertex and PID of the decay products will be measured. SHiP's zero-background goal will be achieved by a combination of detector design, analysis cuts and active vetoes.

The Freiburg group is involved in the R&D activities for the Surround Background Tagger (SBT). It instruments the decay volume walls with liquid scintillator (LAB)-filled cells of variable size (typical

$0.8 \times 1.2 \times 0.3\,\mathrm{m}^3$ and is required to reduce the background from μ/ν deep inelastic scattering. The light generated by particle interactions is read out by two WOMs (wavelength-shifting optical modules) per cell, PMMA tubes inserted into the scintillator guiding the photons to arrays of 40 SiPMs. The group focuses on the realization of a full-scale 2×2 cells prototype for test beam campaigns, contributing to mechanics (vessels, support structure), electronics/readout of the WOMs as well as simulations (see Fig. 3.20).

Future Plans

The **XENON** activities will concentrate on detector operation (in particular the DAQ system under Freiburg's responsibility), possible upgrades, as well as the full exploitation of the science data. The astroparticle group will use its state-of-the-art **low-background facilities** for material selection and the meteorite program. Minor detector improvements are foreseen to continuously optimize their performance.

A MoU has been recently signed between **DARWIN** and the US-based competitors from the LZ experiment to work together towards a joint LXe-based observatory at the DARWIN scale or even larger. The group's LXe detector development activities will mainly focus on this instrument, making use of the local large-scale detector test platform PANCAKE with the clear goal to remain among the leading DARWIN groups. The R&D efforts on alternative TPC designs will also be continued; the recent observation of proportional scintillation signals generated in LXe in the laboratory in Freiburg provides a very interesting case which warrants further study.

The major milestones of the **SHiP** activities will be testbeam campaigns at DESY in late 2022 (single SBT cell) and at CERN in fall 2023 (2×2 cell array). Apart from indispensible insights into detector operation and performance, the prototype will allow developing reconstruction algorithms and tuning the Monte Carlo model. Provided sufficient funding can be secured the SHiP/SBT activities will be expanded.

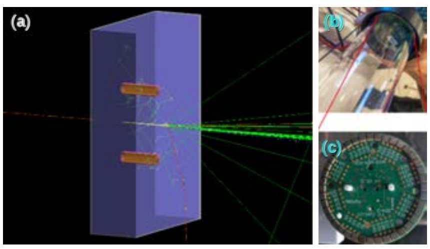


Figure 3.20: Simulation of a 6 GeV electron impinging on a SHiP SBT cell (a). Two WOM tubes (brown, b) read by an array of 40 SiPMs (c) detect the created light.

3.2.9 Experimental Astroparticle and Hadron Physics – Group Fischer

The **Experimental Particle Physics Group** of **Horst Fischer** is concerned with searches of new particles and measurements of the internal structure of the nucleon, both with experiments at CERN.

Research Report

In recent years the focus of the **CERN Axion Solar Telescope** (CAST) shifted from solar axions towards relic axions and chameleons. Two kind of radio frequency cavity detectors were installed to search for non-relativistic axions in complementary mass ranges. The CAST-RADES detector, consisting of 5 sub-cavities coupled by inductive irises, was sensitive for axions with a mass around 34.67μeV [fisch1]. The second detector, CAST-CAPP, consists of four 0.4m long rectangular cavities, each with the ability of a fast frequency tuning in a wide range of 660 MHz to reach out for a mass from 19.74μeV to 22.47μeV. Given the absence of a persistent RF signal, a 90% upper confidence limit was set on the axion-photon coupling down to $g_{a\gamma\gamma} = 8 \times 10^{-14}$ GeV^{-1} (see Fig. 3.21).

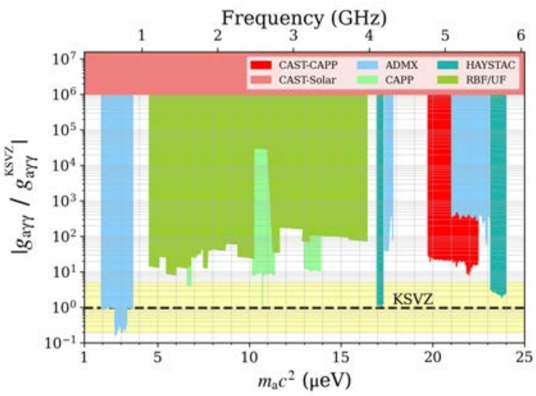


Figure 3.21: Exclusion limit on the axion-photon coupling as function of the axion mass, compared to other axion search results within the mass range 1-25 μeV and predictions by of one of the most popular models (KSVZ).

The so called Chameleon mechanism introduces a scalar field with an effective mass that increases with the local matter density. In high-density regions this characteristic leads to a weak fifth force which can be tested in the laboratory. While this force remains hidden in tests of general relativity it can become significant in low density regions and have cosmological consequences. Chameleons would be produced in the solar tachocline and stream unimpeded to Earth. The KWISP detector looked for tiny displacements of a thin membrane, caused by the mechanical recoil of solar chameleons and measured by the response of an optical resonator. Membrane movements as low as 37.2fm have been excluded, corresponding to a limit on the recoil force of $F_{lim} = 44 \pm 18$pN [fisch2].

In summer 2021 CAST was outphased but the experimental equipment will remain in place to become a visit point for the public.

The **COMPASS** experiment comprises a state-of-the-art spectrometer with a unique polarized target. Here our group is responsible for front-end electronics and has strong participation to the data analysis. COMPASS is one of the well-recognized leaders in the field of measurements related to hadron structure and spectroscopy studies and has been addressing a variety of physics topics related to Transverse Momentum Dependent [fisch8] and Generalized Parton Distributions (GPDs) [fisch4]. Measurements of pseudoscalar or vector mesons produced in hard exclusive lepton-nucleon scattering provide important data for phenomenological parameterization of GPDs. Against widely accepted expectations, strong contributions from transversely polarized virtual photons to the production of spin-0 mesons have been measured [fisch5]. In the GPD formalism, such contributions arise from helicity flip of the active quark coupled to a twist-3 meson wave function. This finding is supported by our observation of unnatural parity exchange in the transition of longitudinally polarized virtual photons to transversely polarized vector mesons [fisch6].

Future Plans

The size of the proton is a fundamental quantity as the proton is the only stable composite system made from quarks and gluons. The spatial extension of the proton's charge can be measured through both the spectroscopy of bound systems and elastic scattering. As both methods should lead to the same result, the disagreement of precision spectroscopy of muonic hydrogen and elastic electron scattering came as big surprise. It has led to many debates on principle issues concerning the measuring methods, experimental effects, data analysis and new physics like lepton non-universality. The **AMBER** Collaboration, successor of COMPASS, aims at a new measurement using for the first time elastic muon-proton scattering to resolve some discrepancies and firmly refute some hypothesis presently discussed [fisch9]. Probing the radius of the proton by muons spares many experimental issues and profits from small necessary corrections owing to radiative processes.

3.2.10 Theory of Particle Physics and Quantum Field Theory – Group van der Bij

It is understood nowadays, that the universe came into existence as a quantum fluctuation of the vacuum followed by a rapid expansion of space; this is known as the inflationary universe scenario. There are various models that can describe inflation. For a correct description one needs to do quantum field theoretical calculations in the presence of gravity and also study the question of quantum gravity itself. Typically one adds extra fields, studies non-minimal couplings of matter with gravity and uses higher order terms in the Riemann-tensor. Different approaches towards quantum gravity can be studied. Recent results gained with gravitational wave detectors point towards a rather large abundance of black holes in the universe, which might be explained by the creation of so-called primordial black holes during inflation.

During the last decades the search for extensions of the standard model was based on the paradigm of the so-called hierarchy problem, a.k.a. the naturalness problem, related to the naive presence of quadratically divergent corrections to the Higgs-boson mass. The formulation and the relevance of the problem was always somewhat unclear, but it led to many rather complicated extensions to the standard model, for instance supersymmetry. These extensions have been refuted by experiment by now. So it is time for a paradigm shift away from naturalness and massive extensions of the standard model towards the question why the standard model is right. So, if one wants to understand why nature is the way it is, one has to look for a new principle.

Research Report

Questions related to quantum gravity, extensions to gravity and effects in the early universe were studied both on the technical level and with respect to observations in the early universe. In ref.[vdbij1, vdbij2] the Wheeler-DeWitt equation was used. The WDW equation is a canonical approach to quantum gravity. Scalar fields can couple to gravity in ways that are different to ordinary minimal coupling. The difference can be quite large and will also change quantum effects. The formalism was developed and applied to the early universe. Effects would show up in the density fluctuation spectrum, that one measures as temperature variations in the cosmic microwave background. The non-minimal couplings increase

the quantum-gravitational effects, however they stay too small to be observable.
It is well known that at the classical level f(R) theories and scalar-tensor theories are equivalent. The extension to the quantum-level was studied in ref.[vdbij3, vdbij4]. Whereas the off-shell formulations maybe different, the on-shell theories were shown to be equivalent at the quantum level.
Galileons are a new class of scalar field models, related to theories where the graviton can become massive. In ref.[vdbij5] quantum effects were calculated and presented in a geometric formulation.
In modified theories of gravity, as used in inflationary models, solutions to the Einstein equations get modified. Such modifications were studied in ref.[vdbij6].
The interplay between models of inflation and the production of primordial black holes was studied in ref.[vdbij7, vdbij8].
Furthermore work was done on Hořava gravity and theories with vector fiields.

As mentioned in the introduction, a principle different from naturalness is needed. In ref.[vdbij9, vdbij10] a slightly extended version of the principle of relativity was introduced, involving also the topology of spacetime. In combination with a non-perturbative gravitational anomaly, some interesting conclusions were reached. The gauge group of nature should be SU(5), there should be exactly three generations of fermions, the standard model is the only allowed low-energy theory in the chiral sector and there is a preferred candidate form of dark matter, namely triplet fermions. This is the only argument in the literature, that explains why there are exactly three generations; the problem goes back to 1936. In general only minimalistic extensions of the standard model are allowed, meaning, extensions that do not change the chiral structure of the standard model. Typical extensions are non-chiral fermions, Stückelberg-like vector bosons and singlets in general. A number of such extensions were studied. The most relevant for LHC-physics is a new class of Higgs-models, where a higher dimensional scalar mixes with the simple Higgs-field. The theory is renormalizable and hardly constrained by present-day experiment. It has the potential to lead to large anomalous Higgs self-couplings, without changing the Higgs-signal itself much. A prediction of the theory is a change in the line-shape of the Higgs boson. This can only be studied with a very large lepton collider, which was originally proposed for this purpose. In the meantime there are large-scale international efforts towards the design of such a collider.

Future Plans

Besides further efforts in model building, in the future we hope to gain a better understanding of the underlying mathematics of the previous results. For this the focus of research will shift more towards mathematical physics. In teaching it is planned to continue the offering of term-paper seminars in mathematical physics together with the mathematics department. So far we had three seminars. The subjects were: exactly solvable models, string theory, classical solutions in gauge theories (fibre bundles).

3.2.11 Theoretical Astroparticle Physics – Group Vogl

The **Theoretical Astroparticle Physics Group of Stefan Vogl** investigates the phenomenology of physics beyond the Standard Model (SM) on the interface between particle and astrophysics. The group was established in November 2020 and currently consists of the group leader and one doctoral researcher (J. Bollig).

The work of the group focuses on dark matter, neutrino physics, and the collider phenomenology of new physics. In particular dark matter is an exciting topic of current research. Astrophysical observations show that luminous matter cannot account for the bulk of the gravitational mass in many systems and a new, "dark" kind of matter is required to explain their behavior. The need for additional gravitating matter has been confirmed spectacularly by cosmology which shows clearly that conventional matter only makes up about one-fifth of the total matter content of the Universe. The known particles cannot explain DM and, therefore, this is a clear sign of physics beyond the SM. The puzzle of what governs the dynamics at the largest scales thus turns into a challenge of our understanding of fundamental physics at the smallest scales. This is very exciting since it makes the search for DM truly interdisciplinary and new insights at either end of the length range can have profound implications on completely different scales.

Research Report

Collider searches, direct detection and indirect detection experiments, astrophysical surveys, and cosmological observations are currently making huge progress. Their success has turned the search for DM into the spearhead of our quest for the fundamental laws of our Universe. However, only a joint effort across the different fields and close collaboration between theory and experiment will allow to make the most of the new data. The research of the group of JProf. Vogl focuses on two strategically chosen topics within this dynamic field.

Dark matter production in the early Universe

From a theoretical perspective, one of the most startling questions regarding DM is its origin. On the one hand, understanding how DM was produced and which role other particles in a possibly extended dark sector played in the early Universe is essential to fill the gaps in our picture of modern cosmology. On the other hand, DM production is also exceedingly important from a practical point of view since many signatures of DM are related to its history in the early Universe. Thus, theoretical insights in the production mechanism guide the expectations for the experimental signatures and provide the ultimate benchmark against which observational progress has to be measured. In order to collect these rewards, a precise description of the evolution of the early Universe is required. Since DM production occurs in a hot and dense environment the appropriate tools are Boltzmann equations. The main ingredients for their solution are the interaction rate of DM Γ, the expansion history of the Universe, and the initial conditions for the evolution.

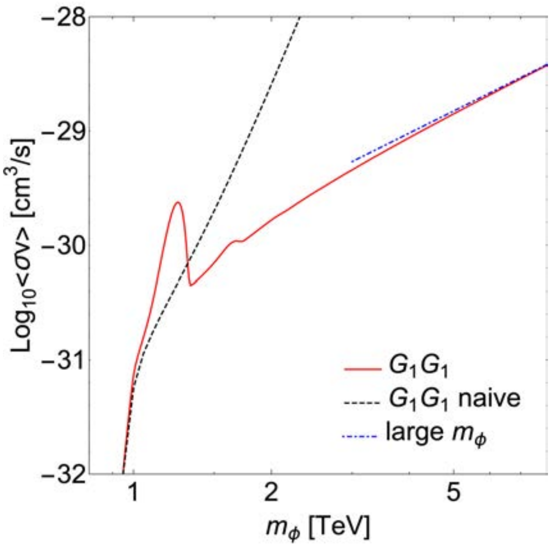


Figure 3.22: The annihilation cross section into two KK-gravitons with (solid, red) and without (dashed, black) proper summation over the KK-tower. A newly derived analytic approximation of the high energy limit is shown by the dotted blue line. For more details see [vogl2].

New effects can have a profound impact on the DM abundance. For example, the impact of bound states in systems with long-range interactions has only come into focus recently. Studies show a strong impact on the expected phenomenology and indicate that bound state assisted freeze-out is an attractive target for ultimate direct detection experiments such as DARWIN [vogl9, vogl7]. In addition, these effects also have to be taken into account for non-thermally produced DM and significantly affect the cosmologically preferred parameter space with important implications for testability at the LHC [vogl1].

In addition, it is crucial to realize that DM production in the early Universe is generally a high energy processes. Therefore, the relic density is more sensitive to UV physics than other observables. The group investigated the UV-sensitivity in a model for gravitationally interacting DM in extra dimensions. The structure of the scattering amplitudes is very subtle in this case [vogl3] and only a careful evaluation of the annihilation rates that takes the full structure of the theory into account allows a reliable prediction of the relic density [vogl2]. This is illustrated in Fig. 3.22 which confronts the full numerical result with an approximation that was used previously and a newly developed approximation for the high mass limit.

Efficient analysis framework for DM phenomenology

The search for DM relies on the combination of a large range of experiments as well as astrophysical and cosmological probes. This plethora of results is both a boon and a challenge since their joint interpretation in a model-independent way is non-trivial. One attempt to tackle this issue that got widely adopted are simplified models. The idea of these models is twofold. First, they act as a "Rosetta Stone" between theory and experiments by providing a simple parametrization of the collider phenomenology in terms of a limited number of degrees of freedom. In addition, this framework allows for a consistent combination of different collider searches and predictions from DM production. It should be noted, however, that the attempt to derive general conclusions with them can produce misleading results unless theoretical consistency conditions and gauge invariance are taken into account [vogl10]. Unfortunately, this also makes them more complicated and reintroduces model-dependent correlations between different observables which can bias experimental searches. These limitations can be addressed by a combination with effective field theory (EFT). Keeping the onshell effects of new degrees of freedom, which are crucial for an accurate description of collider observables, and encapsulating the details of the physics that connects DM and the SM in higher dimensional operators allows keeping the best from both worlds. A first phenomenological study based on this idea is encouraging and it was found that the approach is useful for a model-independent analysis of models with (pseudo-)scalar mediators [vogl5, vogl4].

Neutrino physics

In addition, the group also works on neutrino physics. The observed neutrino masses, which cannot be explained within the SM, mark them as a key area for the search for new physics. However, the elusive nature of neutrinos makes testing new interactions in this sector challenging. A careful combination of different, correlated effects that arise from new interactions between neutrinos and charged SM particles enhances the sensitivity considerably [vogl8]. However, interactions among neutrinos are much more difficult to access and even a very large interaction strength that can affect cosmology remains borderline allowed [vogl6].

Future Plans

The Theoretical Astroparticle Physics group plans to build on its strength in DM phenomenology and deepen this area of research. Directions for future work include:

Testing light dark sectors

There is an increasing number of new searches for light dark sectors. Currently, most searches consider only a few simple models, such as the dark photon with kinetic mixing or a dark scalar mixing with the Higgs. This introduces stringent correlations between different signatures and leads to a biased view of these developments. Therefore, a theoretical framework that allows the robust and efficient analysis of the different searches is of great interest. Hybrid EFT - simplified models are a tool with great promise for DM with weaker-than-weak interactions. To apply this approach here, the set of mediators and effective operators has to be adjusted to the new experimental environment and the new physics contributions to the novel observables have to be computed and confronted with the data.

Cosmological signatures

Astrophysical and cosmological observations provide an alternative way forward. For example, a precise assessment of the evolution of structure can reveal new information about the conditions at the onset of structure formation. The interpretation of the astrophysical data in terms of the underlying fundamental physics depends crucially on the production mechanism in the early Universe. Combining a more detailed study of the origin of DM with novel astrophysical measurements is very promising and will allow us to exploit the power of the ongoing observational program.

3.3 Important Publications and Conference Talks

Group Argyropoulos

Publications

[arg1] ATLAS Collaboration, Measurements of WH and ZH production in the $H \to b\bar{b}$ decay channel in pp collisions at 13 TeV with the ATLAS detector, Eur. Phys. J. C 81 (2021) 178 [arXiv:2007.02873]

[arg2] ATLAS Collaboration, Search for dark matter produced in association with a Standard Model Higgs boson decaying into b-quarks using the full Run 2 dataset from the ATLAS detector, JHEP 11 (2021) 209 [arXiv:2108:13391]

[arg3] S. Argyropoulos, O. Brandt, U. Haisch, Collider searches for dark matter through the Higgs lens, Symmetry 2021 13 (12) 2406 [arXiv:2109.13597]

[arg4] ATLAS Collaboration, Combination and summary of ATLAS dark matter searches using 139 fb^{-1} of 13 TeV pp collision data and interpreted in a two-Higgs-doublet model with a pseudoscalar mediator, ATLAS-CONF-2021-036

Conference Talks

1. S. Argyropoulos, Probing the dark sector with b-quarks with the ATLAS detector, 55th Rencontres de Moriond, Electroweak Interactions & Unified Theories, March 2021

Group Dittmaier

Publications

[ditt1] S. Dittmaier, S. Schuhmacher and M. Stahlhofen, "Integrating out heavy fields in the path integral using the background-field method: general formalism," Eur. Phys. J. C **81** (2021), 826 [arXiv:2102.12020 [hep-ph]].

[ditt2] S. Dittmaier, "Electric charge renormalization to all orders," Phys. Rev. D **103** (2021) no.5, 053006 [arXiv:2101.05154 [hep-ph]].

[ditt3] J. Klappert, F. Lange, P. Maierhöfer and J. Usovitsch, "Integral reduction with Kira 2.0 and finite field methods," Comput. Phys. Commun. **266** (2021), 108024 [arXiv:2008.06494 [hep-ph]].

[ditt4] A. Denner and S. Dittmaier, "Electroweak Radiative Corrections for Collider Physics," Phys. Rept. **864** (2020), 1-163 [arXiv:1912.06823 [hep-ph]].

[ditt5] S. Dittmaier, G. Knippen and C. Schwan, "Next-to-leading-order QCD and electroweak corrections to triple-W production with leptonic decays at the LHC," JHEP **02** (2020), 003 [arXiv:1912.04117 [hep-ph]].

[ditt6] A. Denner, S. Dittmaier, M. Pellen and C. Schwan, "Low-virtuality photon transitions $\gamma^* \to f\bar{f}$ and the photon-to-jet conversion function," Phys. Lett. B **798** (2019), 134951 [arXiv:1907.02366 [hep-ph]].

[ditt7] F. Buccioni, J. N. Lang, J. M. Lindert, P. Maierhöfer, S. Pozzorini, H. Zhang and M. F. Zoller, "OpenLoops 2," Eur. Phys. J. C **79** (2019) no.10, 866 [arXiv:1907.13071 [hep-ph]].

[ditt8] A. Denner, S. Dittmaier, P. Maierhöfer, M. Pellen and C. Schwan, "QCD and electroweak corrections to WZ scattering at the LHC," JHEP **06** (2019), 067 [arXiv:1904.00882 [hep-ph]].

[ditt9] A. Denner, S. Dittmaier and J. N. Lang, "Renormalization of mixing angles," JHEP **11** (2018), 104 [arXiv:1808.03466 [hep-ph]].

[ditt10] L. Altenkamp, M. Boggia and S. Dittmaier, "Precision calculations for $h \to WW/ZZ \to 4$ fermions in a Singlet Extension of the Standard Model with Prophecy4f," JHEP **04** (2018), 062 [arXiv:1801.07291 [hep-ph]].

Conference Talks

1. M. Pellen, "Precise predictions for di-Higgs VBF production", plenary talk at workshop *Higgs Hunting*, Paris, France, Sep 2021 (online).

2. S. Dittmaier, "Electric charge renormalization to all orders", 15th International Symposium on Radiative Corrections (RADCOR) and the XIX Workshop on Radiative Corrections for the LHC and Future Colliders (LoopFest), Tallahassee, USA, May 2021 (online).

3. M. Pellen, "NNLO QCD predictions for W+c-jet production at the LHC", 15th International Symposium on Radiative Corrections (RADCOR) and the XIX Workshop on Radiative Corrections for the LHC and Future Colliders (LoopFest), Tallahassee, USA, May 2021 (online).

4. M. Pellen, "Stress testing the Standard Model via vector-boson scattering at the LHC", invited topical plenary talk at DPG Frühjahrstagung, Dortmund, Germany, March 2021 (online).

5. M. Pellen, "Multi-particle final states at 1-loop EW", *2020 International Workshop on the High Energy Circular Electron Positron Collider*, Shanghai, China, Oct 2020 (online).

6. S. Dittmaier, "Precision Electroweak calculations (Giga-Z,WW, Higgs BRs, etc.)", invited plenary talk at the *Open Symposium – Update of the European Strategy for Particle Physics*, Granada, Spain, May 2019.

7. C. Schwan, "NLO electroweak corrections for WZ scattering at the LHC", *LoopFest XVII*, East Lansing, USA, July 2018.

8. S. Dittmaier, "Electroweak corrections in the Two-Higgs-Doublet Model and Singlet Extensions of the Standard Model", *14th Workshop on Loops and Legs in Quantum Field Theory*, St. Goar, Germany, April/May 2018.

9. P. Maierhöfer, "The next generation of OpenLoops", *14th Workshop on Loops and Legs in Quantum Field Theory*, St. Goar, Germany, April/May 2018.

10. S. Dittmaier, "Precision calculations for $h \to WW/ZZ \to 4$ fermions in the Two-Higgs-Doublet Model with PROPHECY4F", *53rd Rencontres de Moriond – QCD and High Energy Interactions*, La Thuile, Italy, March 2018.

Mandates/Awards

1. S. Dittmaier, Member of the Scientific Advisory Board for the *Les Houches Workshop Series – Physics at TeV Colliders*, since 2014.

2. S. Dittmaier, Theory Convener of the *LHC Electroweak Working Group*, since 2017.

3. S. Dittmaier, Member of the Advisory Committee of the German Federal Ministery of Education and Science (BMBF), 2014–2021.

4. S. Dittmaier, Managing Director of the Institute of Physics, University of Freiburg, 10/2018–3/2021.

5. S. Dittmaier, Member of the Theory Advisory Committee of the *LHC Higgs Cross Section Working Group*, 2016–2019.

Group Fischer

Publications

[fisch1] CAST Collaboration, A. Álvarez Melcón, et al., ”First results of the CAST-RADES haloscope search for axions at 34.67 μeV”, J. High Energ. Phys. **21**, (2021), 75, doi:10.1007/JHEP10(2021)07.

[fisch2] CAST Collaboration, S. Arguedas Cuendis, et al., ”First Results on the Search for Chameleons with the KWISP Detector at CAST”, Phys. Dark Univ. **26**, (2019), 100367, doi:10.1016/j.dark.2019.100367.

[fisch3] H. Fischer, X. Liang, Y. Semertzidis, A. Zhitnitsky, K. Zioutas, ”New mechanism producing axions in the AQN model and how the CAST can discover them”, Phys. Rev. D **98**, (2018), 043013.

[fisch4] COMPASS Collaboration, R. Akhunzyanov et al., ”Transverse extension of partons in the proton probed in the sea-quark range by measuring the DVCS cross section”, Phys. Lett. B, **793**, (2019), 188, doi:10.1016/j.physletb.2019.04.038.

[fisch5] COMPASS Collaboration, M.G. Alexeev et al., ”Measurement of the cross section for hard exclusive π^0 muoproduction on the proton”, Phys. Lett. B, **805**, (2020), 135454, doi:10.1016/j.physletb.2020.135454.

[fisch6] COMPASS Collaboration, M.G. Alexeev et al. ”Spin density matrix elements in exclusive ω meson muoproduction”, Eur. Phys. J. C, **81**, (2021), 126, doi:10.1140/epjc/s10052-020-08740-y.

[fisch7] COMPASS Collaboration, R. Akhunzyanov et al., ”K^- over K^+ multiplicity ratio for kaons produced in DIS with a large fraction of the virtual-photon energy”, Phys. Lett. B, **786**, (2018), 390, doi:10.1016/j.physletb.2018.09.052.

[fisch8] COMPASS Collaboration, M. Aghasya et al., ”Transverse-momentum-dependent Multiplicities of Charged Hadrons in Muon-Deuteron Deep Inelastic Scattering”, Phys. Rev. D, **97**, (2018), 032006, doi:10.1103/PhysRevD.97.032006.

[fisch9] AMBER Collaboration, B. Adams et al., ”Letter of Intent: A New QCD facility at the M2 beam line of the CERN SPS (COMPASS++/AMBER)”, CERN-SPSC-2019-003 (SPSC-I-250), arXiv:1808.00848 (2018).

Group Heinemann

Publications

[hein1] ATLAS Collaboration, Measurements of $W^+W^- + \geq 1$ jet production cross-sections in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector, JHEP **06** (2021) 003.

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

[hein3] S. Carra,V. Goumarre, R. Gupta, S. Heim, B. Heinemann *et al.*, Constraining off-shell production of axionlike particles with $Z\gamma$ and WW differential cross-section measurements, Phys.Rev.D **104** (2021) 9, 092005.

[hein4] ATLAS Collaboration, Emulating the impact of additional proton-proton interactions in the ATLAS simulation by presampling sets of inelastic Monte Carlo events, arXiv:2102.09495, accepted by Comput. Softw. Big Science.

[hein5] H. Abramowicz *et al.* Conceptual design report for the LUXE experiment, Eur. Phys. J. ST **230** (2021) no.11, 2445-2560

[hein6] Z. Bai, T. Blackburn, O. Borysov, O. Davidi, A. Hartin, B. Heinemann, T. Ma, G. Perez, A. Santra and Y. Soreq, *et al.* ”LUXE-NPOD: new physics searches with an optical dump at LUXE”, [arXiv:2107.13554 [hep-ph]], submitted to Phys. Rev. D.

[hein7] R. K. Ellis, B. Heinemann *et al.* "Physics Briefing Book: Input for the European Strategy for Particle Physics Update 2020", [arXiv:1910.11775 [hep-ex]].

[hein8] J. de Blas, M. Cepeda, J. D'Hondt, R. K. Ellis, C. Grojean, B. Heinemann *et al.* "Higgs Boson Studies at Future Particle Colliders", JHEP **01** (2020), 139.

[hein9] B. Heinemann and Y. Nir, "The Higgs program and open questions in particle physics and cosmology", Usp. Fiz. Nauk **189** (2019) no.9, 985-996

[hein10] G. Aad *et al.* [ATLAS], "Measurement of the $Z(\to \ell^+\ell^-)\gamma$ production cross-section in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector", JHEP **03** (2020), 054.

[hein11] M. Aaboud *et al.* [ATLAS], "Measurement of fiducial and differential W^+W^- production cross-sections at $\sqrt{s} = 13$ TeV with the ATLAS detector", Eur. Phys. J. C **79** (2019) no.10, 884.

Conference Talks

1. O. Kuprash, "Measurements of multi-boson production including vector-boson scattering at ATLAS", Blois, 2021.
2. O. Kuprash, "Multibosons production at the LHC (diboson, triboson)", PANIC, 2021.
3. O. Kuprash, Study of the hard double-parton scattering with four-lepton final state in pp collisions at 8 TeV with the ATLAS detector", NEW TRENDS in HIGH-ENERGY PHYSICS, 2019.
4. B. Heinemann, "Physics highlights and challenges - particle physics",Joint ECFA-APPEC-NuPECC Seminar (JENAS), Paris 2019.
5. O. Kuprash, "Soft physics at ATLA and CMSS", LHCP 2018.
6. B. Heinemann, "LHC results relevant for astroparticle physics", TEVPA, July 2018.
7. B. Heinemann, "Physics at Future Colliders: invisible aspects", Invisibles Workshop, May 2021 (online).
8. B. Heinemann, "The potential of electroweak symmetry breaking, The Magic of Physics", Veldhoeven, January 2021 (online).
9. B. Heinemann, "European Particle Physics Strategy Update and Future Prospects", Lecture at the 2021 CERN-Fermilab HCP summer school, Sept 2021
10. B. Heinemann, "LUXE: Proposal for a new experiment using a Laser and XFEL to test quantum physics in the strong-field regime", ExHILP conference, Jena, September 2021.

Mandates/Awards

1. B. Heinemann: Member of Particle Physics Preparation Group for the European Strategy of Particle Physics, 2018-2020
2. B. Heinemann: Member of CERN Scientific Policy Committee, 2017-2023.
3. B. Heinemann: Member of Scientific Committee of the Laboratori Nazionali di Frascati (LNF), 2017-2021
4. B. Heinemann: Member of European Physical Society HEPP Board, 2017-2021
5. B. Heinemann: LBNC Review Panel at FNAL (Batavia/IL, USA), 2016-2019

Group Herten

Publications

[hert1] G. Aad *et al.* [ATLAS], *Measurement of Higgs boson decay into b-quarks in associated production with a top-quark pair in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, arXiv:2111.06712 [hep-ex]].
The associated production of a Higgs boson and a top-quark pair is measured in events characterised by the presence of one or two electrons or muons. The Higgs boson decay into a b-quark pair is used and the signal strength, defined as the ratio of the measured signal yield to that predicted by the Standard Model, is measured.

[hert2] G. Aad *et al.* [ATLAS], *Search for squarks and gluinos in final states with jets and missing transverse momentum using 139 fb^{-1} of $\sqrt{s}$ =13 TeV pp collision data with the ATLAS detector*, JHEP **02** (2021), 143.
A search for the supersymmetric partners of quarks and gluons (squarks and gluinos) in final states containing jets and missing transverse momentum, but no electrons or muons, is presented. The results are interpreted in the context of various R-parity-conserving models where squarks and gluinos are produced in pairs or in association and a neutralino is the lightest supersymmetric particle.

[hert3] M. Aaboud *et al.* [ATLAS], *Measurement of the top quark mass in the $t\bar{t} \to$ lepton+jets channel from $\sqrt{s} = 8$ TeV ATLAS data and combination with previous results*, Eur. Phys. J. C **79** (2019) no.4, 290.
The top quark mass is measured using a template method in the $t\bar{t} \to$ lepton+jets channel (lepton is e or μ) using ATLAS data. Exploiting a three-dimensional template technique, the top quark mass is determined together with a global jet energy scale factor and a relative b-to-light-jet energy scale factor.

[hert4] M. Aaboud *et al.* [ATLAS], *Measurements of differential cross sections of top quark pair production in association with jets in pp collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector*, JHEP **10** (2018), 159.
Measurements of differential cross sections of top quark pair production in association with jets by the ATLAS experiment at the LHC are presented. The measurements are performed as functions of the top quark transverse momentum, the transverse momentum of the top quark-antitop quark system and the out-of-plane transverse momentum using data from pp collisions.

[hert5] M. Aaboud *et al.* [ATLAS], *Evidence for the associated production of the Higgs boson and a top quark pair with the ATLAS detector*, Phys. Rev. D **97** (2018) no.7, 072003.
A search for the associated production of the Higgs boson with a top quark pair ($t\bar{t}H$) is reported. An excess of events over the expected background from Standard Model processes is found with an observed significance of 4.1 standard deviations.

[hert6] M. Aaboud *et al.* [ATLAS], *Search for the standard model Higgs boson produced in association with top quarks and decaying into a $b\bar{b}$ pair in pp collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector*, Phys. Rev. D **97** (2018) no.7, 072016.
A search for the Standard Model Higgs boson produced in association with a top-quark pair, $t\bar{t}H$, is presented. Multivariate techniques are used to discriminate between signal and background events. The signal strength is measured.

[hert7] M. Aaboud *et al.* [ATLAS], *Search for squarks and gluinos in final states with jets and missing transverse momentum using 36 fb^{-1} of $\sqrt{s}$=13 TeV pp collision data with the ATLAS detector*, Phys. Rev. D **97** (2018) no.11, 112001.
A search for squarks and gluinos in final states containing hadronic jets and missing transverse momentum, but no electrons or muons, is presented. Exclusion limits for gluinos and squarks are determined in simplified SUSY models.

Conference Talks

1. Andrea Knue, *The top quark is still going strong (and electroweak)*, Invited Talk (Hauptvortrag), DPG Frühjahrstagung, Heidelberg (Online), March 2022.

2. Andrea Knue, *Top Quark Experimental Overview: The Top Quark is still going strong!*, Plenary Talk, 30th International Symposium on Lepton Photon Interactions at High Energies, Manchester (Online), January 2022.

3. Efstathios Karentzos, *The High Voltage DCS System for the New Small Wheel upgrade of the ATLAS experiment*, 18th International Conference on Accelerator and Large Experimental Physics Systems, Online, October 2021.

4. Manuel Guth, *Search for the Standard Model Higgs boson produced in association with top quarks and decaying into a pair of b-quarks with the ATLAS detector*, Les Rencontres Physique de la Vallée d'Aoste (La Thuile 2021), La Thuile, Online only, March 2021.

5. Manuel Guth, *Optimisation of the ATLAS Deep Learning Flavour Tagging Algorithm*, Conference on Large Hadron Collider Physics (LHCp 2020), Paris, Online only, May 2020.

6. P. Scholer, *Test-beam results performance studies of the ATLAS Micromegas production modules*, MicroPattern Gaseous Detectors Conference, La Rochelle, France, Mai 2019.

7. Andrea Knue, *Measurements of the top quark mass using the ATLAS detector at the LHC*, EPS-HEP 2019, Gent, Belgium, Juli 2019.

8. Stephanie Zimmermann, *ATLAS Phase-1 Upgrades, Overview, Status and Prospects*, HEP 2019 – Conference on Recent Developments in High Energy Physics and Cosmology, NCSR Demokritos, Athens, Greece, April 2019.

9. Veronika Magerl, *Inclusive searches for squarks and gluinos with the ATLAS detector*, Pheno2018, Phenomenology Symposium, Pittsburg, PA, USA, May 2018.

10. Peter Tornambé, *Inclusive searches of squarks and gluinos with the ATLAS detector*, Pheno2018, Phenomenology Symposium, Pittsburg, PA, USA, May 2018.

Mandates/Awards

1. G. Herten: Chair of the ATLAS Muon Institute Board, since 4/2021.

2. G. Herten: Member of the International Advisory Committee of the Future Circular Collider (FCC), 2017 – 2021.

3. A. Knue: Convenor of several Top-Quark analysis groups.

4. S. Zimmermann: Project Leader of the ATLAS *New Small Wheel* upgrade project (6/2013-11/2020).

5. Manuel Guth: ATLAS Thesis Award 2021.

Group Ita

Publications

[ita1] S. Abreu, J. Dormans, F. Febres Cordero, H. Ita and B. Page, "Analytic Form of Planar Two-Loop Five-Gluon Scattering Amplitudes in QCD," Phys. Rev. Lett. **122** (2019) no.8, 082002

[ita2] S. Abreu, J. Dormans, F. Febres Cordero, H. Ita, B. Page and V. Sotnikov, "Analytic Form of the Planar Two-Loop Five-Parton Scattering Amplitudes in QCD," JHEP **05** (2019), 084

[ita3] Z. Bern, H. Ita, J. Parra-Martinez and M. S. Ruf, "Universality in the classical limit of massless gravitational scattering," Phys. Rev. Lett. **125** (2020) no.3, 031601

[ita4] S. Abreu, F. Febres Cordero, H. Ita, M. Jaquier, B. Page, M. S. Ruf and V. Sotnikov, "Two-Loop Four-Graviton Scattering Amplitudes," Phys. Rev. Lett. **124** (2020) no.21, 211601

[ita5] S. Abreu, H. Ita, F. Moriello, B. Page, W. Tschernow and M. Zeng, "Two-Loop Integrals for Planar Five-Point One-Mass Processes," JHEP **11** (2020), 117

[ita6] S. Abreu, J. Dormans, F. Febres Cordero, H. Ita, M. Kraus, B. Page, E. Pascual, M. S. Ruf and V. Sotnikov, "Caravel: A C++ framework for the computation of multi-loop amplitudes with numerical unitarity," Comput. Phys. Commun. **267** (2021), 108069

[ita7] E. Herrmann, J. Parra-Martinez, M. S. Ruf and M. Zeng, “Gravitational Bremsstrahlung from Reverse Unitarity,” Phys. Rev. Lett. **126** (2021) no.20, 201602

[ita8] Z. Bern, J. Parra-Martinez, R. Roiban, M. S. Ruf, C. H. Shen, M. P. Solon and M. Zeng, “Scattering Amplitudes and Conservative Binary Dynamics at $\mathcal{O}(G^4)$,” Phys. Rev. Lett. **126** (2021) no.17, 171601

[ita9] S. Abreu, F. F. Cordero, H. Ita, B. Page and V. Sotnikov, “Leading-color two-loop QCD corrections for three-jet production at hadron colliders,” JHEP **07** (2021), 095

[ita10] S. Abreu, F. F. Cordero, H. Ita, M. Klinkert, B. Page and V. Sotnikov, “Leading-Color Two-Loop Amplitudes for Four Partons and a W Boson in QCD,” [arXiv:2110.07541 [hep-ph]].

Conference Talks

1. H. Ita, Workshop, ‘Taming the Complexity of Multiloop Integrals’, Pauli Center for Theoretical Studies, ETH, ‘Two Loop Numerical Unitarity’, 4-8 June, 2018
2. H. Ita, Elliptics and Beyond Conference, CERN TH-Department, the Niels Bohr Institute (Copenhagen) and the MITP (Mainz), ‘Vector Fields and Integrals’, 7-11 September, 2020
3. H. Ita, Snowmass Community Planning Meeting - Virtual, ‘Automated five-point QCD amplitudes at two-loops’, 5-8 October 2020
4. S. Abreu, LoopFest 2018, Michigan State University, ‘Two-loop amplitudes with numerical unitarity’, July 16-20, 2018
5. B. Page, Rencontres de Moriond, le Thuile, Italy, ‘Computing Planar Five-Gluon Amplitudes with Numerical Unitarity’, March 17-24, 2018
6. B. Page, Loops and Legs, St. Goar, Germany, ‘Planar Two-Loop Five-Gluon Amplitudes from Numerical Unitarity’, April 29 - May 4, 2018
7. M. Ruf, QCD Meets Gravity IV, Northwestern University, Evanston, IL, USA, ‘Classical integrals beyond the conservative region’, November 30 - December 4, 2020
8. V. Sotnikov, CMS Heavy Flavour Tagging Workshop, Brussels, Belgium, ‘Wbb + jets production at NLO QCD’, April 11-13, 2018
9. V. Sotnikov, High Precision for Hard Processes (HP2 2018), Freiburg, Germany, ‘Five-Parton Two-Loop Amplitudes from Numerical Unitarity’, October 1-3, 2018
10. V. Sotnikov, RADCOR 2019, Avignon, France, “Analytic Two-Loop Five-Parton QCD Amplitudes from Numerical Unitarity”, September 9-13, 2019

Mandates/Awards

1. H. Ita, Erasmus Coordinator for the Physics Department, 2014-2021.

Group Jakobs

Publications

[jak1] M. Aaboud *et al.* [ATLAS Collaboration], *Measurements of gluon-gluon fusion and vector-boson fusion Higgs boson production cross-sections in the $H \to WW^* \to e\nu\mu\nu$ decay channel in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, Phys. Lett. B **789** (2019) 508.
First measurements are presented of Higgs boson production cross-sections for gluon fusion and vector-boson fusion times branching ratios in the $H \to WW^* \to e\nu\mu\nu$ decay channel in proton-proton collisions at 13 TeV based on data recorded in 2015 and 2016.

[jak2] G. Aad *et al.* [ATLAS Collaboration], *Measurements of WH and ZH production in the $H \to b\bar{b}$ decay channel in pp collisions at 13 TeV with the ATLAS detector*, Eur. Phys. J. C **81** (2021) no.2, 178.
The production of a Higgs boson in association with a W or Z boson in the above-mentioned decay mode is established with observed (expected) significances of 4.0 (4.1) and 5.3 (5.1) standard deviations, respectively. Cross sections measured as a function of the gauge boson transverse momentum in kinematic fiducial volumes are found to be consistent with the SM expectations.

[jak3] G. Aad *et al.* [ATLAS Collaboration], *Measurements of Higgs boson production cross-sections in the $H \to \tau^+\tau^-$ decay channel in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, [arXiv:2201.08269 [hep-ex]].
Inclusive cross-section measurements, based on the complete Run-2 dataset, in the $H \to \tau^+\tau^-$ decay channel are determined separately for the four dominant production modes; measurements in exclusive regions of the phase space, using the simplified template cross-section framework, are also performed.

[jak4] G. Aad *et al.* [ATLAS Collaboration], *Combined measurements of Higgs boson production and decay using up to 80 fb^{-1} of proton-proton collision data at $\sqrt{s} =$ 13 TeV collected with the ATLAS experiment*, Phys. Rev. D **101** (2020) no.1, 012002.
Combined measurements of Higgs boson production cross sections and branching fractions are presented for the decay modes into $\gamma\gamma$, ZZ^*, WW^*, $\tau\tau$, $b\bar{b}$ and $\mu\mu$ and for decays into invisible final states. Up to 79.8 fb^{-1} of proton-proton collision data collected at $\sqrt{s}$ = 13 TeV with the ATLAS detector are used.

[jak5] G. Aad *et al.* [ATLAS Collaboration], *Search for a scalar partner of the top quark in the all-hadronic $t\bar{t}$ plus missing transverse momentum final state at $\sqrt{s} = 13$ TeV with the ATLAS detector*, Eur. Phys. J. C **80** (2020) no.8, 737.
A search for direct pair production of scalar partners of the top quark (top squarks or scalar third-generation up-type leptoquarks) in the all-hadronic $t\bar{t}$ plus missing transverse momentum final state is presented. Since no significant excess over the SM background expectation is observed, limits based on the complete Run-2 dataset are presented.

[jak6] G. Aad *et al.* [ATLAS Collaboration], *Search for new phenomena with top quark pairs in final states with one lepton, jets, and missing transverse momentum in pp collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector*, JHEP **04** (2021), 174.
A search for new phenomena with top quark pairs in final states with one isolated electron or muon, multiple jets, and large missing transverse momentum is performed. Signal regions are employed to search for two-, three-, and four-body decays of the directly pair-produced supersymmetric partner of the top quark (stop). Additional signal regions are designed specifically to search for spin-0 mediators that are produced in association with a pair of top quarks and decay into a pair of dark-matter particles.

[jak7] M. Aaboud *et al.* [ATLAS Collaboration], *Observation of electroweak production of a same-sign W boson pair in association with two jets in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, Phys. Rev. Lett. **123** (2019) no.16, 161801.
In this publication the observation and measurement is presented of electroweak production of a same-sign W boson pair in association with two jets using 36.1 fb^{-1} of proton-proton collision data recorded at a centre-of-mass energy of $\sqrt{s}$ = 13 TeV.

[jak8] G. Aad *et al.* [ATLAS Collaboration], *Operation and performance of the ATLAS semiconductor tracker in LHC Run 2*, JINST **17** (2022) no.01, P01013 doi:10.1088/1748-0221/17/01/P01013.
During Run 2 at the LHC, the instantaneous luminosity and pile-up conditions were far in excess of those assumed in the original design of the SCT detector. Due to improvements to the data acquisition system, the SCT operated stably and with high efficiency. The performance is discussed in this publication.

[jak9] [ATLAS Collaboration], *Technical Design Report for the ATLAS Inner Tracker Strip Detector*, CERN-LHCC-2017-005.
In this publication, the technical design of all the components of the new ATLAS tracker, for operation at the High-Luminosity LHC, are described in detail.

[jak10] L. Diehl, R. Mori, M. Hauser, J. C. Hönig, L. Wiik-Fuchs, U. Parzefall and K. Jakobs, *Investigation of charge multiplication in irradiated p-type silicon strip sensors designed for the ATLAS phase II tracking detector*, Nucl. Instrum. Meth. A **967** (2020), 163900.
After heavy irradiation, long term annealing and under very high bias voltages, certain silicon particle sensors develop

charge multiplication. This gain is not stable, has a temperature dependence and can lead to signal pulses which exceed the 20 ns shaping time of LHC readout ASICs.

Conference Talks

1. Giulia Gonella, *Tests of the Standard Model with Multi boson final states at the ATLAS detector*, Phenomenology 2018 Symposium (PHENO2018), Pittsburg (USA), May 2018.
2. Philipp Mogg, *Search for top squarks with ATLAS at $\sqrt{s} = 13$ TeV in fully hadronic and semi-leptonic final states*, International Conference on High Energy Physics (ICHEP 2018), Seoul (South Korea), July 2018.
3. Karsten Köneke, *Higgs combination - ATLAS & CMS*, Plenary talk, LHC Days-Konferenz, Split (Croatia), September 2018.
4. Shigeki Hirose, *Higgs boson decays to two fermions and Higgs boson production in association with ttH at the ATLAS experiment*, Lake Louise Winter Institute 2019, Lake Louise (Canada), February 2019.
5. Shigeki Hirose, *The operational experience, challenges and performance of the ATLAS Semiconductor Tracker during LHC Run-2*, The 28th International Workshop on Vertex Detectors, Lopud Island (Croatia), October 2019.
6. Stephen Jiggins, *Higgs boson measurements in third generation decay channels (excl. ttH) with ATLAS and CMS*, 8th Edition of the Large Hadron Collider Physics Conference, Paris (France), - online -, May 2020.
7. Karl Jakobs, *Physics Highlights from the ATLAS Experiment*, Plenary talk, ICHEP 2020 - 40th International Conference on High Energy Physics, Prague (Czech Republic), - online -, July 2020.
8. Dennis Sperlich, *The ATLAS ITk Strip Detector System for the Phase-II LHC Upgrade*, ICHEP 2020, Prague (Czech Republic), July 2020.
9. Leena Diehl, *Investigation of subsequent pulse detection in irradiated silicon sensors*, 16th Trento Workshop on Advanced Silicon Radiation Detectors, Trento (Italy), February 2021.
10. Frank Sauerburger, *Measurement of the Higgs boson coupling to tau leptons in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector at the LHC*, EPS-HEP 2021, July 2021.

Mandates/Awards

1. K. Jakobs, Spokesperson of the ATLAS Collaboration at CERN, March 2017 - Feb. 2021;
2. K. Jakobs, Chair of the European Committee for Future Accelerators (ECFA), since Jan. 2021;
3. K. Jakobs, Editor, Journal of High Energy Physics (JHEP), since Jan. 2021;
4. K. Köneke, Co-Convener of the ATLAS Higgs Physics Group, Oct. 2019 - Sept. 2021;
5. K. Köneke, Member of the Steering Committee of the LHC Higgs Working Group, since Nov. 2021;

Group Schumacher

Publications

[schumach1] ATLAS Collaboration, "Cross-section measurements of the Higgs boson decaying into a pair of τ-leptons in proton-proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector," Phys. Rev. D **99** (2019), 072001 doi:10.1103/PhysRevD.99.072001 [arXiv:1811.08856 [hep-ex]].
The observation of the decay mode of the Higgs boson into a pair of tau-leptons with the ATLAS experiment is reported and cross-section measurments in the major production modes are performed based on the data set from 2015 and 2016.

[schumach2] ATLAS Collaboration, "Measurements of Higgs boson production cross-sections in the $H \rightarrow \tau^+\tau^-$ decay channel in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector," CERN-EP-2021-2017, [arXiv:2201.08269 [hep-ex]], submitted to JHEP.

Cross-section measurements in four production modes are performed using the $H \rightarrow \tau\tau$ decay mode and detailed measurement of cross-section in various phase space regions so called Simplified Template Cross Sections are reported based on the full Run-2 data set.

[schumach3] ATLAS Collaboration, "Combined measurements of Higgs boson production and decay using up to 80 fb^{-1} of proton-proton collision data at $\sqrt{s} = 13$ TeV collected with the ATLAS experiment," Phys. Rev. D **101** (2020) no.1, 012002 doi:10.1103/PhysRevD.101.012002 [arXiv:1909.02845 [hep-ex]].

Measurements of Higgs-boson properties (cross-section, branching ratios, couplings, etc.) from the combination of several Higgs-boson decay modes are reported based on data collected up to 2017. The results are used to constrain the parameter space of Two-Higgs-Doublet Models and Simplified Minimal Supersymmetric Models.

[schumach4] ATLAS Collaboration, "Interpretations of the combined measurement of Higgs-boson production and decay", ATLAS-CONF-2020-053, October 2020.

The first combined measurement of Higgs-boson cross-section and properties based on the full Run-2 data set are used to constrain the model space of several supersymmetric extensions of the SM and are interpreted in the framework of an effective field theory to set limits on various Wilson coefficients.

[schumach5] ATLAS Collaboration, "Combined measurements of Higgs-boson production and decay using up to 139 fb^{-1} of proton-proton collision data at $\sqrt{s}$ = 13 TeV collected with the ATLAS experiment", ATLAS-CONF-2021-053, November 2021

The combined measurement of Higgs-boson production cross sections and branching ratios based on the full Run-2 data set are used to constrain coupling strength modifiers and the model space of several SM extensions and are interpreted in the framework of an effective field theory.

[schumach6] ATLAS Collaboration, "Test of CP invariance in vector-boson fusion production of the Higgs boson in the $H \rightarrow \tau\tau$ channel in proton proton collisions at 13TeV with the ATLAS detector", Phys. Lett. B **805** (2020), 135426 doi:10.1016/j.physletb.2020.135426 [arXiv:2002.05315 [hep-ex]].

The invariance of Higgs-boson production via vector-boson fusion under the combined CP transformation is tested exploiting the $H \rightarrow \tau\tau$ decay mode. The method of the Optimal Observable is applied. No hints for CP-violation are observed and the most stringent limit on the parameter describing CP-violating effects is extracted.

[schumach7] ATLAS Collaboration, "Searches for lepton-flavour-violating decays of the Higgs boson in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector," Phys. Lett. B **800** (2020), 135069 doi:10.1016/j.physletb.2019.135069 [arXiv:1907.06131 [hep-ex]].

The results from searches for lepton flavour violating decays (LFV) of the Higgs boson based on the data from 2015 and 2016 are reported. No hints for LFV are observed and most stringent limits on LFV branching ratios are extracted.

[schumach8] U. Schnoor, F. Bührer, F. Fischer, G. Fleig, A. Gamel, M. Giffels, T. Hauth, M. Janczyk, K. Meier and G. Quast, *et al.* "Dynamic Virtualized Deployment of Particle Physics Environments on a High Performance Computing Cluster," Comput. Softw. Big Sci. **3** (2019) no.1, 9 doi:10.1007/s41781-019-0024-5 [arXiv:1812.11044 [physics.comp-ph]].

The integration of the HPC cluster NEMO in the workflows of the ATLAS and CMS experiments via virtualisation techniques is reported. The advancement of the ROCED tool for transparent, automatized, and on-demand integration of the HPC resource and the evaluated performance of the virtualized environment is discussed.

[schumach9] M. Böhler, R. Caspart, M. Fischer, O. Freyermuth, M. Giffels, S. Kroboth, E. Kuehn, M. Schnepf, F. von Cube and P. Wienemann, "'Transparent Integration of Opportunistic Resources into the WLCG Compute Infrastructure," EPJ Web Conf. **251** (2021), 02039 doi:10.1051/epjconf/202125102039

The efficient and transparent integration of several opportunistic resources into existing compute infrastructures with the tools COBalD and TARDIS is reported. The challenges, employed solutions and experiences gained with the provisioning of opportunistic resources from several resource providers like university clusters, HPC centers and cloud setups are discussed.

[schumach10] A. Di Girolamo *et al.* "Preparing distributed computing operations for the HL-LHC era with Operational Intelligence", Front. Big Data, Vol 4, 2022, doi:10.3389/fdata.2021.753409,

https://www.frontiersin.org/article/10.3389/fdata.2021.753409,
The Operational Intelligence project aims to increase the level of automation in computing operations and reducing human interventions by ”smart”solutions. Machine learning, data mining, log analysis, and anomaly detection are only some of the tools which have been evaluated. A suite of operational intelligence services to cover various use cases: workload management, data management, and site operations have been developed and are described.

Conference Talks

1. Anton J. Gamel, ”Integration of a heterogeneous compute resource in the ATLAS workflow” CHEP 2018, July 2018, Sofia, Bulgary
2. Kathrin Becker, “Higgs Boson Properties as a Window to New Physics”, Invited talk at Spring meeting of the German Physical Society, March 2019, Aachen, Germany.
3. David Hohn, “Measurements of Higgs boson production in decays to two tau leptons with the ATLAS detector”, European Physical Society Conference on High Energy Physics (EPS-HEP), Juli 2019, Ghent , Belgium. ATL-PHYS-PROC-2019-151.
4. Kathrin Becker, “ATLAS results on H(125) Higgs fermion decays”, HiggsHunting 2019, Juli 2019, Paris/Orsay, France. ATL-PHYS-SLIDE-2019-518.
5. Alena Lösle, “Test of CP invariance in vector-boson fusion production of the Higgs boson using H to tau tau decays at the ATLAS experiment”, 8th International Conference on New Frontiers in Physics (ICNFP 2019), August 2019, Kolymbari, Kreta, Griechenland. ATL-PHYS-SLIDE-2019-665
6. Alena Lösle, “Test of CP invariance in vector-boson fusion production of the Higgs boson using H to tau tau decays at the ATLAS experiment”, Higgs Couplings HC2019, September 2019, Oxford, UK. ATL-PHYS-SLIDE-2019-720
7. Felix Bührer, ”Integration of NEMO into an existing particle physics environment through virtualization”, 5th bwHPC-Symposium, April 2019, Freiburg, Germany.
8. Dirk Sammel, ”How to bring HTC data to HPC resources - A caching solution for the ATLAS computing environment in Freiburg”, 7th bwHPC-Symposium, November 2021, Ulm.
9. Valerie Lang, ”Long-term monitoring of delivered luminosity and calibration stability in ATLAS”, LHC Lumi Days 2019, Juni 2019, CERN/Geneva, Switzerland.
10. Fabian Becherer, ”Combined Higgs boson measurements and their interpretations in Effective Field Theories and new physics models with the ATLAS experiment”, LXXI International conference ”NUCLEUS – 2021. Nuclear physics and elementary particle physics. Nuclear physics technologies”, September 2021, St. Petersburg, Russia.

Mandates / Awards

1. M, Schumacher, Member of the GridKa Overview Board (German WLCG Tier-1 center) since 11/2011.
2. M. Schumacher, Representative of KET in the Advisory Board for Digitization in the Research Field ”Universe and Matter” to the Federal Ministry for Research and Education (BMBF) in Germany since 1/2017.
3. M. Schumacher, Weston Visiting Professor at the Weizmann Institute of Science, Rehovot, Israel, 11/2019 – 3/2020.
4. M. Schumacher, Spokesperson of the BMBF Cooperative Research Compound ”“Federated Computing for the ATLAS- and CMS-Experiments at the LHC in Run-3” since 10/2021,
5. M. Schumacher, Deputy Chair of the “Committee for Particle Physics in Germany (KET)” since 11/2021.

Group Schumann

Publications

[schumann1] J. Billard, M. Boulay, S. Cebrián, L. Covi, G. Fiorillo, A. Green, J. Kopp, B. Majorovits, K. Palladino, F. Petricca, L. Roszkowski, M. Schumann, "Direct Detection of Dark Matter – APPEC Committee Report", accepted by Rep. Prog. Phys., arXiv:2104.07634.

APPEC is the European body to steer Astroparticle Physics. The Dark Matter Committee was charged to assess the status and future of direct searches for dark matter in the form of WIMPs or axions. This report summarizes the work of the committee and makes recommendations for the future.

[schumann2] E. Aprile et al. (XENON Collaboration), "Projected WIMP Sensitivity of the XENONnT Dark Matter Experiment", JCAP **11** (2020) 031.

XENONnT is low-background dark matter detector with a 5.9 t active liquid xenon target. It was constructed in 2020. This article is based on detailed simulations (which were largely done in Freiburg) and presents its unpreceded sensitivity to WIMP dark matter.

[schumann3] E. Aprile et al. (XENON Collaboration), "Excess Electronic Recoil Events in XENON1T", Phys. Rev. **D 102** (2020) 072004.

An excess of electronic recoil events (i.e., signatures of particles scattering off electrons) in the range of 1-7 keV was observed with the XENON1T experiment ($> 3\sigma$ significance), thanks to its unprecedented low background level. The unexpected signal could either be caused by a new background (e.g., ^{3}H) or new physics (e.g., solar axions, axion-like particles, a finite neutrino magnetic moment.

[schumann4] L. Althueser, S. Lindemann, M. Murra, M. Schumann, C. Wittweg, C. Weinheimer, "VUV Transmission of PTFE for Xenon-based Particle Detectors", JINST **15** (2020) P12021.

PTFE (Teflon) is an important electrically insulating construction material for low-background detectors. It has a rather low intrinsic radioactivity, however, the use of the material still needs to be minimized. In this work we measured the transmission of VUV light through PTFE and concluded that a 3 mm thick PTFE layer is sufficient to optically separate the XENONnT TPC from the environment.

[schumann5] F. Agostini et al. (DARWIN Collaboration), "Sensitivity of the DARWIN observatory to the neutrinoless double beta decay of ^{136}Xe", Eur. Phys. J. **C 80** (2020) 808.

The future DARWIN observatory will contain almost 4 t of ^{136}Xe in its acive liquid xenon target. This allows searching for the neutrinoless double beta decay of ^{136}Xe without isotopic enrichment. This work evaluates the sensitivity for this channel and was mainly done in Freiburg.

[schumann6] Å.V Rosén, B.A. Hofmann, M. von Sivers, M. Schumann, "Radionuclide activities in recent chondrite falls determined by gamma-ray spectrometry: implications for terrestrial age estimates", Meteorit. Planet. Sci. **55** (2020) 149.

We operate the low-background gamma spectrometer GeMSE in a small underground laboratory. It is also used to identify short-lived isotopes (^{48}V, ^{51}Cr, ^{7}Be, ^{22}Na, ^{54}Mn ^{44}Ti) in meteorites which allows for their terrestrial age-dating and to find correlations between falls. In this work we analyzed 10 meteorite samples.

[schumann7] E. Aprile et al. (XENON Collaboration), "Light Dark Matter Search with Ionization Signals in XENON1T", Phys. Rev. Lett. **123** (2019) 251801.

The sensitivity to low-mass WIMP dark matter (DM) can be enhanced by analyzing only the charge signals from a dual-phase xenon TPC. This increases the background level but decreases the threshold. This work excludes new regions in the parameter spaces for DM-nucleus scattering for DM masses m within 3–6 GeV/c^2, DM-electron scattering for $m > 30$ MeV/c^2, and absorption of dark photons and axion-like particles for m within 0.186–1 keV/c^2.

[schumann8] E. Aprile et al. (XENON Collaboration), "The XENON1T Data Acquisition System", JINST **14** (2019) P07016.

The data acquisition system of the XENON1T dark matter experiment reads all signals above $\sim$0.3 photoelectrons asynchronously without a global trigger. Subsequent event identification and reconstruction on a computer cluster allows for the lowest possible threshold. The system was developed by the Freiburg group and is presented in this work.

[schumann9] E. Aprile et al. (XENON Collaboration), ”Observation of two-neutrino double electron capture in ^{124}Xe with XENON1T”, Nature **568** (2019) 532.

Two-neutrino double electron capture is a rare second-order weak transition. This process was observed at 4.4σ in ^{124}Xe with a half-life of 1.8×10^{22} y. This is the rarest process ever measured directly and demonstrates the great potential of liquid xenon based experiments to detect very rare events.

[schumann10] E. Aprile et al. (XENON Collaboration), ”Dark Matter Search Results from a One Tonne×Year Exposure of XENON1T”, Phys. Rev. Lett. **121** (2018) 111302.

The first dark matter search ever with an exposure of 1 t×yr and an ultra-low background rate. No significant excess over background is found excluding new parameter space for spin-independent elastic WIMP-nucleon interaction cross sections for WIMP masses $m \geq 6\,\mathrm{GeV}/c^2$, with a minimum of $4.1\times10^{-47}\,\mathrm{cm}^2$ at $m = 30\,\mathrm{GeV}/c^2$ (90% CL). This result is still one of the most stringent constraints on WIMP dark matter to date.

Conference Talks

1. M. Schumann, ”SHiP”, talk at *Physics Beyond Colliders* General Working Group Meeting, CERN/Online, December 2021.
2. M. Schumann, ”Dark Matter Direct Detection: Experimental Review”, invited highlight talk at TAUP 2021, Valencia/Online, October 2021.
3. M. Schumann, ”Highlights from Direct Dark Matter Direction”, invited review at ICRC 2021, Berlin/Online, July 2021.
4. M. Schumann, ”Direct Detection: A short review ... and the XENON1T excess”, invited review at Kashiwa Dark Matter Symposium, Tokyo/Online, November 2020.
5. A. Elykov, ”Latest XENON1T results & a glimpse into the future with XENONnT”, talk at ICHEP 2020, Prague/Online, July 2020.
6. M. Schumann, ”XENON and DARWIN”, invited talk at 41st International School on Nuclear Physics, Erice, September 2019.
7. M. Schumann, ”Direct Detection: Status and Prospects of High-Mass WIMP searches”, invited review at Zurich Phenomenology Workshop, Zurich, January 2019.
8. F. Kuger, ”DARWIN - The ultimate WIMP Detector”, talk at IDM, Providence, July 2018.
9. M. Schumann, ”Dark matter detection with large LXe/LAr detectors”, invited review at workshop *Dark Matter at the Dawn of Discovery?*, Heidelberg, April 2018.
10. D. Coderre, ”Upcoming Results from XENON1T”, talk at Moriond Electroweak, La Thuile, March 2018.

Mandates/Awards

1. 2017: ERC Consolidator Grant ”ULTIMATE”
2. Since 2018: Co-Spokesperson DARWIN Collaboration
3. 2019-21: APPEC Dark Matter Committee (to define European Strategy for direct dark matter detection)
4. Since 04/2021: Managing Director and Vice-Dean, Institute of Physics, Freiburg

Group van der Bij

Publications

[vdbij1] C. F. Steinwachs and M. L. van der Wild, “Quantum gravitational corrections from the Wheeler–DeWitt equation for scalar–tensor theories,” Class. Quant. Grav. **35** (2018) no.13, 135010.

[vdbij2] C. F. Steinwachs and M. L. van der Wild, “Quantum gravitational corrections to the inflationary power spectra in scalar–tensor theories,” Class. Quant. Grav. **36** (2019) no.24, 245015.

[vdbij3] M. S. Ruf and C. F. Steinwachs,“ Quantum equivalence of f(R) gravity and scalar-tensor theories,” Physical Review D **97**, 044050 (2018), Editors’ suggestion.

[vdbij4] M. S. Ruf and C. F. Steinwachs, “One-loop divergences for f(R) gravity,” Physical Review D **97**, 044049 (2018), Editors’ suggestion.

[vdbij5] L. Heisenberg and C. F. Steinwachs, “Geometrized quantum Galileons,” Journal of Cosmology and Astroparticle Physics **02**, 031 (2020).

[vdbij6] E. Hernandéz-Lorenzo and C. F. Steinwachs, “Naked singularities in quadratic f(R) gravity,” Physical Review D **101**, 124046 (2020).

[vdbij7] A. Gundhi, C. F. Steinwachs and S. V. Ketov, “Primordial black hole dark matter in dilaton-extended two-field Starobinsky inflation,” Physical Review D **103**, 083518 (2021).

[vdbij8] A. Ghundi and C. F. Steinwachs, “Scalaron-Higgs inflation reloaded: Higgs-dependent scalaron mass and primordial black hole dark matter,” European Physics Journal C **81**, 460 (2021).

[vdbij9] J. J. van der Bij, “Physics after the discovery of the Higgs boson,” Acta Phys. Polon. Supp. **11** (2018), 397.

[vdbij10] J. J. van der Bij, “The Principle of Global Relativity,” Acta Phys. Polon. B **52** (2021) no.6-7, 627.

Conference Talks

1. C. Steinwachs, Online workshop on Quantum Gravity: Recent developments in QG, plenary talk: Naked singularities in quadratic f(R) gravity. 04/2020.
2. C. Steinwachs, SISSA Trieste, Heat kernel technique and renormalization in curved spacetime. 10/2019.
3. C. Steinwachs, DESY Hamburg, DESY Theory Workshop 2019: Quantum field theory meets gravity, plenary talk: Towards a unitary and renormalizable quantum theory of gravity. 09/2019.
4. C. Steinwachs, ECT* Trento, Functional and Renormalization Group Methods (FRGIM 2019): Towards a unitary and renormalizable quantum theory of gravity. 09/2019.
5. C. Steinwachs, Newcastle University, Heat-kernel technique for operators with degenerate principle part. 07/2019.
6. C. Steinwachs, ETH Zürich, Heat-kernel technique and renormalization in curved spacetime. 05/2019.
7. C. Steinwachs, Albert Ludwig University Freiburg, physics colloquium (inaugural lecture): Towards a unitary and renormalizable quantum theory of gravity. 05/2019.
8. C. Steinwachs, Physics Centre Bad Honnef, 678 WE-Heraeus seminar: Hundred years of gauge theory, plenary talk: Higgs field in cosmology. 08/2018.
9. C. Steinwachs, Albert Ludwig University Freiburg, physics colloquium (habilitation lecture): Quantum fields and gravity - a unified perspective. 04/2018.

Group Vogl

Publications

[vogl1] J. Bollig and S. Vogl, "Impact of bound states on non-thermal dark matter production," [arXiv:2112.01491 [hep-ph]]

The impact of bound state formation on the production of non-thermal dark matter is analyzed in models with charged next to lightest states in the dark sector. We find that the cosmologically preferred parameter space changes considerably once these corrections are included.

[vogl2] A. de Giorgi and S. Vogl, "Dark matter interacting via a massive spin-2 mediator in warped extra-dimensions," JHEP **11** (2021), 036 [arXiv:2105.06794 [hep-ph]]

We investigate the production of gravitationally interacting dark matter in an extra dimensional model. Building on the results of [vogl3] we perform the first full computation of dark matter annihilation into Kaluze-Klein-gravitons.

[vogl3] A. de Giorgi and S. Vogl, "Unitarity in KK-graviton production: A case study in warped extra-dimensions," JHEP **04**, 143 (2021) [arXiv:2012.09672 [hep-ph]]

This work analyzes the structure of the amplitudes for massive spin-2 particle pair production in an extra-dimensional model. We show that the sum over internal KK-graviton propagators leads to intricate cancellations which cure unitarity issues that arise in models with a single massive spin-2 particle.

[vogl4] G. Arcadi, A. Bally, F. Goertz, K. Tame-Narvaez, V. Tenorth and S. Vogl, "EFT interpretation of XENON1T electron recoil excess: Neutrinos and dark matter," Phys. Rev. D **103**, no.2, 023024 (2021) [arXiv:2007.08500 [hep-ph]]

We study the electron recoil excess observed by XENON1T in an EFT framework. A dark matter interpretation of the signal is found to be disfavored while novel neutrino interactions allow for a good fit of the data. These interactions are subject to severe constraints from other observables that can only be avoided in certain corners of parameter space.

[vogl5] T. Alanne, G. Arcadi, F. Goertz, V. Tenorth and S. Vogl, "Model-independent constraints with extended dark matter EFT," JHEP **10**, 172 (2020) [arXiv:2006.07174 [hep-ph]]

We investigate the phenomenology of the recently proposed extended dark matter effective field theory. This framework remains applicable at collider energies by including a mediator particle in addition to the dark matter and maintains correlations dictated by gauge invariance in a 'model-independent' way.

[vogl6] V. Brdar, M. Lindner, S. Vogl and X. J. Xu, "Revisiting neutrino self-interaction constraints from Z and τ decays," Phys. Rev. D **101**, no.11, 115001 (2020) [arXiv:2003.05339 [hep-ph]]

Neutrino self-interactions could have a profound impact on cosmology. We derive upper limits on the strength of such an interaction using data from terrestrial experiments. We focus on the invisible width of the Z and leptonic τ decays in a model with a light new scalar. A cosmologically relevant interactions strength is found to remain borderline allowed.

[vogl7] S. Biondini and S. Vogl, "Scalar dark matter coannihilating with a coloured fermion," JHEP **11**, 147 (2019) [arXiv:1907.05766 [hep-ph]]

We analyse the phenomenology of a real scalar dark matter candidate interacting with quarks via a coloured fermionic mediator. Non-relativistic effective field theory is used to treat non-perturbative effects in the early Universe. The parameter space compatible with the dark matter relic abundance is confronted with experimental results. Most experimentally allowed thermal relics can be probed by a future Darwin-like experiment.

[vogl8] J. Heeck, M. Lindner, W. Rodejohann and S. Vogl, "Non-Standard Neutrino Interactions and Neutral Gauge Bosons," SciPost Phys. **6**, no.3, 038 (2019) [arXiv:1812.04067 [hep-ph]]

Non-Standard Neutrino Interactions (NSI) arising from a flavor-sensitive Z' boson of a new $U(1)'$ symmetry are studied. We find that kinetic $Z-Z'$ mixing gives vanishing NSI in long-baseline experiments if a direct coupling between the $U(1)'$ gauge boson and matter is absent. In contrast, $Z-Z'$ mass mixing generates such NSI but requires new states that participate both in EW and $U(1)'$ symmetry breaking.

[vogl9] S. Biondini and S. Vogl, "Coloured coannihilations: Dark matter phenomenology meets non-relativistic EFTs," JHEP **02**, 016 (2019) [arXiv:1811.02581 [hep-ph]]

We employ a state of the art calculation of the relic density which makes use of a non-relativistic effective theory framework and calculate the effective annihilation rates by solving a plasma-modified Schrodinger equation. We determine

the cosmologically preferred parameter space and confront it with current experimental limits and future prospects for dark matter detection.

[vogl10] G. Arcadi, M. Lindner, F. S. Queiroz, W. Rodejohann and S. Vogl, “Pseudoscalar Mediators: A WIMP model at the Neutrino Floor,” JCAP **03**, 042 (2018) [arXiv:1711.02110 [hep-ph]]
At leading order, dark matter interacting via peudoscalar mediators is essentially unobservable in direct detection experiments. We compute the one-loop contribution to the effective dark matter-nucleon interaction. This higher order correction dominates the scattering rate completely and can naturally lead to a direct detection cross section in the vicinity of the neutrino floor which makes this dark matter candidate an attractive target for future experiments.

Conference Talks

Only talks given since November 2020 are listed.

1. S. Vogl, ”Spin-2 mediated dark matter”, New Physics from the Sky @ GGI, 2021, Florence, Italy

3.4 Bachelor, Master and Phd Theses

Group Dittmaier

Habilitations

1. Philipp Maierhöfer, “Tools for the automated calculation of scattering processes”, May 2021.

PhD Theses

1. Gernot Knippen, “Next-to-leading-order QCD and electroweak corrections to WWW production at proton–proton colliders”, Oct 2019.
2. Michele Boggia, “Precise predictions for Higgs physics in a singlet extension of the Standard Model”, April 2018.

Master Theses

1. Jan Schuler, “Mixed NNLO QED-QCD corrections to the Higgs-boson decay $H \to b\bar{b}$”, Dec 2021.
2. Robin Feser, “Phenomenology of models with radiatively generated neutrino masses at the LHC”, Jan 2021
3. Stefan Rode, “Mixed NNLO QCD-electroweak radiative corrections to the Higgs-boson decay $H \to b\bar{b}$”, May 2019.
4. Jonas Rehberg, “Precision calculations in a gauged singlet extension of the Standard Model”, June 2019.
5. Sebastian Schuhmacher, “Effective field theory for a heavy-singlet extension of the Standard Model”, Nov 2019.
6. Paul Haider, “Automated amplitude generation for physics beyond the Standard Model”, Dec 2019.
7. Jan Schwarz, “Mixed QCD$\times$EW radiative corrections to hadronic Z-boson decays”, Oct 2018.
8. Ivona Kafedjiska, “The dipole subtraction formalism for photon radiation off W bosons”, Aug 2018.

Bachelor Theses

1. Zainab Chokr, “The anomalous magnetic moment of the muon and physics beyond the Standard Model”, July 2021.
2. Chiara Hubner, “Effektive Feldtheorien für schwere Fermionen”, July 2021.
3. Yannick Stoll, “Predictions for loop-induced photon photon scattering at the LHC”, Aug 2020.
4. Gegor Suchan, “Numerical evaluation of polylogarithms”, Aug 2020.
5. Robin Feser, “Loop-induced Higgs-boson decays in extensions of the Standard Model”, Aug 2018.

Group Fischer

PhD Theses

1. A. Elykov, ”Background Modeling and Data Acquisition for XENON Detectors”, December 2021.
2. M. Gorzellik, ”Cross-section measurement of exclusive π^0 muoproduction and firmware design for an FPGA-based detector readout”, March 2018.

Master Theses

1. S. Scherrers, ”Extraction of the exclusive J/ψ photoproduction cross section at COMPASS, CERN”, September 2019.

2. J.N. Köhne, ”Der Franck-Hertz-Versuch in der Schule”, January 2018.

Bachelor Theses

1. T. Molzberger, ”Readout of the Silicon Pixel Detectors of the AMBER Experiment at CERN”, September 2021.
2. D. Rifert, ”Measurement of Natural Radioactivity”, February 2021.
3. J. Alt, ”Installation of a data acquisition system for a xenon time projection chamber”, March 2020.
4. J. Hermes, ”Assembly and optimization of a KWISP detector”, November 2018.

Group Heinemann

PhD Theses

1. Jorge Andres Sabater Iglesias (also at DESY), ”Welcome to Twin Particles: From Novel ZZ Estimate to Searches for Supersymmetric Sleptons and Higgsinos using the ATLAS Run-2 Data and at the High-Luminosity LHC”, April 2021. `https://cds.cern.ch/record/2798641`

Master Theses

1. Jose Fernandez Pretel, ”Estimation of electron charge misidentification background for the same-sign WW measurement with the ATLAS detector at $\sqrt{s} = 13$ TeV”, 2021.

Bachelor Theses

1. Vincent Kliem, ”Studien zur Reduzierung des Untergrundes bei der Messung der Produktion von zwei W-Bosonen der selben Ladung am ATLAS-Detektor am LHC”, 2019.

Group Herten

PhD Theses

1. Patrick Scholer, *Tracking Performance of Micromegas Chambers for the ATLAS New Small Wheel Project*, March 2022.
2. Manuel Guth, *Search for $t\bar{t}H(H \to b\bar{b})$ production in the lepton+jets channel and quark flavour tagging with deep learning at the ATLAS experiment*, March 2021.
3. Veronika Magerl, *Search for Gluinos and Squarks in RPC and RPV SUSY Models with the ATLAS Detector at $\sqrt(s) = 13$ TeV*, Februar 2020.
4. Thorwald Klapdor-Kleingrothaus, *Untersuchung zum Arbeitspunkt und Performance von Micromegas Detektoren im ATLAS Experiment am CERN*, January 2019.
5. Peter Tornambè, *Search for Supersymmetry with multiple leptons in the final state*, January 2019.
6. Fabio Cardillo, *Search for Supersymmetry in Events with Two Same-Sign Leptons or Three Leptons with the ATLAS Detector at $\sqrt(s) = 13$ TeV*, June 2018.
7. Manfredi Ronzani, *SUSY in strong production: Search for SUSY in final states with jets and missing transverse momentum with the ATLAS detector*, April, 2018.

Master Theses

1. Daniel Bahner, *An Improvement of the Jet-Parton Assignment in the $t\bar{t}H(b\bar{b})$ Process at $\sqrt{s} = 13$ TeV using Deep Neural Networks and Symmetry-Preserving Attention Networks*, Dezember 2021.
2. Thea Engler, *Training of an extended b-tagging algorithm with neural networks*, Dezember 2020.
3. Felicia Volle, *Improvement of the $t\bar{t}H(b\bar{b})$ event reconstruction using machine-learning techniques*, September 2020.
4. Ksenia Solovieva, *Characterising the VMM3 Readout Chips and Response of Gain and Energy Resolution to Pressure in Micromegas Detectors*,Juli 2019.
5. Yanwen Hong, *Impact of Humidity on Deformations of FR-4 Based Detector Elements in the ATLAS New Small Wheel*,Juli 2019.
6. Moritz Springer, *Studien zur Abschätzung des $ttbb$-Untergrunds für die Reaktion $pp \to t\bar{t}H(H \to b\bar{b})$*, Februar 2019.
7. Vladislavs Plesanovs, *ATLAS New Small Wheel Project - Front-End Board Cooling*, November 2018.
8. Manuel Guth, *Signal Region Optimisation Studies Based on BDT and Multi-Bin Approaches in the Context of Supersymmetry Searches in Hadronic Final States with the ATLAS Detector*, April 2018.

Bachelor Theses

1. Kilian Berger, *Investigation of systematic uncertainties in a top-quark mass measurement at 13 TeV at the ATLAS experiment*, August 2019.
2. Joschka Birk, *Improvement of the top-quark reconstruction for the top-quark mass measurement using machine learning techniques*, Juli 2019.
3. Phillip Stöcks, *Gas Studies with different Ar:CO2 ratios using a prototype Micromegas Detector for the ATLAS New Small Wheel Upgrade*, Bachelorarbeit, September 2019.
4. Thea Sophie Engler, *Investigation of discriminating variables to improve the $t\bar{t}H(H \to b\bar{b})$ search*, April 2018.

Group Ita

PhD Theses

1. Wladimir Tschernow, 'Feynman Integrals for Five-Point Two-Loop One-Mass Amplitudes in QCD', March 2022
2. Evgenij Pascual, 'Two-Loop Amplitudes for Processes Involving Photons at Hadron Colliders', October 2021
3. Michael Ruf, 'Precise Predictions for Graviational Binary Systems from Scattering Amplitudes', September 2021
4. Jerry Dormans, 'On the automation of NNLO QCD corrections', February 2020
5. Vasily Sotnikov, 'Scattering Amplitudes with the Multi-Loop Numerical Unitarity Method', December 2019
6. Felix Anger, 'Automation for Associated Production of Multi-Jet Events at NLO', April 2018

Master Theses

1. Maximilian Klinkert, 'Integration-by-Parts Relations for High Multiplicity and Non-Planar Two-Loop Topologies', December 2018

Bachelor Theses

1. Tobias Lippold, 'Black Hole Scattering Observables from Scattering Amplitudes', August 2021

Group Jakobs

Habilitations

1. Dr. Karsten Köneke, *Electroweak Interactions, the Higgs Boson, and the Search for new heavy Bosons*, May 2018.
2. Dr. Susanne Kühn, *Semiconductor Detectors for High Energy Physics Experiments*, May 2018.
3. Dr. Frederik Rühr, *Searching for Supersymmetric Partners of the Top Quark at ATLAS*, February 2019.

PhD Theses

1. Christian Lüdtke, *The Search for Direct Top-Squark Production in Hadronic Final States with the ATLAS Detector at* $\sqrt{s}$ *= 13 TeV*, November 2018.
2. Hannah Arnold, *Search for a CP-Odd Higgs Boson Decaying to Zh in pp Collisions at* $\sqrt{s}$ *= 13 TeV and Development of a b-Jet Tagging Calibration Method for c Jets at the ATLAS Experiment*, March 2019.
3. Theo Megy, *Measurement of the Higgs-boson Coupling to tau-leptons and Combined Measurements of Higgs-boson Properties at* $\sqrt{s}$ *= 13 TeV with the ATLAS Detector*, September 2019.
4. Giulia Gonella, *Observation and measurement of the electroweak* $W^{\pm}W^{\pm}jj$ *Process in proton-proton collisions at* $\sqrt{s}$*=13 TeV with the ATLAS detector*, October 2019.
5. Ralf Gugel, *Measurement of Higgs boson production via gluon fusion and vector-boson fusion in the* $H \to WW^*$ *decay mode with the ATLAS experiment at the LHC at* $\sqrt{s}$ *= 13 TeV* , December 2019.
6. Philipp Mogg, *The search for top-squark pair production with the ATLAS detector at* $\sqrt{s}$ *= 13 TeV in the fully hadronic final state*, February 2020.
7. Julian Wollrath, *Search for supersymmetry with top-squarks and ATLAS data at a centre-of-mass energy of 13 TeV*, April 2021.
8. Simona Gargiulo, *Measurement of the Higgs boson coupling to b-quarks in the associated production with a vector boson with the ATLAS detector*, April 2021.
9. Moritz Wiehe, *Development of a Two-Photon Absorption - TCT system and Study of Radiation Damage in Silicon Detectors*, October 2021.
10. Cedric Hönig, *Investigation of nitrogen enriched silicon sensors and characterization of passive CMOS strip sensors* , October 2021.

Master Theses

1. Leena Diehl, *Investigation of Charge Multiplication in Irradiated Silicon Strip Sensors after Long Annealing Times*, November 2018.
2. Juan Sebastian Useche, *Radiation dose simulation and verification for X-ray backscattering applications*, January 2021.
3. Christina Schwemmbauer, *A Setup for Time Dependent Measurements of Silicon Sensors*, December 2021.

Bachelor Theses

1. Franziska Moos, *Untersuchung von mit Stickstoff angereicherten strahlenharten Siliziumsensoren*, Oktober 2018.
2. Johannes Hinze, *Analysis of Higgs boson decays into two W bosons in the final state with a muon, a large-R-jet and missing transverse energy with the ATLAS detector*, August 2019.
3. Fabian Lex, *Electrical characterisation of a new type of silicon strip sensors*, September 2020.
4. Montague King, *Investigations on Detection Efficiency in the Bond-Pad-Region of ATLAS ITk Modules with a Laser*, October 2020.
5. Markus Österle, *Studien der Partonschauer-Unsicherheiten für die H $\rightarrow$ WW Messung in ATLAS*, October 2020.
6. Lennart Heinen, Optimization of the event classification of $H \rightarrow \tau\tau$ decays at the ATLAS experiment using feedforward neural networks, March 2021.

Group Schumacher

PhD Theses

1. Alena Loesle, "Measurement of the Higgs-boson production cross-sections and test of CP Invariance in vector-boson fusion production in the H $\rightarrow \tau_{lep}\tau_{lep}$ mode with the ATLAS Detector", July 2020.
2. Dirk Sammel, "Measurement of the Higgs-boson production cross-sections and test of CP Invariance in vector-boson fusion production in the $H \rightarrow \tau_{lep}\tau_{had}$ mode with the ATLAS Detector", October 2020.

Master Theses

1. Daariimaa Battulga, "Search for CP-violation in gluon fusion production of the Higgs boson using the $H \rightarrow \tau_{lep}\tau_{had}$ decay at $\sqrt{s}$ = 13 TeV with the ATLAS detector", November 2019.
2. Emanuel Dorbath, "Search for lepton-flavour violation in $pp \rightarrow X \rightarrow \tau e(\tau\mu)$ decays with the ATLAS experiment", Mai 2020.

Bachelor Theses

1. Leonie Hermann,"JUPYTER NOTEBOOK: A proof-of-principle notebook using ATLAS dijet data", September 2018.
2. Severin Sylla, "Vergleich von Methoden zum Test der CP-Invarianz der Higgs-Bosonproduktion in Vektorbosonfusion $pp \rightarrow Hjj$", August 2019.
3. Ye Joon Kim, "Optimizing a classification neural network for selecting events from Higgs-boson production in vector-boson fusion in the decay mode $H \rightarrow \tau\tau \rightarrow e\mu 4\nu$ at the ATLAS experiment", August 2020.
4. Alexandra Spitzer, "Studien zur Verbesserung der Sensitivität für Tests der CP-Invarianz in der Higgs-Boson-Produktion via VBF am ATLAS-Experiment durch Verwendung neuronaler Netzwerke zur Rekonstruktion des Higgs-Boson-Viererimpulses", December 2021.

Group Schumann

PhD Theses

1. Arianna Rocchetti, XENONnT: assembly, backgrounds and sensitivity to $0\nu\beta\beta$ decay of ^{136}Xe, 2021. `https://freidok.uni-freiburg.de/data/223691`

2. Patrick Meinhardt, Commissioning, Operation, and Characterization of a small-scale liquid xenon TPC and R&D studies on single-phase TPC operation, 2021.

Master Theses

1. Mariana Rajado Nunes da Silva, Low Background Rare Event Searches with Liquid Xenon Detectors, 2021.
2. Robin Glade-Beucke, Characterization of XeBRA's Dual-Phase TPC for DARWIN R&D, 2021.
3. Jaron Grigat, A robust and versatile slow control system for small- to medium-size experiments, 2020.
4. Julia Müller, The Gas System for the DARWIN Demonstrator, 2020.
5. Alexander Bismark, Simulation and Characterization of a LXe TPC for DARWIN R&D, 2019.
6. Florian Tönnies, R&D towards the DARWIN full diameter demonstrator, 2019.

Bachelor Theses

1. Dominik Rifert: Measurement of Natural Radioactivity, 2021.
2. Wolfgang Boemke: Collection and Transfer Efficiency Assessment of the MonXe Radon Emanation Chamber, 2021.
3. Johannes Alt: Installation of a data acquisition system for a xenon time projection chamber, 2020.
4. Anne Becker: Conceptual Optimization of the GeMSE Muon Veto, 2020.
5. Lukas Grunwald: A Capacitive Liquid Nitrogen Levelmeter for the GeMSE HPGe γ-screening facility, 2020.
6. Thomas Kok: Monte Carlo Data Comparison of the New GeMSE Background Spectrum, 2019
7. Ingolf Kaufmann: Development of a setup required for filling, operating and recuperating a hermetic TPC, 2019.
8. Luisa God: Efficiency Studies for the MonXe Radon Emanation Chamber, 2019.
9. Baris Kiyim: Liquid Nitrogen Ohmic Levelmeter for GeMSE, 2019.
10. Christina Schwemmbauer: Construction and Installation of a PMT based ^{83m}Kr Decay Counter, 2018.
11. René Kirsch: Development of a PIN diode based Radon Detector, 2018.

Group van der Bij

Habilitations

1. Christian Steinwachs, Quantum fields, gravity and renormalization in curved spacetime, 2019.

PhD Theses

1. Matthijs van der Wild, Inflation and Quantum Geometrodynamics in scalar-tensor theories, 2019.

Master Theses

1. Max Ammer, Wave equations in binary black hole space-time, 2018.
2. Lokesh Mishra, Theories of massive gravity in 2+1 dimensions, 2018.

Group Vogl

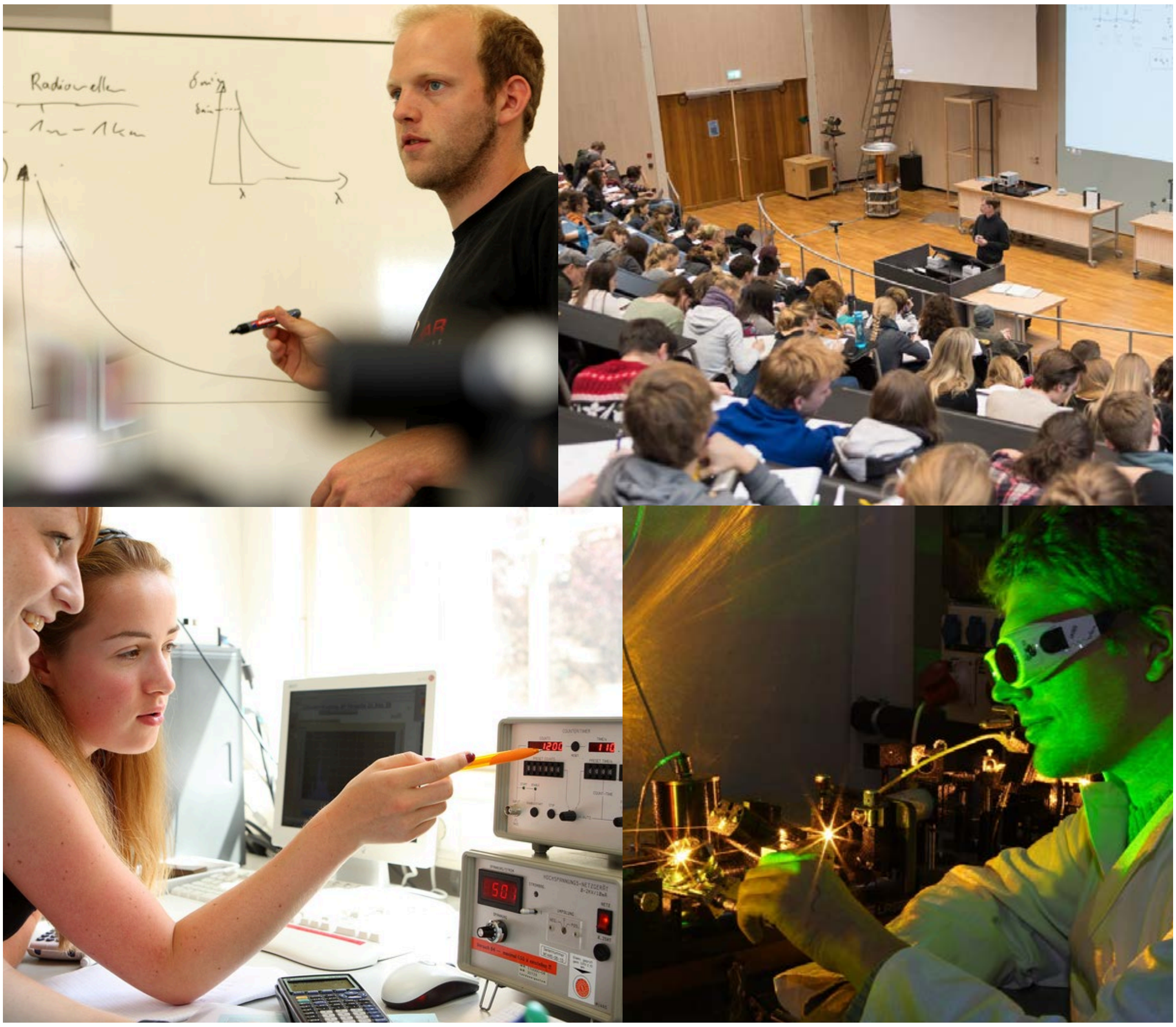
Only theses awarded by the University of Freiburg are listed.

Bachelor Theses

1. S. Machnitzky, “Quantenstatistikeffekte bei Freeze-In Produktion von Dunkler Materie”, 2021.

Part III

Teaching



Chapter caption: From top left to bottom right: Tutor teaching in exercises class; Experimental physics lecture in the large lecture hall; Students in the beginners physics lab; Student working on his master's project. (image credits: B. Bender, M. Herrmann).

1.1 Overview

The Institute of Physics offers its students a broad variety of courses ranging from mathematical preparatory classes, over bachelor- and master-level courses to specialized physics lectures and seminars. The subjects cover topics from fundamental basic principles to practical applications with early exposure to contemporary research. Since basic knowledge in physics is also required in many other natural science disciplines our institute contributes to external study programs by offering dedicated lectures and laboratory classes to several other faculties.

Various course formats are offered in order to teach the students basic and advanced topics of physics as well as to train the students' mathematical and experimental skills necessary to conduct their own research. Fundamental and specialized physics content is taught in different **lectures**, with the number of participants ranging from 50–350 in the introductory lectures to 10–15 in advanced elective courses. In all degree programs the lectures are generally accompanied by **tutorials/exercises** offered in groups with typically fewer than 15 participants each. In our bachelor and master programs, **seminars** are implemented as central modules, where students give talks on a topic of current research. These formats train the participants in handling scientific literature and in presenting and discussing scientific topics. Each term, the research groups offer various seminars for bachelor students and term paper seminars for master students covering all three main research fields at the institute. In several practical **laboratory courses** for bachelor and master students the participants perform basic and advanced physics experiments in teams of two and obtain hands-on experience in running lab experiments, as well as analyzing and presenting their results. For their **final thesis work**, the students join a research group at the Institute of Physics or at one of the associated and participating research institutes.

At the Institute of Physics students can currently enrol in the following modular degree programs:

- **Bachelor of Science (BSc) Physics**
  The BSc program started in the winter term of 2008/09. It encompasses six semesters with a total workload of 180 ECTS credit points (CP). The degree program was accredited in 2015 and re-accredited in 2021.

- **Master of Science (MSc) Physics**
  The English-taught MSc program in Physics started in the winter term of 2011/12. It encompasses four semesters with a total workload of 120 ECTS CP. The degree programme was accredited in 2015 and re-accredited in 2021.

- **Master of Science (MSc) Applied Physics**
  This English-taught MSc programme has been established in the winter term of 2016/17. It encompasses four semesters with a total workload of 120 ECTS CP. This degree program explicitly includes contributions from other faculties of the university, the university medical center and the local Fraunhofer Institutes. The degree program has been successfully accredited in 2021.

- **Polyvalent two-subject Bachelor Physics (with teacher training option)**
  This Bachelor program started in the winter term of 2015/16. In this program students study physics in combination with a second subject. It encompasses six semesters with a total workload of 180 ECTS credit points (75 CP for each subject and 30 CP for didactics and Bachelor thesis). The Polyvalent Bachelor in combination with the Master of Education has substituted the previous teaching degree for secondary schools (*Erstes Staatsexamen* / first state examination) in winter term 2015/16. It was accredited in 2015 and re-accredited in 2021.

- **Master of Education (MEd)**
  The program started in the winter term of 2018/19. It encompasses four semesters with a total workload of 120 ECTS CP. In combination with a second subject, the program qualifies for teaching physics at secondary schools. The degree program has been successfully accredited in 2021.

Figure 1.1: Students working in the beginners physics lab (image credits: B. Bender).

1.2 Degree Programs

1.2.1 BSc Physics

To enrol in the BSc program no specific requirements have to be fulfilled by the candidates apart from the general qualification for university entrance. However, they have to take part in an online self-assessment (`http://www.osa.uni-freiburg.de/physik`) in order to check whether their interests and expectations about the study program are sufficient and realistic.

The compulsory part of the course program provides basic knowledge and key competences in mathematics, theoretical physics, experimental physics and laboratory work. These classes also include an introductory course to scientific programming and basic knowledge in statistics, electronics and detection techniques. The remaining fifth of the course program can be chosen according to the preferences of the students. This allows the students to specialize already during the BSc program and to get a first glimpse into modern research topics by choosing up to two specialized lectures and a seminar topic. 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, it is required that one or two classes are chosen from a non-physics discipline. An overview of the BSc course program is given in Fig. 1.2. The BSc studies are completed by the bachelor thesis work. Students perform for the first time a small and independent research project during a period of three months in one of the research groups at the Institute of Physics or at the associated institutes. The students' bachelor project closes with documenting their work and their scientific results in a written thesis and giving a faculty-public presentation on their thesis work.

The overall drop-out rate is on the order of 60%–70% with only a third of the enrolled students finishing their degree (see Fig. 1.9). However, as there are no specific admission requirements, a significant fraction of the enrolled students do not seriously plan to study physics, but use their enrollment for orientation, and to obtain student status. Based on the registrations to our courses, tutorials and final exams, we estimate that these students amount to about 15% of all first semester students, so that the realistic drop-out rate is at the level of 45% to 55%, which is consistent with numbers from BSc Physics programs at other German universities. The large majority of these students leave the challenging course program already during the first year. Most of the students who drop out of the BSc program do not leave the university, but enrol in a different discipline, e.g. in engineering sciences. In this case most of the accomplished academic achievements in the BSc physics program can usually be transferred to the new program so that the students can begin the new discipline in an advanced semester.

1.2.2 MSc Physics

The MSc program in Physics is taught in English in order to provide additional skills in the dominating academic language English to the native German students and to attract students from non-German-speaking countries. Application to the MSc program is possible in both winter and summer terms. The selection and admission process is executed by the MSc Admission Committee, which evaluates whether the admission criteria are met by the applicants.

The MSc Physics program (see overview in Fig. 1.3) provides a comprehensive scientific education in advanced physics, together with a research focus on a particular field during the final research traineeship and master thesis. During this final one-year phase students participate in a research project of one of the research groups at the Institute of Physics or at the associated institutes.

In the first MSc year, participants consolidate their knowledge in advanced theoretical and experimental physics. Advanced quantum mechanics and the advanced laboratory are mandatory classes. The students can choose each term among various "Term Papers", where they learn to give oral presentations in English on a topic of modern research, accompanied by a written "paper-style" summary in English. Three courses have to be chosen 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) programs of other faculties. During the second year, the students carry out their Research Traineeship and their Master Thesis project. The study program concludes with the submission of the MSc thesis and a faculty-public presentation of the results.

Starting 2022 the institute will offer optional specializations within the MSc Physics program, allowing the students to select their courses in order to obtain a certain specialization, which will be certified on their final transcript of records. Currently, optional specializations are offered in **"Atomic, Molecular and Optical Physics"** and in **"Particle Physics"**. A

FS	Mathematik Module		Theoretische Physik A - C	Experimental-physik A - D	Physiklabore A + B	Mündl. Prüfungen	Wahlpflicht-module	∑ ECTS
1	Lineare Algebra I 9 ECTS	Analysis I 9 ECTS		Experimental-physik I 6 ECTS	Wissenschaftl. Programmieren 5 ECTS			29
2	Mathematik I für Studierende der Physik 9 ECTS		Theoretische Physik I 7 ECTS	Experimental-physik II 6 ECTS	Physiklabor für Anfänger I 6 ECTS	Experimental-physik A *(Orientierungs-prüfung)* 4 ECTS		32
3	Mathematik II für Studierende der Physik 9 ECTS		Theoretische Physik II 7 ECTS	Experimental-physik III 7 ECTS	Physiklabor für Anfänger II 6 ECTS	Theoretische Physik A 4 ECTS		33
4			Theoretische Physik III 8 ECTS	Experimental-physik IV 7 ECTS	Experimentelle Methoden 5 ECTS		Fachfremdes Wahlpflicht-modul 8 ECTS	28
5			Theoretische Physik IV 8 ECTS	Experimental-physik V 7 ECTS	Physiklabor für Fortgeschrit-tene 7 ECTS		Seminar 4 ECTS BOK 4 ECTS	30
6	Bachelorarbeit und Kolloquium 10+2 ECTS						Spezial-vorlesungen 7 + 5 ECTS BOK 4 ECTS	28

Figure 1.2: Module plan of the six semester (3-year) BSc course program showing all required modules and allocated ECTS credit points.

Term	Modules				
1	Advanced Quantum Mechanics 10 CP	Advanced Physics 1 9 CP	Advanced Physics 3 9 CP		Master Laboratory 8 CP
2		Advanced Physics 2 9 CP	Elective Subjects 9 CP	Term Paper 6 CP	
3	**Research Traineeship** 30 CP				
4	**Master Thesis** (Thesis and Presentation) 30 CP				

Figure 1.3: Recommended module plan of the four semester (2-year) MSc Physics program.

Term	Modules				
1	Advanced Experimental Physics 9 CP	Applied Physics 18 CP		Term Paper 6 CP	Master Laboratory Applied Physics 8 CP
2	Advanced Theoretical Physics 9 CP		Elective Subjects 10 CP		
3	**Research Traineeship** 30 CP				
4	**Master Thesis** 30 CP				

Figure 1.4: Recommended module plan of the four semester (2-year) MSc Applied Physics program.

specialization in Condensed Matter Physics is in the planning phase and will probably follow next year.

Currently, 120 students are enrolled in the master program. By advertising the study program e.g. on the web pages of the *Deutscher Akademischer Austauschdienst DAAD* (German Academic Exchange Service), we were able to steadily increase the fraction of international students from initially a few % to currently 36%. The drop-out rate in the master program has continuously been at a low level of only a few percent.

1.2.3 MSc Applied Physics

Initiated by the suggestion of the Scientific Advisory Board (SAB) the Institute of Physics implemented a master program in Applied Physics in 2015. In this context, funding for a new professorship for "Applied Theoretical Physics - Computational Physics" could be successfully acquired through the "Master 2016" program of the Baden-Württemberg Ministry of Science, Research and the Arts. The position was filled by Joachim Dzubiella in 2018.

The module plan of the MSc Applied Physics program is shown in Fig. 1.4. In the first year, participants consolidate their knowledge in advanced experimental and theoretical physics. They can choose among various Term Paper seminars and may select from a variety of elective courses in physics, or from the master programs of other faculties. In the large *Applied Physics* module and in the *Master Laboratory Applied Physics* courses and experiments are contributed to a substantial extent by other faculties and external institutes (e.g. the University Hospital, Fraunhofer Institutes, KIS), offering the possibility for specialization in a particular area of applied physics, such as optical technologies, physics in the life science, or interactive and adaptive materials. In their final year the students pursue their Research Traineeship and their Master Thesis project. The study program concludes with the submission of the MSc thesis and a faculty-public presentation of the results.

Starting 2022 the institute will offer an optional specialization in **"Quantum Science and Technology"** within the MSc Applied Physics program. By selecting their courses students are able to obtain this specialization, which will be certified on their final transcript of records.

Currently, 45 master students are enrolled in the program. With 68% international students the program appears especially interesting for applicants from abroad, who are attracted by the exceptional variety of elective lecture courses. Many of the lectures in the module *Applied Physics* and some of the experiments in the dedicated *Master Laboratory Applied Physics* are offered by colleagues from outside the Institute of Physics, including the Fraunhofer Institutes and other faculties such as Biology, Medicine, Environment & Natural Resources, or the Technical Faculty. The drop-out rate in the master program is continuously at a low level of only a few percent.

1.2.4 Polyvalent Bachelor & Master of Education (MEd)

Starting with the winter term of 2015/2016 the former Teaching-studies program (*Staatsexamen*) in the federal state of Baden-Würtemberg was replaced by a consecutive bachelor-master study program. In the frame of the bachelor program *Polyvalent two-subject Bachelor* prospective teachers are able to study two major subjects in a single bachelor degree. An overview of the study program in physics comprising 80 ECTS credit points is shown in Fig. 1.5. By selecting the teacher-training option the program incorporates in addition to the classes in the scientific disciplines (lectures, tutorials and lab courses) also didactics courses in each of the two major subjects, classes in general educational sciences and a school internship. The final bachelor thesis can be written in either of the main subjects.

If physics is one main subjects it is generally recommended to select mathematics as second subject, since in this case the required mathematical knowledge is covered and no additional mathematics lectures have to be selected. In this case the students can freely choose two elective courses in physics instead, allowing to gain some specialized physics knowledge.

The drop-out rate in the Polyvalent Bachelor program is currently at the same level as in the BSc program. Also in this case, most of the students dropping out do not leave the university, but enrol in a different discipline, where the accomplished academic achievements can usually be transferred.

Starting in the winter term of 2018/2019 the Master-of-Education (MEd) was implemented as a consecutive master program for graduates of the Polyvalent Bachelor (with teaching-training option). The program comprises courses in the scientific discipline physics, in physics didactics, classes in general educational sciences, and an internship at a secondary school of 12 weeks duration. The final master thesis can be written in either of the main subjects, or alternatively in educational sciences. A detailed overview of the MEd course program is given in Fig. 1.6.

The university has entered a cooperation with the *Pädagogische Hochschule* (PH, University for Education) in Freiburg, so that students of the Polyvalent

FS	Mathematik Modul	Theoretische Physik A + B	Experimental-physik A - C	Physiklabor	Mündl. Prüfungen	Option Lehramt	Σ ECTS
1	Mathematik für Ingenieure I 5 ECTS		Experimental-physik I 6 ECTS				11
2	Mathematik für Ingenieure II 5 ECTS		Experimental-physik II 6 ECTS		Experimental-physik A *(Orientierungs-prüfung)* 4 ECTS		15
3			Experimental-physik III 7 ECTS	Kleines Physiklabor für Anfänger:innen I 4 ECTS		Fachdidaktik I 2 ECTS	11
4		Theoretische Physik I 7 ECTS	Experimental-physik IV 7 ECTS	Kleines Physiklabor für Anfänger:innen II 4 ECTS			18
5		Theoretische Physik II 7 ECTS			Theoretische Physik A 4 ECTS	Fachdidaktik II 3 ECTS	11
6		Kompakte Fortgeschrittene Theoretische Physik 7 ECTS	Bachelorarbeit Physik und Kolloquium 10+2 ECTS *oder* Kolloquium 2 ECTS			Einführung Bildungs-wissenschaften 3 ECTS *und* Orientierungs-praktikum 7 ECTS	9

Figure 1.5: Overview of the course program in Physics of the Polyvalent two-subject Bachelor.

Sem.	Fachwissenschaft Physik		Fachdidaktik
1	Experimentalphysik V 7 ECTS		Kontextorientierung und Physik im Alltag 2 ECTS
2	Spezialvorlesung nach Wahl 5 ECTS	Physiklabor für Fortgeschrittene Lehramts-studierende 5 ECTS	
3			Labor für Demonstrationsversuche (Block) 4 ECTS
4	**Masterarbeit Physik** (optional im anderen Fach oder in den Bildungswissenschaften) 15 ECTS		Fachdidaktik der Physik der Kursstufe 3 ECTS Fachdidaktik: Modulabschlussprüfung 1 ECTS

Figure 1.6: Recommended module plan of the four semester (2-year) MEd Physics program.

Bachelor and the MEd programs attend their basic and advanced courses in physics didactics at the PH.

Starting in the winter term of 2022 the Institute of Physics will introduce the MEd Physics also as an ”Extension Subject” (Erweiterungsfach) which can be studied in addition to a MEd with two other main subjects. The Extension Subject is offered with two options: 90 ECTS credits / 4 semesters (Erweiterungsbeifach) or 120 ECTS credits / 5 semesters (Erweiterungshauptfach). The first option enables graduates to teach physics at German high-schools up to grade 9 (Sekundarstufe I) and the latter to grade 12 (Sekundarstufe II).

1.3 Numbers and Figures

The evolution of the new enrollments in each course program since the introduction of the BSc program in 2008/09 is summarized in Fig. 1.7. The number of enrollments in the BSc program has steadily increased over the initial years with minor variations reaching an average level of around 90 beginners per academic year over the past few years. Enrollments in the MSc programs follow a similar trend, having consolidated at approximately 50 beginners per academic year. Note that the numbers for 21/22 only include master students having started in the winter

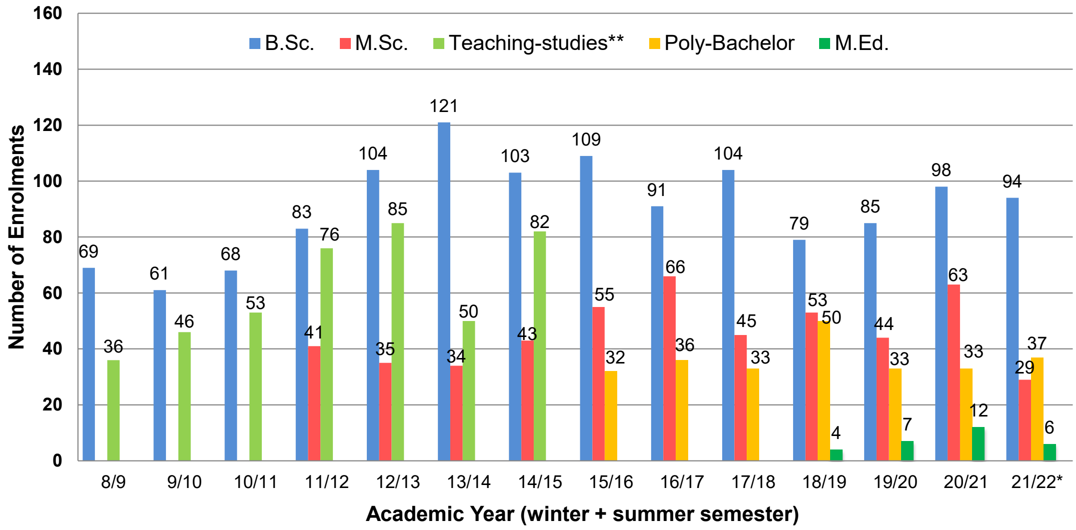


Figure 1.7: New enrollments in our degree programs per academic year. Enrollment to the BSc and Poly programs is possible only for the winter terms, to the MSc and MEd programs for winter and summer terms. (*For the academic year 21/22 only MSc and MEd-enrollments for the winter semester are included. **In 2015/16 the Teaching-studies program was replaced by the new polyvalent Bachelor in combination with the Master of Education, which started in winter semester 2018/19.)

semester 2021/22. The total number is expected to increase to around 50 with the new enrollments for the summer semester 2022. A detailed view with the beginners in each semester separated for the two Master programs MSc Physics and MSc Applied Physics is shown in Fig. 1.8.

The number of beginners in the Polyvalent Bachelor, which has replaced the Teaching-study program in 2015/16, has consolidated at a level of 30–40 each year. This is significantly lower than the number of enrollments in the final years of the former Teaching-training studies, a trend also observed in other disciplines and also at other universities in Baden-Württemberg.

The number of degrees awarded (see Fig. 1.9) shows some fluctuations over the years with the BSc and MSc degrees having finally replaced the Diploma. We believe that the minimum in 20/21 can be attributed to the fact that many students sojourned (or at least slowed down) their studies during the corona pandemic due to the difficult conditions. We expect the number of degrees to increase again in the near future.

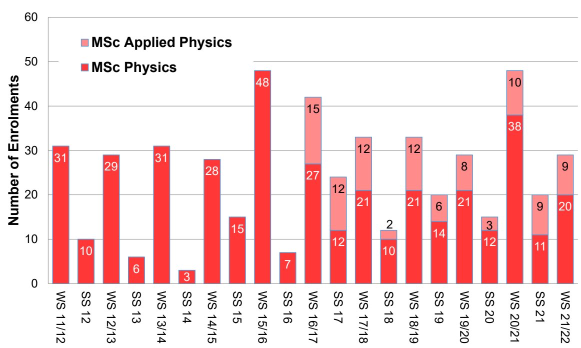


Figure 1.8: New enrollments in our MSc programs per semester.

1.4 Postgraduate Studies / PhD Program

A significant fraction of master graduates continues with postgraduate studies aiming for the PhD degree "Dr. rer. nat." awarded by the joint Faculty for Mathematics and Physics. Since 2016 at the University of Freiburg new PhD regulations are in effect, which require that the candidate and his or her supervisor sign a supervision agreement prior to the PhD project. In this document the candidate and supervisor agree on regular official meetings where they assess the progress of the PhD project and discuss the next steps and time-line.

For obtaining a PhD degree no structured course program is mandatory. However, at the Institute of Physics two Research Training Groups and one Research Unit, funded by the *Deutsche Forschungsgemeinschaft DFG* (German Science Foundation), are currently hosted, which offer an educational program

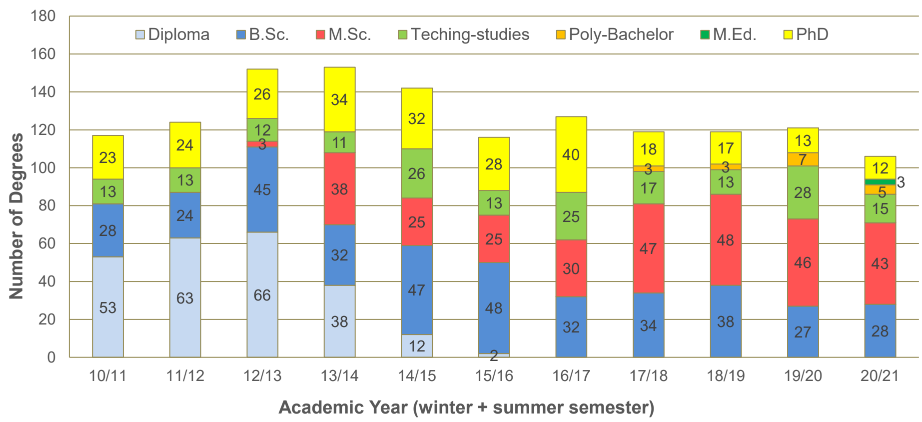


Figure 1.9: Number of degrees awarded by the Institute of Physics since winter semester 2010.

for the participating PhD students including specialized lectures, seminars, topical workshops and meetings. The Research Training Group (RTG 2044) "Mass and Symmetries after the Discovery of the Higgs Particle at the LHC", the Research Training Group (IRTG 2717) "Dynamics of Controlled Atomic and Molecular Systems DynCAM", and the DFG Research Unit (FOR 5099) "Reducing Complexity of Non-equilibrium Systems" cover all three main research areas at our institute.

In total 126 PhD students are currently performing research for their dissertation in physics, about two thirds directly at the Institute of Physics and one third at the associated research institutes or in the group of a co-opted member.

1.5 Teaching Export

The Institute of Physics supplies the largest share in teaching support to other departments and faculties at the University of Freiburg. Basic physics knowledge is mandatory in course programs or recommended as an elective subject in nine BSc, five MSc and three *Staatsexamen* programs, i.e. in BSc Biology, BSc and MSc Chemistry, MSc Chrystalline Materials, BSc Embedded Systems Engineering, BSc Environmental Sciences, BSc Geography, BSc and MSc Geology, BSc and MSc Computer Science, Bsc and MSc Mathematics, BSc Microsystems Engineering, and state examinations in Medicine, in Dentistry, and in Pharmacy. In some of the programs, the external students participate in the basic experimental physics lectures of the regular BSc physics program, e.g. students from computer science and mathematics. However, for students from other natural sciences, and from medicine and pharmacy dedicated lectures, tutorials and laboratory classes are offered. Nearly one thousand students from all over the university participate in these dedicated lectures and laboratory courses each year.

1.6 Office for Studies

The Office for Studies is the central contact point for the students at the Institute of Physics. The examination office constitutes a central part of this office, offering advice and information on examination details and procedures during the regular consultation-hours as well as by email. Two study advisors offer individual advice and guidance with respect to planning the curriculum and to general aspects of the study programs. One advisor is responsible for the BSc/MSc programs and one for the Polyvalent Bachelor/MEd programs. Both also coordinate the course programs. The head of the Office for Studies is the Dean of Studies, who is responsible for all affairs related to teaching and examinations. In addition three professors, one from each main research area, offer consultations on specific questions related to the particular research field.

1.7 Quality Management

All lectures are evaluated with a questionnaire towards the end of each semester. The survey is pursued by the central evaluation service (ZES) of the university. In addition the student representatives (Fachschaft) regularly organize a separate evaluation of tutorial classes. The evaluations consist of a statistical analysis and a compilation of individual comments by the students. Direct feedback is given to the lecturers and to the tutors.

New developments and structural changes in the

Figure 1.10: Physics lecture in the large lecture hall.

course programs 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 of the academic staff and four professors.

1.8 Support for Students

1.8.1 New Students

The body of student representatives (Fachschaft Physik) offers various forms of assistance to students, particularly to new students at the start of their studies and during their first semesters. They provide practical help in organizing the students' life and in planning their studies and their individual time tables. Before the beginning of the winter term, a one-week long "Welcome and Kick-Off event" is organized, which helps students make the transition from school to university. The welcome week of the Fachschaft incorporates guided tours of the natural science campus, the libraries and the physics institute, as well as an overnight stay at a local lodge, where the new students get to know each other and connect to students in higher semesters.

Welcome and introduction seminars are organized by the Dean of Studies and the study counsellors during the first week of each teaching period. The presentations give an overview of the study program, the examination procedures and regulations and the various options to obtain advice and support. General help is also provided by the central Service Centre for Studies (SCS).

The Institute of Physics has implemented a mentoring program for first year students where professors and lecturers meet with up to five students each, several times during the first year of their studies. In these meetings students and mentors discuss their expectations, in particular also the requirements in terms of personal responsibility and motivation of the students. Furthermore, these meetings enable the students to personally get to know one of the professors or lecturers which is typically difficult in the large first year's lectures. We hope that this program will especially be of value for students who have the talent to study physics but do not succeed to deal with the challenges of the transition from school to university.

1.8.2 Gender and Diversity

The fraction of female students in the course programs is currently at the level of 29% (BSc), 27% (MSc), 27% (Polyvalent Bachelor), and 32% (MEd). These numbers have significantly increased since the last reporting period in 2017.

In order to increase the number of female students in physics and to help women in organizing their studies and career planning, specific programs have been implemented:

Each year a special open day originally for pupils at secondary schools is organized, where they are informed about the study programs and the research activities at the institute and also have the possibility to participate in small practical workshops organized by the research groups. Originally, the event was only available for female pupils but has been opened recently also for male pupils. The institute aims to especially deploy female PhD students as supervisors of the workshops, who may act as role models for the students.

A specific mentoring program MeMPhys (mentoring in mathematics and physics) has been established at the Faculty for Mathematics and Physics. Each interested student is mentored by an experienced student in a tandem approach. In addition, specific seminars and social events are organized by coordinators of the MeMPhys program in cooperation with the faculty member responsible for equal opportunities. Although this program was initially designed only for female students, the event has now been opened for all genders.

1.8.3 International Students

Dedicated support is provided to students from foreign countries, who enrol in the MSc programmes or spend several months in Freiburg with an international exchange program. The International Office of the university provides general help, particularly related to questions concerning housing and visa issues. It also provides support for students participating in the European exchange program ERASMUS. The Institute of Physics also has an ERASMUS coordinator (Prof. Dzubiella took over this responsibility from Prof. Ita in 2021). He is organizing the cases of about 15–20 students per year who participate in the student exchange program and go for one or two terms to one of the partner universities abroad, and of the 5–10 incoming students from foreign countries who are visiting the Institute of Physics.

The *Studierendenwerk Freiburg Schwarzwald* (Student Services Freiburg) offers advice to students looking for an apartment or a possibility to finance their stay in Freiburg. Language courses in German are offered regularly at various levels by the *Sprachlehrinstitut SLI* (Language Teaching Centre). Help with the regulations for applications and enrollments is provided by the International Admissions and Services (IAS) in the Service Centre for Studies (SCS).

Currently the ratio of international students in the BSc program is less than 3%, as the program requires them to have advanced proficiency in German (C1-level). The English-taught MSc programs are attracting much more students from abroad, with a fraction of currently 45% internationals (MSc Physics and MSc Applied Physics combined). .

1.9 Outreach - Promoting the Physics Programs

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 programs at our institute and to inform the public about the research activities.

Each year an ”Open Day” for interested pupils from secondary schools is organized by the Office for Studies. The pupils are informed about the content of the various course programs 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. Specific lectures covering aspects of experimental and theoretical physics adapted to the level of secondary school students are held by professors. About 100 pupils attend this event each year.

In the module *Berufs- und Studienorientierung am Gymnasium BOGY* (Orientation for Profession and Studies at Secondary Schools) pupils at the age of sixteen to seventeen have to visit a service provider, company, research institute or research group at a university to perform an internship for one week. Each year on average ten pupils choose to join a research group at the Institute of Physics for this project.

Six researchers at the Institute of Physics act as jury members and judges at the annual ”Jugend forscht” contest, a school and youth competition in the field of natural sciences and technology where talented schoolchildren work on their own projects. They present their results at an annual event. The Institute of Physics awards two 3-day research internships at our institute as special prizes for successful participants at the state level competition of ”Jugend forscht”.

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

The particle physics groups participate in the international Master Classes ”Hands on Particles Physics”, organized simultaneously at 210 institutes in 52 countries worldwide every year in March. Secondary school pupils have the opportunity to attend lectures on particle physics and to perform analyses of data from collider experiments during the course of one day. At the end of each day, the participants join an international video conference for the discussion of their results. In addition, teachers can also invite scientists from the Institute of Physics to visit their school for a day and perform the Master Classes on site. On average five such visits take place every year.

Other activities for the general public include the participation in the biannual two-day long Science Market centrally organized by the University of Freiburg in the centre of the city and the well attended public Christmas Lectures in physics every year.

A comprehensive list of the outreach activities of the Institute of Physics is given in Chapter V.

Part IV

Infrastructure

Chapter caption: Newly renovated seminar room in the physics library.

1.1 Buildings of the Institute

With few exceptions all facilities used by and available to the researchers, students, and administration of the Institute of Physics are located at the Physics Campus (see overview map in Fig. 1.1). This campus is part of the University's Natural Sciences Campus (Institutsviertel), just about 1000 m away from the Freiburg city center. The institute and its facilities are distributed over several buildings.

With its eleven floors, the *Physics High-Rise* (Physik Hochhaus) provides office spaces for theoretical and experimental research groups, some smaller, basic experimental laboratories, the offices of the IT support group, as well as two large lecture halls and several seminar rooms for tutorial classes in the first floor. The eleventh, top floor hosts the institute's Common Room which is mainly used as a student workspace.

The *Gustav-Mie Building* (Gustav-Mie Gebäude) offers high-quality experimental lab spaces and further offices. Chemical labs and clean rooms are also located here. In addition, the Gustav-Mie building hosts the advanced laboratory courses with the corresponding experiments on the second floor, as well as computer pools for students, a seminar room and the students' "social room".

The *Low-Rise Building*, which connects the Physics high-rise and the Gustav-Mie building, provides space for the mechanical and electrical workshops, the mechanical/laser engineering laboratory and the electronic design and development lab. In addition, the laboratories of four experimental research groups are located here on an interim basis as they are outdated in terms of accessibility, appliances and safety. The tower of the old Van de Graaf accelerator, that has been dismantled already in the last century, remained essentially unused in the last years. It was fully refurbished and since spring 2018 it now hosts the laboratory of the Astroparticle Physics group.

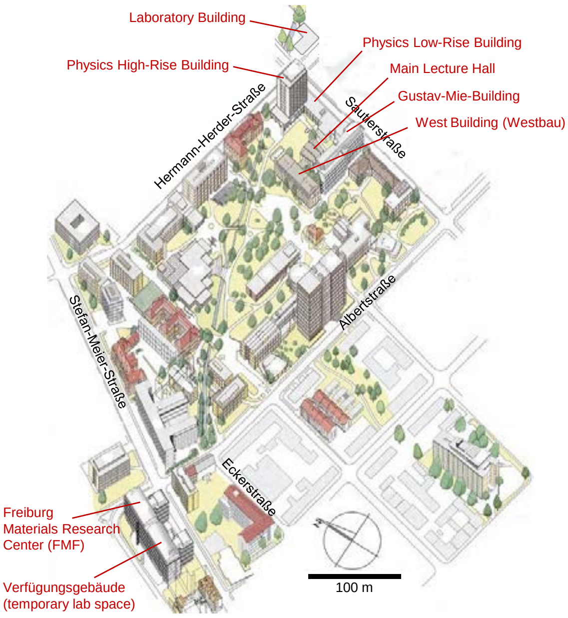


Figure 1.1: Map of the Natural Sciences Campus of the University (Institutsviertel) with the physics buildings being labeled.

Figure 1.2: The new room for parents and their kids in the basement of the West Building after its completion in February 2022.

The *West Building* (West Gebäude) houses additional seminar rooms, the offices of the institute and the student administration, the library of the Institute of Physics, and the offices of some theoretical research groups. Furthermore, there are two meeting rooms furnished with modern multimedia equipment, plenty of work space for students (in and outside of the library) and (new since 2022) a room dedicated to parents and their kids, see Fig. 1.2. The *Fachschaft Physik* (body of student representatives) has its own rooms in the basement of the building.

The *Main Lecture Hall* (Großer Hörsaal Physik) is located in a dedicated building in the center of the physics campus (see Fig. 1.3). It also provides additional rooms for the preparation and storage of demonstration experiments. The building with a capacity of ∼350 seats has been renovated from February to December 2017 and is equipped with state-of-the-art building automation and modern multimedia equipment.

The *Laboratory Building* (Praktikumsgebäude) just across the road from the highrise hosts the experimental setups and lab spaces of the introductory

Figure 1.3: Experimental physics lecture in the Main Lecture Hall (*Großer Hörsaal*).

physics laboratory courses for physics students and students of other natural sciences (teaching export to study programs in molecular medicine, medicine, dentistry, pharmacy, biology, chemistry, etc.).

The available space for offices and laboratories is not sufficient to accommodate all research groups and support units of the institute. After the transformation of the former accelerator tower into a laboratory, there is currently no further space available at the physics campus. For this reason, the laboratories and offices of two experimental research groups (Sansone, von Issendorf) are located in the Verfügungsgebäude adjacent to the Freiburg Materials Research Center (Freiburger Materialforschungszentrum, FMF) since many years (see Figure 1.1).

This leads to the very unfortunate situation that these groups are located in rented space, separated by a distance of 500 m from the workshops and support groups while hampering the direct contact with the physics students and colleagues.

1.2 General Organization

The Institute of Physics is organized as a "Department System", which provides central management of personnel, finances and other resources. The procurement of research equipment is in the hands of the individual groups, possibly in cooperation with the University's central purchasing department.

An essential element of the Department System is that in addition to their individual resources, all full professors participate equally in a common "pool of resources". It provides central infrastructure such as administration, technical services (workshops, engineering expertise, IT support, technical staff), liquid nitrogen supply and further resources. A similar pool also exists for scientific personnel from which positions can be allocated based on demand (largely reflecting the institute's obligations from hiring negotiations), as well as for financing the joint infrastructure and short term needs of individual groups.

The institute's administration comprises the senior manager who also acts as head of administration, the deputy senior manager/head of technical services and four administrators. It manages the human and financial resources, including the various third-party funding from mostly the DFG, BMBF, and EU. Dedicated team assistants, most of whom are working part-time, support the research groups and the administration.

1.3 Technical Support Department

The scientific work at the Institute of Physics is supported by a technical support department, shown in Fig. 1.4. Following an internal evaluation process in 2020, its structure has been adapted to meet future requirements of the working groups. The following adjustments have been made:

- Establishment of a new overarching service unit "Mechanics" which includes the mechanical workshop as well as a newly established engineering unit. Leader of the unit is Dipl. Ing. M. Stoll.

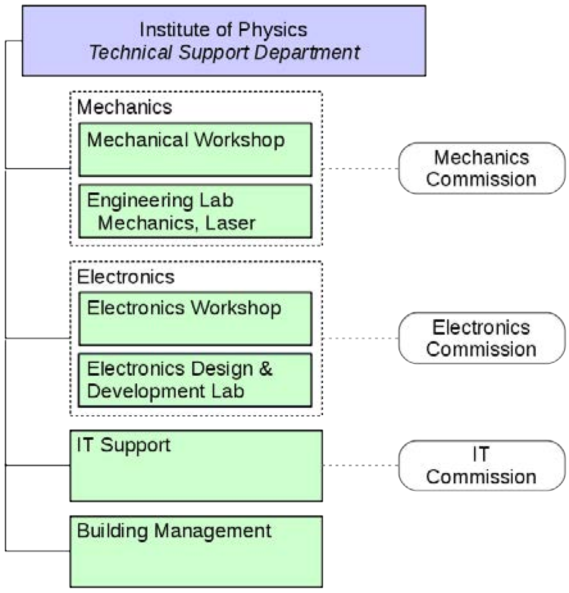


Figure 1.4: Organization chart of the technical services of the Institute of Physics which have been updated in the last years to meet the changing needs of the scientific groups.

- Two engineers, for mechanical engineering and laser systems, have been hired on permanent positions to bring crucial expertise to the institute that was not available so far. These positions also help with knowledge transfer and to support long-term projects.
- Establishment of a new overarching service unit ”Electronics” which includes the electronics workshop as well as the electronics design and development laboratory. Leader of the unit is Dr. K. Mahboubi.
- The group leader position for the electronics workshop has been finally filled successfully (D. Wagner), after years of interim solutions.
- One position in the electronics design and development laboratory has been upgraded to a full engineering position.
- The IT support group (led by G. Endress) has been strengthened by ensuring that the IT expert hired by the institute is actually working at the institute. (The last years have seen unsatisfactory solutions with personnel delegated from/to other university units.)

In total, no new positions have been added to the support department but all adaptions of the structure were established using positions from the support units. (In some cases temporary financing solutions using other positions had to be identified to bridge gaps until retirements etc.) The transition to the new organizational system is now completed and the users are happy with it.

The Mechanics Unit, with the Mechanical Workshop (MW) and the Engineering Laboratory for Mechanics and Lasers, and the Electronics Unit, with the Electronics Workshop (EW) and the Electronic Design and Development Laboratory, offer highly specialized technical services and are essential resources for the experimental physics groups. They traditionally constitute a central cornerstone of physics research in Freiburg and their work is internationally recognized thanks their contribution to large-scale multi-national projects such at ATLAS at CERN or XENON at LNGS as well as bilateral projects, e.g., with UBC Vancouver. The mechanical and electronic workshops regularly train young apprentices as *Feinwerkmechanikern/innen* (precision mechanics, typical 8 positions) or electricians (typical 4 positions).

The IT group provides computing support and advice mainly to the theory groups and some of the experimental research groups. The unit also supports the central administration and maintains the IT/multimedia infrastructure for teaching etc.

All three units regularly report to commissions which consist of three full professors and the representatives of the respective units. These commissions report to the Institute Board about the performance of the support units and advise the Institute's management in terms of strategical decisions and funding requirements.

The fourth unit ”Building Management” takes care of the institute's buildings and infrastructure. The unit is of particular importance since the institute with its partly very old buildings accommodates a large number of experimental laboratories and workshops which need continuous, close support by experts that know the infrastructure very well and also serve as contact points towards the relevant technical units at the University level.

1.3.1 Mechanics

The unit Mechanics supports the researchers starting from the design phase of a project, by advice and discussions, CAD design as well as engineering support, to production, assembly/installation and maintenance.

Mechanical Workshop

The mechanical workshop has 19 members (plus apprentices). It serves the experimental groups in all their requirements to build and operate their experiments. The full integration of the workshop into the institute allows for the efficient realization of prototypes, time-critical components, special shapes and new developments, and facilitates solving complicated experimental problems via continuous interaction between workshop personnel and scientists. It considerably reduces experimental down-times and allows the Freiburg groups to take leading roles in the construction of international large-scale projects. If required, the number of workshop members also allows for mass production of parts. The workshop is conveniently located on the first two floors of the Low-Rise Building, which allows young researchers at the PhD level, but also already during the BSc or MSc thesis, to directly interact with machining experts to realize their own projects.

The workshop team also operates the forklift truck and the various cranes of the institute, and provides general support in any larger logistic operations as well as installation campaigns.

The workshop is equipped to manufacture all sorts of high-precision parts, up to sizes of $1.5 \times 0.7\,\mathrm{m}^2$ (see Fig.1.5). The available manufacturing tools allow achieving essentially any specification currently attainable by state-of-the-art mechanical manufactur-

Figure 1.5: 5-axis milling center in the Mechanical Workshop at the Institute of Physics.

ing technology. Besides the usual lathe and milling tools the mechanical workshop currently operates

- seven CNC milling centers; three of them with 4- and 5-axis control;
- two CNC turning centers with driven tools; and one standard CNC turning center;
- 3-D printer for rapid prototyping;
- welding equipment for stainless steel, aluminum and copper;
- sheet metal working machines for complex designs.

Simultaneous 5-axis manufacturing is possible thanks to a CAD/CAM cross linking. Sophisticated parts can be treated by clamping, which enhances the manufacturing efficiency and quality.

Engineering Laboratory

After evaluating the current and future needs of the experimental physics groups, the engineering laboratory within the service unit Mechanics was founded in mid 2021. It consists of a mechanical engineer and a laser engineer who closely interact with the mechanical workshop as well as the relevant people in the electronics unit.

The mechanical engineer (Dipl. Ing. Ochoa) takes over complex design projects and in particular assists design decisions using detailed mechanical modelling. The laser engineer (Dr. Niebuhr) supports all groups of the Institute of Physics that use lasers for their experiments, e.g., by maintenance of laser systems and conducting optical simulations.

1.3.2 Electronics

Electronics Workshop

The electronics workshop consists of seven technicians. After a long period with interim solutions the unit has now again a dedicated workshop head: Mr. Delon Wagner was hired in fall 2021. Some restructuring of the rooms of the unit also occurred in 2021; this is accompanied by efforts to modernize the workshop and the work-organization – a process that is still ongoing.

The core expertise of the electronics workshop is the development and production of instruments and measurement systems with a special emphasis on CAD-aided printed circuit board (PCB) layout routing and in-house production of two-layer print boards and well as the procurement of multi-layer PCBs and SMD parts. This is done in close collaboration with the electronics design and development laboratory. The workshop additionally offers a wide range of services, starting from counseling in all electronics related questions, management and provision of electronic parts, assembly of cables and connectors, and repair and maintenance of custom-made and commercial equipment. If required, equipment in the research laboratories is also being checked in terms of safety.

To this end the workshop is equipped with all required standard tools and machines. PCBs with a small number of electronic components are produced by hand using stereo microscopes. For projects involving many components, protoypes or small batch series, an automatic pick & place machine (Fritsch PlaceALL 510) is employed. It features a broad range of components and allows for a flexible realization of complex projects. For such projects, the workshop also operates a large high-end reflow soldering oven (Rehm) while smaller ones are handled using a compact table-top oven.

Also offered are custom Arduino-based microcontroller boards for rapid developments. These boards are compatible with the Arduino IDE. Program code can also be created on this platform in the electronic workshop. Here also the most powerful microcontroller of this platform are used.

1.3.3 Electronic Design and Development Lab

This group comprises of four electronics engineers supporting the experimental groups of the Institute of Physics in their research and development programs. It offers a number of immediate benefits to researchers, from providing consulting to developing

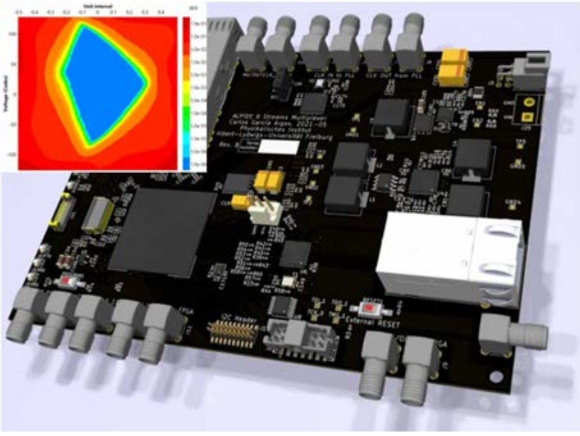


Figure 1.6: A Kintex-7 FPGA data acquisition board design example. Inset: Eye diagram for a 10 Gbps link using the Xilinx Integrated Bit Error Tester.

fully-customized electronic systems which are commercially not available.

The electronic design and development lab provides researchers with access to advanced electronics, assists with integrating electronics technology into research projects, and aids in electronics technology transfer to users by providing ongoing technical support, consulting, proof of concept and proposals for technical solutions. The group's expert designers offer a full design service, starting at the requirements specifications phase up to full production. Working in many electronics domains, from analog through digital, including RF designs and ultra-sensitive sensor electronics, the group masters in low-noise high-performance signal conditioning and power electronics, high speed FPGA, microcontroller, microprocessor and DSP based applications.

The team develops solutions that involve hardware design, and firmware and software development, according to the requirements of the experiments and following best practices. It operates a cleanroom for semiconductor sensors applications (see Section 1.5.2), including wire bonding and pull testing for quality control. Some highlights of electronics designed and/or developed during the last four years include:

- Acquisition, interface and control circuit board for high-speed read-out of custom high density silicon pixel sensors based on high-end FPGA devices.

- Microprocessor-based universal controller for hot-cathode ionization vacuum gauges utilizing processor and DSP cores implementing interfaces and fast PID algorithm.

- Stand-alone, fast, Programmable TTL Pulse Pattern Generator, Delay Generator, Digital Word Generator and Timing Module enabling the generation of complex pulse and pattern sequences for, e.g., spectrometry, and related resonance and test technologies.

- FPGA/microprocessor based very fast PID engines for various applications such as laser beam stabilization/collimation/focusing.

- Microcontroller based multi-channel low impedance/capacitance measurement system, as part of the Quality Control and Assurance for the production of the ATLAS ITk Strips Upgrade production.

- High voltage/current fast switching modules to drive various capacitive and inductive loads.

- Microcontroller based read-out systems for power supplies and interlock systems, with USB or Ethernet interface controllers.

- Various multi-stage low-noise and high bandwidth amplifier and filter designs.

- Several photodiode driver circuits, for instance for laser focusing applications.

- Frequency mixer and various filters/amplifiers for RF applications.

In many cases, the projects realized in past years have led to designs that can be adapted to meet new and/or common requirements of the Freiburg researchers. This is a big advantage of in-house designed, custom-built and tested equipment.

1.3.4 IT Support Group

The institute's IT support group of four computer specialists represents a central service unit of the institute. It was founded in 2016 by combining IT experts from individual research groups into a dedicated team, in order to exploit synergies and to optimize expertise and the availability of support. It serves the needs of a large fraction of the institute, including the theoretical and many experimental groups and the administration. However, due to limited manpower, not all experimental groups can benefit from the IT support group. Mr. Wyneken, a long-term IT expert (Linux, network administration) will retire in 2022; his succession was already solved in late 2021 by the early hire of Mr. Beh to ensure sufficient overlap time.

The tasks of the group include:

- maintenance, configuration and trouble-shooting of computers and other IT infrastructure;
- operation of complex IT infrastructures;
- administration of UNIX/Linux, OSX and Windows based clients and servers;
- hardware and software installations for personnel computers;
- procurement of IT components;
- assistance in IT and network questions and coordination with other faculties and the computer center ("Rechenzentrum");
  item coordination, administration and deployment of Wolfram Mathematica and OriginLab campus licenses;
- maintenance, configuration and trouble-shooting of multimedia facilities;
- administration of institute copiers

1.3.5 Building Management

The building management team is responsible for the maintenance and servicing of building installations and infrastructure such as heating, ventilation, air-conditioning, small repairs, postal delivery services and further tasks such as interaction with external companies working on the institute premises. It is handled by a janitor and a desk officer, who is based in the entry area of the Physics High-Rise. Further advice, planning and implementation of building technology installation is offered by the *Technisches Gebäude Management* (technical building management), a central service unit of the university. The building management team is supported by members of the mechanical workshop on a regular basis.

1.4 Facilities for Teaching and Students

The central administration unit for students, the "Office for Studies" (for details see Part III, Sect. 1.6), is located in the West Building and comprises two officials at the examination office supporting the dean of studies, the program coordination and the student advisers (one for BSc/MSc physics students, one for students who want to become physics teachers). Detailed additional academic counseling is provided

Figure 1.7: Indoor and outdoor areas of the "Common Room" on the top floor of the physics high-rise building.

by three professors, representing the three main research areas of the institute.

Three large lecture halls are available to the Institute of Physics on its own premises: the main lecture hall (340 persons, see 1.3 on page 196), and lecture halls I (150 persons) and II (60 persons) on the first floor of the Physics High-Rise Building. A total of six seminar rooms with capacities ranging from 15 to 40 persons are available in the buildings of the institute. In order to compensate for space shortcomings, especially in highly-demanded time slots in the morning or the early afternoon, student seminars or tutorials are occasionally also held in the seminar/common rooms of individual research groups for a full semester. Two Computer Pools with a total of 34 workplaces for students are available in the Gustav-Mie Building.

The basic laboratory courses for physicists and the for students of medicine, dentistry, pharmacy and other natural sciences are all held in the Laboratory Building (for location see Fig. 1.1), where the experimental setups are distributed over four floors. A

Figure 1.8: The newly renovated seminar and work space in the physics library.

graduated full-time staff member is in charge of organizing all basic laboratory courses assisted by a laboratory course technician. The 25 experiments for the advanced laboratory classes are located in the Gustav-Mie Building, and maintained by another technician. The teaching and laboratory team is completed by an assistant responsible to develop and prepare the demonstration experiments in the main lecture hall.

The Institute of Physics provides ample space for both learning and recreation. A large Common Room (Fig. 1.7) at the top floor of the Physics High-Rise offers a relaxed atmosphere for students to meet with other students or teaching staff and scientific personnel. It provides a stunning view over Freiburg and the surrounding mountain ridges and is equipped with tables, whiteboards and a small kitchen and is regularly used by students for discussions, preparation for lectures and tutorials, or relaxing.

A social room in the Gustav-Mie Building is equipped with a black board and desks, as well as kitchen equipment. It is regularly used for studying, student gatherings or meetings, but can also be booked for tutorial classes. Several other rooms at the institute premises are also available as dedicated student workplaces: six newly created smaller rooms in the basement of the West Building providing more privacy and the public areas in front of the large lecture halls. The student representatives of the *Fachschaft Physik* occupy separate rooms in the basement of the West Building.

1.5 Other Infrastructure

1.5.1 Physics Library

The Physics Library occupies the entire first floor of the West building. It is organized as a reference library (*Präsenzbibliothek*), and is open to researchers 24 hours a day, seven days a week and to students during the week when it is staffed by a team member of the central University Library. Apart from providing scientific literature it also offers silent work space and a newly renovated seminar room which can also be used for smaller institute events such as award ceremonies (see Fig. 1.8).

1.5.2 Clean Room Facilities

The Gustav-Mie building houses an industrial-style class 10000 clean room of approximately 100 m^2. About 15 m^2 of it are equipped with class 100 laminar flow boxes. It is primarily used for testing and manipulating semiconductor wafers and detectors made from, e.g., Silicon, GaAs, or CdTe. It is also well adapted to handling delicate electronic boards. The clean room is equipped with a Delvotec ultrasonic wire bonder (see Fig. (see Fig. 1.9), a wire pull tester, an automatic probe station, a semi-automatic metrology microscope and a dispensing robot.

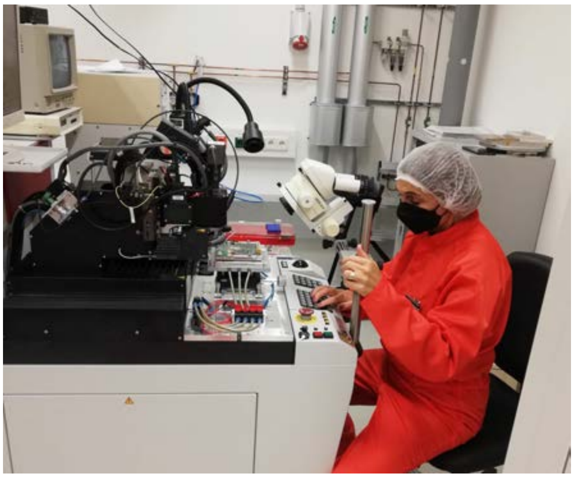


Figure 1.9: I. Veiga (group Jakobs) in the clean room connecting a CMOS silicon sensor with its readout ASICs, operating the Delvotec G5 ultrasonic wire bonder

A smaller class 100000 cleanroom with an area of 12 m^2 is located in the astroparticle physics laboratory where it is used to construct and maintain liquid-xenon based detector prototypes. It was designed such that large components of up to $\sim$2 m size can be easily brought into the room.

1.5.3 Computing Infrastructure

Major computing hardware of the Institute of Physics is located in two server rooms in the basement of the High-Rise and the Gustav-Mie building. The majority of the installed systems are operated by the institute's IT support group; the rest by the research groups that own the systems. The two computer rooms for students are also operated by the IT support group. They offer 34 PC workstations and some printers. Additional computing infrastructure, e.g., web and mail servers, wiki-services, home-directory storage space with automated backup functionality, etc. is provided by the University IT Services (computing center/"Rechenzentrum").

Very significant additional resources for research activities are provided via four high-performance computing (HPC) clusters in the *bwForCLuster* initiative funded by the state of Baden-Württemberg (BW) and the German Research Foundation (DFG); it can be used by all scientists at universities in Baden-Württemberg. The Freiburg University IT Services (Rechenzentrum) hosts and operates the HPC cluster *NEMO* for the particle physics, neuroscience, microsystem engineering and material science communities. The clusters comprises 18'000 logical cores, five NVIDIA GPU machines, mass storage of approximately 1 PB and an uplink to the *BaWue network* of 100 Gbits/s.

The application for the next generation HPC cluster *NEMO-2* was successful; it will start operation in winter 2022/2023. In addition, the mass storage system *bwSFS* (also funded by BW and DFG) providing several PB capacity for data archiving and data storage was installed in 2021. It serves the needs of the NEMO communities and the three consortia in the context of the DFG-funded National Research Data Infrastructure NFDI with participation from Freiburg: BioDATEN, DataPLANT and PUNCH4NFDI. Several research groups of the Institute of Physics participated in the applications for *NEMO-2* and *bwSFS* and are main users of these IT infrastructures.

For the research activities in the four experimental ATLAS groups (Heinemann, Herten, Jakobs, Schumacher) the dedicated high throughput computing (HTC) cluster *ATLAS-BFG* (Black Forest Grid) is available. It offers 3 PB of fast parallel mass storage and a CPU power of 3200 logical cores. It is hosted at the University IT Services and operated by one of the ATLAS groups.

Part V

Activities of the Institute

Chapter caption: Various outreach activities of the Institute of Physics such as presentations at ”Science Days”, the annual Christmas lecture and public lectures for school classes (Image credits: M. Herrmann, Badische Zeitung).

During this reporting period, albeit also impaired by the world-wide pandemic situation in 2020 and 2021, members of the Institute of Physics have (co-)organized various international and national conferences, workshops, symposia as well as PhD schools which are listed below in Sections 1.1 and 1.2. Some of them have been co-organized by the *Freiburg Institute for Advances Studies (FRIAS)*. Researchers from Freiburg have also been invited to teach at PhD schools organized elsewhere (Sect. 1.3).

The institute offers several regular colloquia and seminar series in the different research areas, listed in Sect. 1.4. The *Freiburger Physikalisches Kolloquium* is the institute's main colloquium that is targeted at all institute members from first year student to professors and covers all research areas of physics and relevant neighboring fields. It takes place every Monday afternoon during the semester and is followed by an informal wine-and-pretzel get-together which provides an ideal forum for scientific exchange between scientists and students. Every research group hosts at least one regular internal group seminar; these events are not listed.

As part of our outreach activities scientists from our institute are actively promoting physics in general and the institute's research areas in particular at local schools, in public lectures, or at science fairs, see Sects. 1.5 and 1.6. The goal is to excite interested students and encourage them to enrol in physics or other natural sciences, as well as to familiarize high school teachers with the topics of current research. Another important aspect of the outreach activities is to increase the awareness of the general public that physics, science and evidence-based decision making is important for society.

The various activities are listed in the following.

1.1 Conferences

- **Spring Meeting of the German Physical Society, Section AMOP**, Erlangen, 4-9 March 2018; Rostock, 10-15 Mar 2019; Hannover 8-13 Mar 2020 (cancelled due to COVID-19); Chair of Scientific Organsiation: A. Buchleitner
  `https://erlangen18.dpg-tagungen.de/`
  `https://rostock19.dpg-tagungen.de/`
  `https://www.dpg-verhandlungen.de/year/2020/conference/hannover/parts?lang=en`

- **High Intensity Lasers and High Field Phenomena**Topical Meeting of OSA-OPTICA
  Strasbourg, France, 26-28 March 2018. Program Chair: Giuseppe Sansone.
  Washington, DC, United States 16–20 November 2020. General Chair: Giuseppe Sansone.

- **TeVPA 2018**, Berlin (Germany), 27.-31.08.2018. Convener dark matter session: M. Schumann
  `http://tevpa2018.desy.de`

- **High Precision for Hard Processes (HP2 2018),** Freiburg, Oct 2018
  Local Organizing Committee: S. Abreu, S. Dittmaier, F. Febres Cordero, H. Ita, P. Maierhöfer
  (`https://indico.cern.ch/event/694599/`)

- **Axion-WIMP (PATRAS)**, DESY (2018), Freiburg (2019), Online (2021).
  International Organization Committee: M. Schumann, H. Fischer
  `http://axion-wimp.desy.de/`.

- **Higgs Hunting Conference**, IJCLab/Paris (2018, 2019 and 2020),
  International Advisory Committee: K. Jakobs and M. Schumacher

- **IEEE NSS/MIC Conferences**, Sidney (2018), Manchester (2019), Boston (2020), Online (2021). Referee for Nuclear Science Symposium: M. Schumann
  (`https://nssmic.ieee.org`)

- **LHCP - Large Hadron Collider Physics Conference**, Bologna (2018), Puebla/Mexico (2019), Paris (2020), Paris (2021). International Advisory Committee: K. Jakobs

- **ICHEP - International Conference on High Energy Physics**, Seoul (2018), Prague (2020), Bologna (2022). International Advisory Committee: K. Jakobs

- **First Fall Meeting of the German Physical Society – "Quantum Science and Information Technologies"**, Freiburg, 23-27 September 2019,
Chair of programme committee and local organiser: A. Buchleitner & QOS
`https://freiburg19.dpg-tagungen.de/`
- **Memory Effects in Dynamical Processes**, Vienna, Austria, June 2021
Organizing Committee: A. Kuhnhold (Freiburg), H. Meyer, T. Schilling (Freiburg), C. Dellago
(`https://www.esi.ac.at/events/e413/`)
- **ICRC 2021**, Berlin, July 2021, Local Organization Committee: M. Schumann
`https://icrc2021.desy.de/`

1.2 Workshops, Symposia and Schools

- **Meeting on Extreme Atomic Systems – EAS**, Riezlern, 19-22 Feb 2018, 18-21 Feb 2019, 27-30 Jan 2020, Organisers: J.-M. Rost, T. Pfeifer, A. Buchleitner (Freiburg)
(`https://www.pks.mpg.de/~eas/`)
- MITP Workshop **Probing Physics Beyond the Standard Model with Precision,** Mainz, Feb/March 2018
Organizers: A. Denner, S. Dittmaier (Freiburg), T. Plehn
(`https://indico.mitp.uni-mainz.de/event/122/`)
- **Joint Project Group FRIAS – Nagoya IAR, Kick-off meeting *Quantum information processing in non-Markovian complex quantum systems QIPQC***, 14-17 May 2018, FRIAS, Organisers: F. Buscemi, M. Hayashi, H.-P. Breuer (Freiburg), A. Buchleitner (Freiburg). Co-organized by FRIAS.

  Joint Project Group FRIAS – Nagoya IAR, International Workshop *QIPQC19*, 9-12 December 2019, Nagoya, Organisers: F. Buscemi, M. Hayashi, H.-P. Breuer (Freiburg), A. Buchleitner (Freiburg).
Co-organized by FRIAS.
- **3rd and 4th IRTG 2079 (CoCo) Summerschool: Coherent dynamics of cold molecular ensembles. Theoretical and experimental methods**,
Brand, Austria (29.7.-3.8.2018); Kelowna, Canada (29.7.-4.8.2019)
(`https://www.irtg-coco.uni-freiburg.de/events/summer-schools-irtg-coco`)
- **Herbstschule für Hochenergiephysik,** Maria Laach; September 2018, September 2019, July 2021
Organizers: S. Bethke, S. Dittmaier (Freiburg), T. Mannel
(`https://www.maria-laach.tp.nt.uni-siegen.de/archiv.php?ID=31`,
`https://www.maria-laach.tp.nt.uni-siegen.de/archiv.php?ID=32`,
`https://www.maria-laach.tp.nt.uni-siegen.de/archiv.php?ID=33`)
- **RTG 2044 Annual Workshops**, Kinzigtal (25.-26.9.2018); Bonndorf (25.-27.10.2019); Freiburg (online, 7.-9.10.2020); Freiburg (27.-29.9.2021). Organizers: PIs of RTG2044.
- **RTG 2079 (CoCo) Annual Meetings**, Freiburg (23.-27.7.2018); Vancouver (5.-9.8.2019).
Organizers: PIs of RTG2079.
(`https://www.irtg-coco.uni-freiburg.de/events/annual-conventions-1`)
- **Annual Meeting of the Cooperative Research Focus (Forschungsschwerpunkt) ErUM-FSP ATLAS**, Freiburg, 4-7 September 2018, Organisers: B. Heinemann, G. Herten, M. Schumacher, C. Weiser et al..
- **Herbstschule "Quantum-Enhanced Imaging and Spectroscopy",** Physikzentrum Bad Honnef, September 2018; Organizers: F. Kühnemann (Freiburg), M. Selmke
(`https://www.iof.fraunhofer.de/de/veranstaltungen/quilt-autumn-school.html`)
- **Advances in Open Systems and Fundamental Tests of Quantum Mechanics**, 684. WE-Heraeus-Seminar, Bad Honnef, Germany, 2-5 December 2018, Organizers: B. Vacchini, H.-P. Breuer and A. Bassi
(`https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2018/advances-in-open-systems-and-fundamental-tests-of-quantum-mechanics/`)

- **DFT Spring School 2019** in Freiburg, 18-21 March 2019,
Organizers: A. Härtel (Freiburg), D. de las Heras, M. Oettel, R. Roth, M. Schmidt, G. Amati (Freiburg)
(`https://www.soft.uni-freiburg.de/events/dft-spring-school`)

- **Workshop ”Quantum Transport in Nanoscale Molecular Systems”**, Telluride Science Research Center, Telluride, USA, July 2019 and July 2021; Organizers: F. Evers, M. Thoss (Freiburg), L. Venkataraman
(`https://www.telluridescience.org/meetings/workshop-details?wid=922/`)

- **CECAM Flagship Workshop “Learning the Collective Variables of Biomolecular Processes”**,
INRIA Paris, July 2019, Organizers: L. Delemotte, J. Henin, T. Lelievre, G. Stock (Freiburg)
(`https://www.cecam.org/workshop-details/92`)

- **Freiburg-Nagoya-Strasbourg International Summerschool 2019 on ”Sustainability, Ethics and Transformation”**, Freiburg, 16-20 September 2019, Organisers: G. Neuhaus, A. Buchleitner, V. Robert.

- **Workshop ”Sensing with Quantum Light”,** Physikzentrum Bad Honnef, September 2019; Kremmen b. Berlin, September 2020; Organizers: S. Ramelow, F. Kühnemann (Freiburg), M. Selmke
(`https://www.iof.fraunhofer.de/en/events/sensing-with-quantum-light.html`,
`sql20.hu-berlin.de/`)

- **QUTIF Research School on ”Ultrafast Dynamics in Atoms, Molecules, Nanostructures and Solids”**, Freiburg, 7-10 October 2019, Organisers: G. Sansone and F. Stienkemeier
(`https://www.qutif.de/freiburg19.php`)

- MITP Summer School **The Amplitude Games,** Mainz, July 2021 (online)
Organizers: C. Bogner, C.S. Machado, M. Stahlhofen (Freiburg), Z. Ször, S. Weinzierl
(`https://indico.mitp.uni-mainz.de/event/204/`)

- **Les Houches School on Dark Matter**, Les Houches, July/August 2021,
Scientific Advisory Committee: M. Schumann
(`https://indico.cern.ch/event/949654`)

- **754th WE Heraeus Seminar ”Sensing with Quantum Light”,** Physikzentrum Bad Honnef, September 2021; Organizers: S. Ramelow, F. Kühnemann (Freiburg)
(`https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2021/`
`sensing-with-quantum-light/`)

- **Symposium ”Hot topics in cold molecules: From laser cooling to quantum resonances (SYCM)”,** DPG Meeting of the Atomic, Molecular, Plasma Physics and Quantum Optics Section (SAMOP) (virt. conf.), September 2021; Organizers: K. Dulitz (Freiburg), T. Langen, M. Zeppenfeld, S. Truppe, G. Meijer
(`https://www.dpg-verhandlungen.de/year/2021/conference/samop/part/sycm/session/1`)

- **CECAM Flagship Workshop “Learning the Collective Variables of Biomolecular Processes”**,
INRIA Paris, July 2019, Organizers: L. Delemotte, J. Henin, T. Lelievre, G. Stock (Freiburg)
(`https://www.cecam.org/workshop-details/92`)

1.3 Lectures at Physics and Interdisciplinary Schools

- **A short introduction to quantum chaos**, Department of Physics, University of Cyprus, Nikosia, Mar 2018, Lecturer: A. Buchleitner

- **Quantum Theory II**, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, 26 Mar-11 Apr 2019, Lecturer: A. Buchleitner

- **Transatlantic Questions**, Arbeitsgruppe auf der Sommerakademie Neubeuern, Studienstiftung des deutschen Volkes, 29 Jul-10 Aug 2019, Lecturer: A. Buchleitner (together with Michael C. Kimmage).

- **Dark Matter**, University of Erlangen: Astroparticle School 2018, Obertrubach-Bärnfels, Oct 2019, Lecturer: M. Schumann.

- **Spectral properties of complex quantum systems**, ICTP School on “Quantum Information Theory and Thermodynamics at the Nanoscale” (SMR 3426), Al Hoceima, Morocco, 24-28 Feb 2020, Lecturer: A. Buchleitner

- **Renormalization for Pedestrians**, Fall workshop of the RTG 2044 “Mass and Symmetries after the Discovery of the Higgs Particle at the LHC”, Freiburg, Oct 2020 (online), Lecturer: H. Rzehak

- **Optical Traps for Ions Ultracold Atoms and the Onset of Sympathetic Cooling**, Winter School on Physics with Trapped Charged Particles, Les Houches, Feb 2021, Lecturer: T. Schaetz.

1.4 Colloquia and Seminars at the IoP

- **Physics Colloquium**: During the semester, weekly Mondays, University of Freiburg, 2018-2021; Organizers: Professors of the Institute of Physics,
  `http://www.physik.uni-freiburg.de/aktuelles/vortraegekolloquien/physikkolloq`

- **Seminar Series on "Particle Physics"** within the RTG 2044 "Mass and Symmetry after the Discovery of the Higgs Particle at the LHC": During the semester, bi-weekly Wednesdays, 2018-2021; Organizers: S. Dittmaier, H. Fischer, G. Herten, B. Heinemann, H. Ita, K. Jakobs, A. Knue, U. Parzefall, M. Schumacher, M. Schumann, S. Vogl,
  `http://www.grk2044.uni-freiburg.de/seminars`

- **Seminar within the IRTG 2079 "Cold Controlled Ensembles in Physics and Chemistry"**: During the semester, weekly, 2018-2021; Organizers: F. Stienkemeier, T. Momose, et al.
  `https://www.irtg-coco.uni-freiburg.de/events/seminar-series`

- **Seminar "Fundamental Interactions"**: During the semester, weekly Tuesdays, 2018-2021; Organizers: S. Dittmaier, H. Ita, J.J. van der Bij, S. Vogl,
  `http://portal.uni-freiburg.de/ag-dittmaier/seminars/fundi`

- **Seminar of the DFG Research Unit “Reducing complexity of nonequilibrium systems”**: During the semester, weekly Wednesdays, since 2021; Organizers: G. Stock, M. Thoss,
  (`https://www.for5099.uni-freiburg.de/`)

1.5 Lectures and Events for the General Public

- **“Weihnachtsvorlesung” (public Christmas lecture)**, every year, three lectures each, in December 2018, 2019 (canceled in 2020/21 due to the Covid-19 pancemic); Lecturer: H. Fischer; Experiments: H. Wentsch

- **Particle Physics Show of the University of Bonn: "From Rutherford to Higgs – A Journey through particle physics"**, Freiburg, four shows on October 1-2, 2019,
  Organizer: M. Schumacher for the RTG-2044.

- **Optical Trapping of Ion Coulomb Crystals**, Nature - Webinar sponsored by Andor, Online July, 2018, Lecturer: T. Schaetz.

- **"Wäre die Welt nicht einfacher ohne Quanten zu verstehen?"**, Campus Talk - ARD alpha, television broadcasting, March 2020, Lecturer: T. Schaetz.

- **Exploring the Dark Universe**, Havering Astronomical Society (UK), Online, 07.01.2021,
  Lecturer: M. Schumann.

- **Pint of Science: "What is darker than dark?"**, Freiburg, 21.05.2019, Presenter: M. Schumann.

1.6 Lectures, Presentations & Events for High-school Teachers and Students

- **Open day presentations ("Tag der offenen Tür")**, every year, Nov 2018-2021;
  Organizers/Lecturers: J. Timmer, T. Filk, M. Walther
- **Presentations of the Institute of Physics, CERN and jDPG at "Science Days"**, Germany's largest science festival for school classes at the Europa-Park Rust near Freiburg, October 2018, 2019, 2021; Organizers: M. Walther, H. Dummin, A. Woitzik, and researchers from Particle Physics;
  `http://www.science-days.de/science-days/`
- **Freiburg Study Information Day ("Freiburger Hochschultag")**, November 2018-2020;
  About 500 students from 17 high schools in the Freiburg area attend lectures on the study programs offered at the University of Freiburg; Information event of the IoP by M. Walther.
- **Breakfast for school students ("Schülerfrühstück")**; Once a year;
  Hosted by the Young German Physical Society (jDPG); Organizers: T. Filk, A. Woitzik
  About 20 students meet with three professors of the IoP in the institute's Common Room. The participating students can discuss physics and ask questions and may join a lecture and lab tour.
- **Junior Studies for high school students ("Schülerstudium")**, University of Freiburg;
  Every year about one to two extremely talented high schools students participate in the junior study program, where they attend lectures and tutorials parallel to their school classes. Passed exams will be accredited if they later enrol at the university.
- **BOGY - internship for high-school students at the IoP**, every year, students apply for a one-week internship at the institute where they visit and work with various research groups; participating groups and researchers: H. Fischer, T. Schaetz, B. von Issendorff, K. Dulitz, F. Stienkemeier, G. Reiter, K. Jakobs, C. Weiser, U. Parzefall, M. Schumann, A. Buchleitner, A. Woitzik, C. Fuchs, T. Filk
- **"Physik hautnah - die IRTG Schulbotschafterin"**, on request a female MSc student visits schools in the Freiburg area to attract high-school students (in particular female students) for physics studies; initiated by the IRTG 2079 `https://www.irtg-coco.uni-freiburg.de/events/public-outreach/physik-hautnah-die-irtg-schulbotschafterin`
- **Several lectures at high schools in the Freiburg area**, about two to five per year,
  Lecturers: T. Filk, H. Fischer, A. Woitzik
- **Master Classes for High-school students at the Department for Particle Physics of the IoP**, University of Freiburg, 2018-2020; Organizers: A. Knue, V. Lang, L. Wiik-Fuchs
- **One-day visits by high-school classes**, Introductory lecture and lab tours organized by various groups at the IoP
- **Excursions to CERN for school classes from Freiburg**, 1-2 per year, Organizer: H. Fischer
- **Physikalisches Kolloquium PARS Physik**, Stuttgart, physics teacher training event, 29.11.2019,
  Lecturer: M. Schumann.
- **Information event about the teacher's profession**, 14.01.2019,
  `https://www.physik.uni-freiburg.de/aktuelles/studnews/studinfo-LehramtPhysik-jDPG`
- **Lehramtsseminar**; June 2019; Preparatory seminar for teaching students; A weekend conference with lectures and workshops on the teaching profession with about 20 participants from all over Germany; Organizers: C. Fuchs, A. Woitzik, jDPG
- **Workshop at the DPG student conference on quantum information processing**, 2021;
  Lecturer: A. Woitzik

- **Development of web applet "Quantum Penny Flip"**; `https://www.quantumpennyflip.com/`, Web application for teachers and students funded by teaching prize 2021; Developer: A. Woitzik
- **Jugend Forscht**; Members of the institute participate as referees at this yearly competition series in which high-school students present their own research projects; 2018-2021: Referees: H. Fischer, S. Lindemann, J. Dierle; since 2021: C. Bartels, M. Walther.
  Since 2020, the Institute of Physics sponsors two special prices for excellent participants in the competition at state level. The prices are 3-day-long research stays at the institute in Freiburg.

Physikalisches Institut
Hermann-Herder-Str. 3
79104 Freiburg
www.physik.uni-freiburg.de

Albert-Ludwigs-Universität Freiburg