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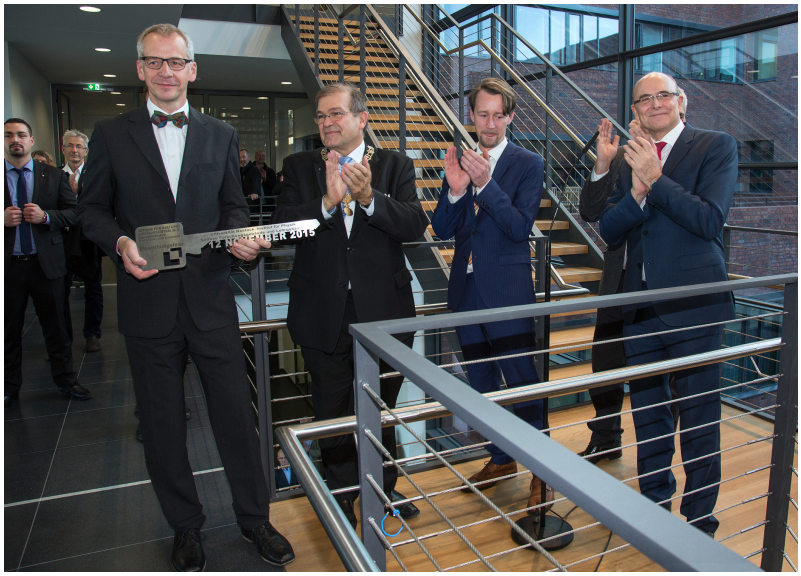
1 Overview of the Institute

by Prof. Dr. Oliver Kühn
Managing Director, Institute of Physics

This research report covers the activities of the Institute of Physics at the University of Rostock during the years 2013 – 2015. The tradition of the institute starts in 1874 when Ludwig Matthiessen was appointed to the first chair of Physics, a position he held for more than 30 years. During these years the institute expanded considerably such that a new physics building was needed. The latter, being situated in the city center, was opened in 1910. It had to last for more than one hundred years, until Physics moved to the Südstadt-campus in August 2015, where it was officially opened on the 12th of November.

The new institute has been planned and realized by Gerber Architects, Dortmund. It consists of a laboratory building and a teaching complex, being connected by a bridge over the Campus Street leading from the university library to the LIKAT on the campus. On 4900 m^2 the research building houses 50 modern laboratories and a fine-mechanical workshop.

The locations of the new buildings of the Institute of Physics and the science building of the Department of Light, Life, and Matter (LL&M) on the Südstadt campus. (source: Prof. K.-H. Meiwes-Broer)



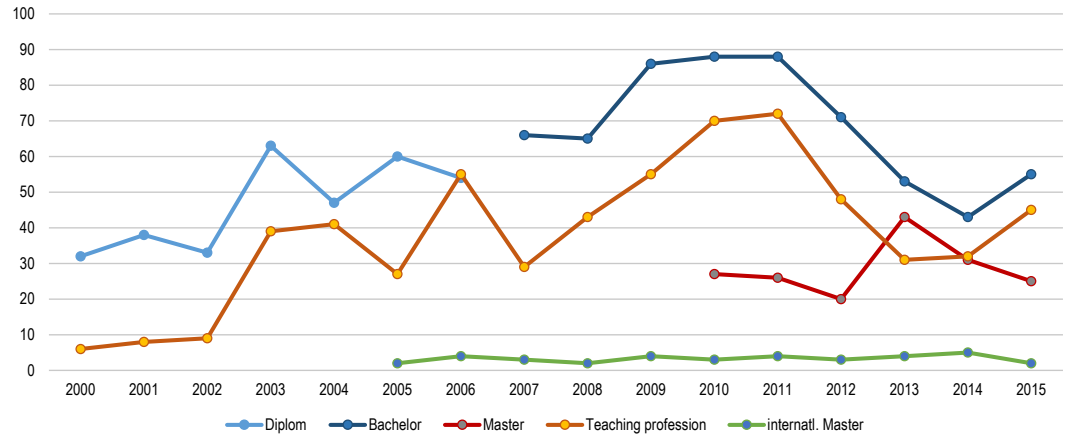
Opening ceremony of the new Physics buildings on November, 12 2015; from left: Prof. Kühn, Prof. Schareck (Rector of Rostock University), M. Brodkorb (Minister of Education), E. Sellering (Prime Minister) (source: ITMZ, Universität Rostock).

At the heart of the teaching building is a large lecture hall for 200 students. Two smaller lecture halls, seminar rooms and the practical training unit complete this 1800 m^2 building. Next to the teaching building there is the research complex of the Department Life, Light and Matter of the Interdisciplinary Faculty. It hosts five competence centers for interdisciplinary projects including the engineering and medical faculties.

The Institute of Physics in 2015 has its focus on experiment and theory in the areas Optics and Photonics, Interfaces and New Materials, and the Physics of Atoms, Molecules, Clusters, and Plasmas. Expertise in Maritime and Atmospheric Physics is contributed by two adjunct external Leibniz institutes, i.e. the Baltic See Research Institute (IOW) and the Institute for Atmospheric Physics (IAP). The research profile is completed by a Leibniz-Professorship for Bioelectrics at the Institute for Plasma Science and Technology in Greifswald.

During the period of this report the faculty members included five C4, three C3, four W3, one W2, and two W1 professors. The scientific staff was completed by 6 lecturers (Privatdozenten). In November 2015 Prof. Heinrich Stolz retired. Newly appointed were Prof. Dr. Jorge L. Chau as Professor for Experimental Atmospheric Physics at the IAP (2013) and Prof. Markus Meier as Professor for Physical Oceanography at the IOW (2015).

The research projects of the Institute of Physics received support by external sources from various organizations such as Deutsche Forschungsgemeinschaft (DFG), Bundesministerium für Bildung und Forschung (BMBF), European Union (EU) as well as by programs within the scope of the Hochschulbauförderungsgesetz (HBFG)



Number of freshmen at the Institute of Physics. Note that the official number of Master students include only those who enroll in the winter term. As of 2012 those students are included who started in the previous summer term.

and by industry. The major part of operational expenses of the institute was financed by these external financial sources. Here, the averaged budget per year was about 4.3 Mio Euro in the accounting period. Among the collaborative grants the Sonderforschungsbereich (SFB) 652 "Strong Correlations and Collective Effects in Radiation Fields" continued to provide the platform for the joined research of ten groups from the institute, one from the Institute of Chemistry and three from the University of Greifswald. Furthermore, two interdisciplinary projects within the BMBF program "Spitzenforschung und Innovation in den neuen Bundesländern", which had started at the end of 2009, were successfully completed in 2014. "Light2Hydrogen" (with participation of the groups of Profs. Meiwes-Broer, Kühn, Lochbrunner) investigated fundamental aspects of photocatalytic water splitting. REMEDIS ("Regional Development of Medical Innovation and Research" with participation of the groups of Profs. Meiwes-Broer and Lochbrunner) was focused on the development of new micro implants.

The Institute of Physics offers several study programs, i.e. Physics Bachelor and Master of Science, teaching profession in Physics and Astronomy for gymnasium and regional schools, and an International Master program. In 2015 the latter has been restructured and focussed to the Physics of Life, Light and Matter. Our institute continues to be an attractive place for studying Physics in Germany. This fact manifests itself in the excellent rankings during the last years. For example, the recent CHE ranking of the Zentrum für Hochschulentwicklung places Physics in Rostock into the top-level group in the categories "getting started", "supervision", "library", and "IT infrastructure". Together with the opening of the new Physics building, this might be the reason for the positive trend concerning the number of freshmen (see above diagram).

In the reporting period 44 students received their doctor's degree. Opportunities

for PhD students to broaden their education beyond the specific topic are offered by the integrated graduate school of the SFB 652 in the area of light-matter interaction.

The Institute of Physics places emphasis on various outreach activities to communicate science to the society and to raise the interest in studying Physics. For instance, Physics Navigators provide answers about study related questions to interested pupils. Further activities include the yearly "Physics Day", the "Long Night of Sciences", "Science and Sail", the "Girls Day" and "Physch", Physics and school.

The auditorium on occasion of the opening lecture given by Prof. Ludger Wöste, Freie Universität Berlin. (source: Prof. K.-H. Meiwes-Broer)

Finally, this report was written not only for statistical purposes, but to trigger interest in study and research at the Institute of Physics of the University of Rostock.

2 Research Activities

2.1 Optics and Photonics

2.1.1 Nonlinear Optics

Head: Prof. Dr. Fedor Mitschke

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	Hartmuth Reichwagen	Theresa Kopplow
	Manja-Carina Schulz	
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MSc Graduates:	Sonia Gholami	Sven Kraft
	Maria Lubs	Bennet Krebs
	Jan Froh	
BSc Graduates:	Maria Pierce	Nils Thomas
	Philip Pisowocki	Bennet Krebs

General Outline of the Field of Research

We study nonlinear dynamical processes in the realm of optics. *Nonlinear* means that optical properties of a material are modified by the irradiated light so that a light beam itself modifies the conditions of its propagation. *Dynamical* refers to short time scales; we routinely deal with femtosecond processes. Lasers are a central concept here in a twofold way: They provide the light required to excite nonlinear processes, but their inner workings involve nonlinear processes too.

Our focus in recent years has been on the nonlinear interactions which occur when a short pulse of light travels down an optical fiber. Given the right conditions, very special pulses called *solitons* can arise. After their first experimental demonstration in 1980 solitons have found their way into commercial applications in optical telecommunications ca. 2001. As the demands on the data-carrying capacity of fiber-optic cables keep rising rapidly, the fundamental limitations for time-honored binary transmission have now been reached, and it has become mandatory to use coding 'beyond binary'.

Soliton Molecules

Soliton-soliton interaction, first experimentally described by the group head in 1986, remains an issue of some debate when higher-order corrections to the propagation equation must be included. A few years ago we discovered that there exists a stable solution which is a compound state of two bright solitons. This compound, called the *soliton molecule*, suggests a way to create an optical coding of data that goes beyond the binary format. Such procedure would increase the data-carrying capacity of fibers so that the impending capacity bottleneck is mitigated.

At the very end of the previous report period this group had demonstrated by way of proof-of-principle experiment that solitons can be combined to soliton molecules, and these in turn can provide a quaternary coding of data. Four symbols (no pulse, single soliton, two-pulse molecule, three-pulse molecule) have been demonstrated. We followed up on that first report by a detailed investigation [1]. The setup is shown schematically in Fig. 2.1.

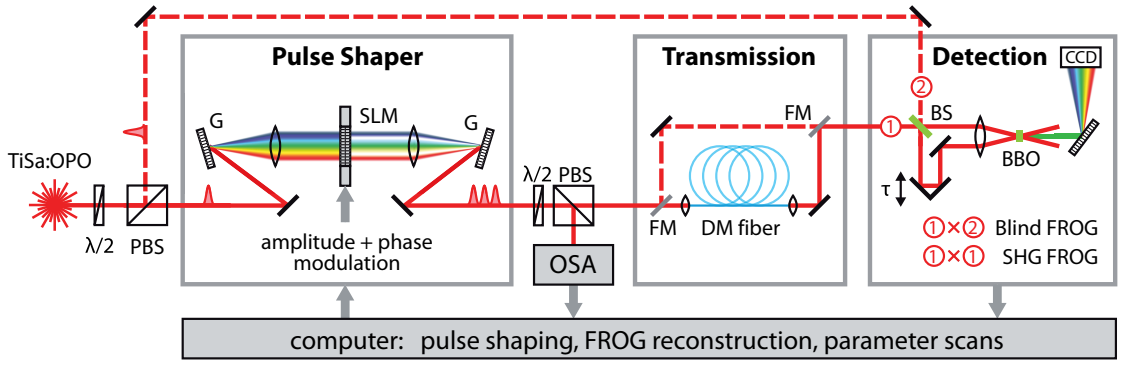

Fig. 2.1: Experimental setup for the demonstration of soliton molecules. The desired initial pulse shape is carved from the pulses delivered by the laser (an TiSa:OPO system). The pulse shaper contains a liquid crystal-based spatial light modulator (SLM), lenses and gratings (G). OSA: optical spectrum analyzer, $\lambda/2$: half wave retarder, PBS: polarizing beam splitter. Flip mirrors (FM) steer either the fiber input or the fiber output signal towards data acquisition. BS: beam splitter, BBO: frequency-doubling crystal, CCD: camera. Both autocorrelaton and cross correlation measurements are provided; the latter require a sample of the laser pulse as a reference. Both pulse shaping and data acquisition are computer-controlled for automated parameter scans.

Solitons in optical fibers are described by the Nonlinear Schrödinger Equation. In idealized circumstances, analytic solutions exist. However, for realistic fibers of the 'dispersion-managed' type (DM fiber) there are no closed solutions of the wave equation. There is also no analytic answer to the question how to find the optimum pulse shape for the soliton molecules. We employed a self-searching strategy, which finds the best form, taking all deviations from ideality into account. At the core of this method there is an optimization procedure for which a genetic algorithm was determined to be slightly better suited than a Nelder-Mead algorithm [2, 3].

The most striking aspect of the inner working of the soliton molecule is the binding force which results from Kerr interaction and gives rise to a stable equilibrium at a certain separation of the participating individual pulses. We had demonstrated this earlier mathematically by perturbation analysis. Meanwhile we could vastly improve the accuracy of that approach by taking the true, optimized pulse shape into account. This led to the discovery that there are actually more equilibria that the pulses in a soliton molecule may attain; with growing separation they alternate in their stability. It was reassuring that this conclusion could be corroborated in the experiment [4].

Akhmediev Breather

A continuous light wave in an optical fiber may become unstable, depending on the sign of the dispersion parameter. This instability leads to the continuous wave getting modulated at a certain power-dependent frequency, which typically takes values of hundreds of Gigahertz to several Terahertz. The process is well known as *modulational instability*, or MI. However, a full mathematical framework to describe it lay dormant after its first formulation in the 1980's until it was revived only a couple of years ago.

The mathematical model for MI is the *Akhmediev Breather*; we had contributed to its understanding in the previous report period. The item left missing then was the connection between the modulated wave which can look like a pulse train, and a sequence of soliton pulses. Various conjectures had been put forward over the last decades. We could finally settle this issue: The MI solution of the Nonlinear Schrödinger equation does contain solitons, but these can in no way be identified with the pulses in the Akhmediev Breather. After all, a soliton is one type of solution, and the Akhmediev Breather is a different type of solution of the same equation, and neither type can be written as a linear combination of solutions of the other type. However, one can decompose the Akhmediev Breather by applying perturbations to it; this lets true solitons emerge [5].

Rogue Waves

In the context of solitons in a highly nonlinear optical fiber, an intense debate has started a few years ago concerning optical *rogue waves*. Reports of giant ocean waves which may damage or sink even large ships existed for centuries; in recent years it became evident that there is actually truth in these reports. Under certain circumstances, pulses in an optical fiber can also attain an unusually high peak power; apparently there is some analogy. We found that in the presence of linear waves (called 'radiation' in the soliton community), interaction between solitons and radiation can have the surprising property that the weak radiation creates a barrier which the powerful pulses cannot cross [6].

Ultrashort Pulse Measurement Technique Refined

Earlier cooperation between the group of Prof. Stolz, the Institute of Mathematics (Prof. Tasche) and this group resulted in a novel technique to assess amplitude and phase of femtosecond light pulses, which was introduced ca. 2007. The technique had already been shown to be superior to competing techniques, among which *frequency resolved optical gating*, or FROG, is the best known [7]. There is an issue about the reliability of a FROG reconstruction when the pulse shape contains zeroes in either temporal or spectral domain. We expanded our previous work to provide better criteria for the reliability [8].

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2.1.2 Experimental Quantum Optics

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	Mirjam Samelin	Oskar Schlettwein	Hannes Sobottka
	Wolfram Stamm		
BSc Graduates:	Kai Barnscheidt	Karsten Bölts	Tom Ettrich
	Christian Reiher	Dieter Schick	Jakob Studer

General Outline of the Field of Research

Optical systems are particularly suitable for the fundamental investigation of quantum phenomena as well as their applications. Light with distinct properties can be generated, confined, guided, transmitted and detected easily in many cases. Also, the interaction of light and matter can be well controlled in certain scenarios. Today's communication largely relies on optical channels in the classical regime. Future communication networks will involve some quantum physics for adding communication security or boosting the channel capacity. Hence, studying the quantum properties of optical systems and also the distinction of quantum and classical effects in optics is interesting from a fundamental point of view as well as with respect to technology.

The Experimental Quantum Optics group was started in April 2012 at the University of Rostock. Hence, this report is not a collection of results but more about ongoing work.

Squeezed Light Sources

We set up two different kinds of squeezed light sources. On the one hand we implemented two continuous wave sources based on the optical parametric amplification. We used bulk lithium niobate as well as periodically poled potassium titanyl phosphate as nonlinear materials with a laser wavelength of 1064 nm. These sources are well established in the quantum optical community and serve as working horses for the preparation of nonclassical states of light in a single quantum mode and quantum optical entanglement of two or more

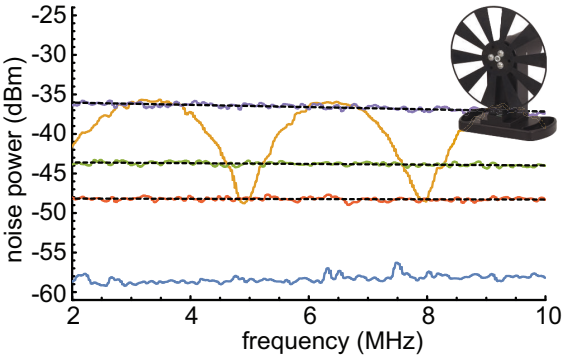

Fig. 2.2: Measurement of quantum fluctuations below the shot noise (green line) prepared by optical parametric (de-)amplification.

modes. In order to incorporate the squeezed light source on the individual photon level, choppers were used to suppress all necessary control beams intermittently. Even with the chopped control we could generate a descent amount of squeezing, see Fig. 2.2.

On the other hand, we investigated the quantum properties of mode-locked femtosecond pulses in the telecommunication wavelength regime upon propagation through an optical fibre inflicting nonlinear effects such as the Kerr effect onto the propagating light fields. We were able to implement an interferometric scheme for the preparation and detection of squeezed light based on the Kerr effect, see Fig. 2.3, which also is a well-established method in the community. Based on this preliminary work we set out to implement a quantum tomography scheme and investigate the multi-mode quantum properties of *optical soliton molecules*.

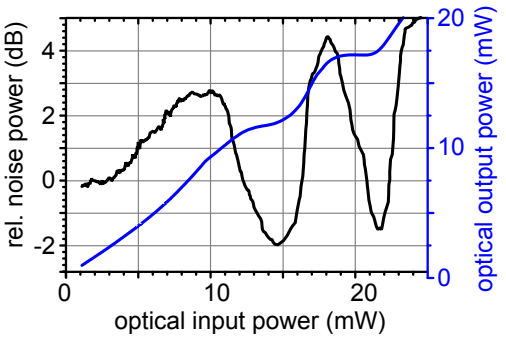

Fig. 2.3: Sub-shot noise fluctuations caused by the Kerr effect in an optical fibre. The noise power is normalised to the shot noise level.

We are currently working on the combination of several squeezed light modes in order to form entangled states of light, which we want to use for an experimental discrimination of effects like entanglement itself, quantum discord and nonclassical correlations.

Click Statistics of Multi-Pixel Photon Counters

Counting photons is one of the major challenges in the field of optical quantum information science. Advancing demands on the performance of true photon number-resolving detectors go beyond the abilities of state-of-the-art devices. In many cases a multitude of single photon detectors is used in order to achieve a photon number resolution. However, it is generally impossible to infer the true photon statistics from the click statistics. If only statistical information about the quantum state is required for a certain task, the Theoretical Quantum Optics group (Sec. 2.1.4) has developed a way to extract crucial properties, such as the nonclassicality, by considering the click statistics rather than the photon number statistics.

We extended the idea by studying commercially available detectors in great detail. We could obtain the statistics for up to 96 clicks, see Fig. 2.4, with carefully designed electronic amplifiers and appropriate filtering. Based on that we can understand how the click statistic is influenced by unwanted but inevitable effects like crosstalk, temporarily blinded pixels, after pulses to name just a few. We demonstrated, with experimental evidence, that neither is the statistical information acquired with these devices insufficient for discriminating quantum states, nor is the nonlinear detection

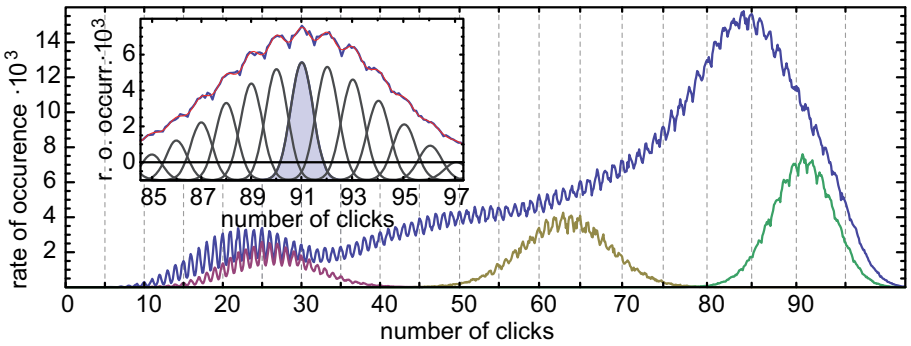

Fig. 2.4: With a carefully designed electronic front end and appropriate filtering, we were able to discriminate up to 96 simultaneous clicks in a 10×10 detector array.

mode a disadvantage compared to true photon counters. We developed a model for detector characteristics including dark counts, blinded pixels and cross talk, which enables us to extract vital information about the incident light with intensities two orders of magnitude higher than commonly applied. Thus, these detector arrays can even bridge the gap between the single photon and linear detection. We are currently developing a nonclassical light source for visible light which is suitable to be detected with these detectors.

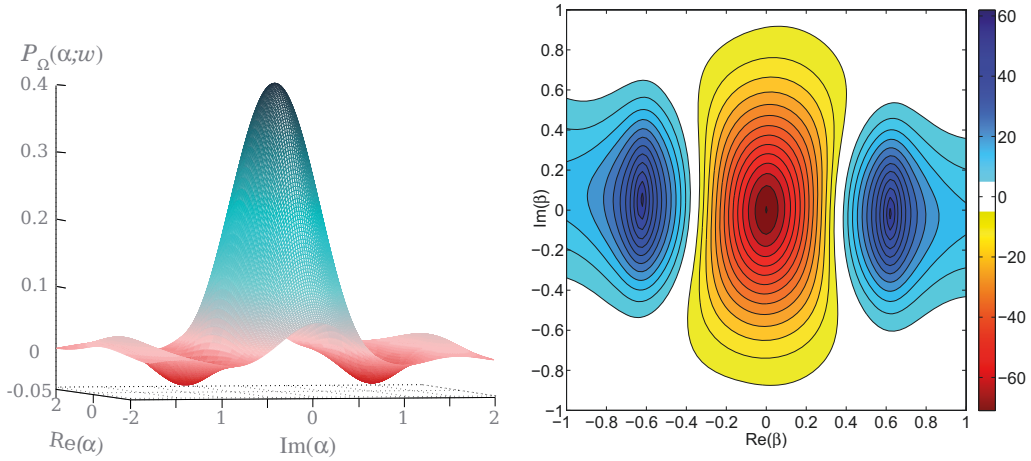

Fig. 2.5: Based on the experimental data which we produced in the lab, we could apply two distinct methods to verify the nonclassical character of our squeezed light sources. Left: Nonclassicality measured in the negative parts of the regularised P-function. Right: Statistical significance (negative values indicate the presence of nonclassicality) gained from the generalized Bochner matrix.

Detection of Nonclassicality

We used our squeezed light sources, which we characterised carefully, for the preparation of the input states of two new methods for the observation of nonclassicality devised by the Theoretical Quantum Optics group (Sec. 2.1.4).

The detection of nonclassicality is essentially based on quantum tomographic data obtained from a squeezed state of light in the laboratory. In contrast to previous experiments, we implemented the quantum tomography such, that the detection phase was varied continuously rather than in discrete steps. For a valid tomography it is crucial to know the detection phase for each sample precisely. For this purpose we tracked the mean optical power in one of the detector ports, which allowed us to determine the nonlinear variation of the detection phase over time. The results of two different nonclassicality detection methods are shown in Fig. 2.5.

The next step will be not only to detected but also to quantify the nonclassicality of a given experimental state. There is a theoretical recipe to do the quantification by counting the coherent elements needed in superposition to form a given state. However, even the weakest squeezed state exhibits an infinite amount of nonclassicality with this recipe. We are going to modify the recipe from the experimental point of view by counting only those elements forming the superposition, which can be detected with statistical significance based on an experimental set of data.

A proper normalisation by either the measurement time and bandwidth or the total amount of data will allow a comparison between the amount of nonclassicality produced in different experiments.

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2.1.3 Quantum Optics of Macroscopic Systems

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	Dipl.-Phys. Robin Schmidt	MSc Johannes Block
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	Thomas Stielow	

General Synopsis

The research in the group led by Prof. Stefan Scheel is focussed on the interaction of quantized light with macroscopic objects, with particular emphasis on Casimir-type dispersion forces. In this context, we have been investigating the role of Casimir–Polder interactions between atoms and molecules, and material gratings in interferometry [1–3], as well as with carbon-based materials such as graphene and carbon nanotubes [4–6]. Complex dielectric structures are included by a Born series expansion of the dyadic Green function which is shown to converge rapidly [7].

We have extended the concept of Casimir–Polder interactions beyond second-order perturbation theory to include resonant effects and the influence of atomic motion [8–11]. We have shown that, in nanostructured environments such as in close proximity to nanofibers, a chiral lateral Casimir–Polder force can be created that results from directional spontaneous emission [12].

In the dilute limit, the Casimir–Polder interaction reduces to the van der Waals interaction between microscopic particles. Their interaction potential can in turn be influenced and hence partially controlled by material boundaries [13, 14]. In excited systems, the van der Waals interaction leads to the phenomenon of Rydberg blockade which we have recently observed for the first time in excitons in the semiconductor cuprous oxide [15].

Rydberg excitons in Cu_2O

Excitons in semiconductors are quasiparticle bound states that are formed between an electron and a hole. Recently, together with colleagues from the TU Dortmund, we have been able to study highly excited Rydberg excitons in the semiconductor cuprous oxide (Cu_2O). Single-photon absorption spectroscopy reveals a series of resonances that could be identified as excitons with P-type envelope wavefunctions with principal quantum numbers up to $n = 25$ (Fig. 2.6a). Such a wavefunction extends over $2\,\mu$m and covers approximately 10 billion crystal unit cells (Fig. 2.6d). These states are nonetheless very stable, their lifetimes scale with n^{-3} [15].

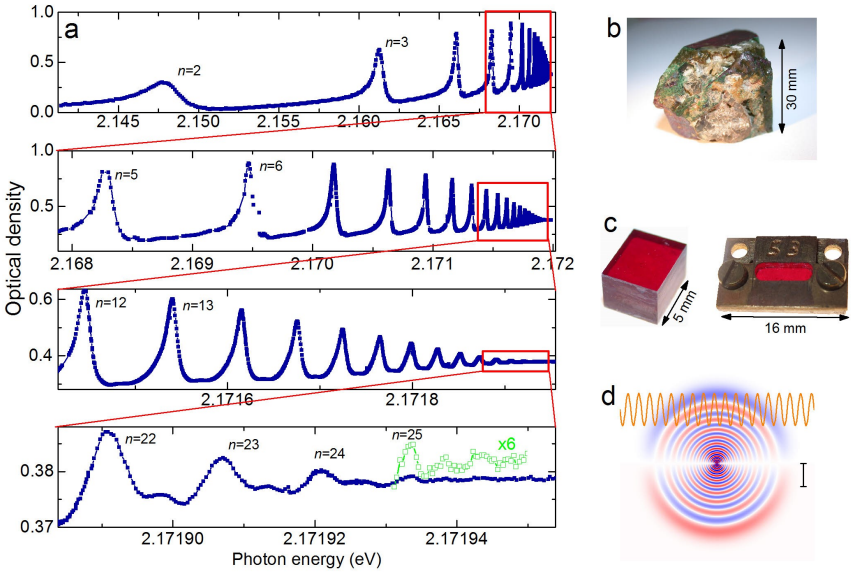

Fig. 2.6: Absorption spectra of excitons with principal quantum numbers up to $n = 25$ in cuprous oxide. Taken from Ref. [15].

Due to their large spatial extent (their size scaling as n^2), Rydberg excitons are extremely sensitive to external fields. Their polarisability scales as n^7, which results in giant van der Waals interactions between them ($C_6 \propto n^{11}$). The result is the phenomenon of Rydberg blockade that is well-known from atomic physics, but hitherto not yet being observed in a solid-state system. The effect of this blockade is the dramatic loss of oscillator strength for the excitation of excitons with larger n, but without broadening the resonance lines. We have already gained a good understanding of the mechanism involved in the blockade effect based on modelling the exciton wavefunctions by hydrogen-like wavefunctions. Further investigations in the detailed level structure and the interactions between the excitons point towards the development of a quantum coherent system in a solid-state bulk material.

Controlled dispersion interactions in nanostructured environments

Dispersion interactions result from the (ground-state or thermal) fluctuations of the electromagnetic field and lead to forces between neutral, but polarisable objects such as atoms, molecules or macroscopic bodies with a dielectric permittivity. These interactions are short ranged and rather weak, but at nanometer distances they dominate all other forces except for the electrostatic force. As dispersion interactions are mediated by (virtual) photons, any change in the dielectric environment in which they propagate will alter these Casimir-type forces. Nanostructured environments are particularly suited for this task.

An example is shown in Fig. 2.7a, where a cesium atom is assumed to be placed

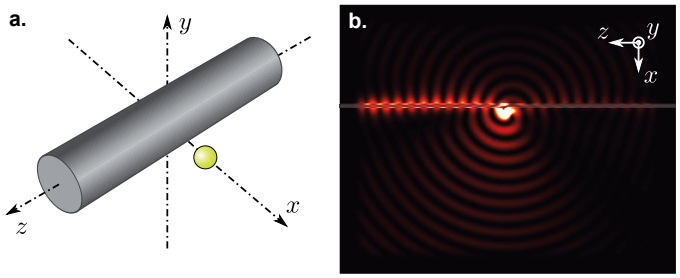

Fig. 2.7: A cesium atom is located close to a nanofiber (a). If the atom is initially prepared in the state $|6^2P_{3/2,F=5,m_F=5}\rangle$, it can only decay to the state $|5^2S_{1/2,F=4,m_F=4}\rangle$ by emitting a σ^+-polarized photon. The spontaneous emission is strongly asymmetric (b), leading to a unidirectional lateral force on the atom along the fiber. Taken from Ref. [12].

near a nanofiber that carries an evanescent optical mode. Upon excitation of the atom to the state $|6^2P_{3/2,F=5,m_F=5}\rangle$, it can only decay to the state $|5^2S_{1/2,F=4,m_F=4}\rangle$ by emitting a σ^+-polarized photon. The spontaneous emission pattern is strongly asymmetric (Fig. 2.7b) and leads to a chiral interaction that results in a unidirectional lateral Casimir–Polder force on the atom along the fiber [12]. This lateral force is unique as it does not require corrugated surfaces, but acts along a translationally invariant structure by virtue of the highly asymmetric emission pattern.

Dispersion forces between atoms or molecules are also mediated by electromagnetic fields that result from quantum-mechanical ground-state fluctuations. These van der Waals interactions can therefore in principle be controlled by altering the dielectric environment in which the electromagnetic fields propagate [13]. An experimentally feasible geometry is a hollow fiber in which two atoms are placed on the fiber axis (Fig. 2.8). The total dispersion potential between the atoms can be decomposed into contributions from free-space propagation of the virtual photons ($U^{(0)}$) and contributions arising from one ($U^{(\mathrm{cross})}$) or two ($U^{(\mathrm{sc})}$) scattering events at the vacuum-fiber interface. Figure 2.8 shows the waveguide-mediated van der Waals coupling between two emitters in a subwavelength hollow metallic cylinder (black)

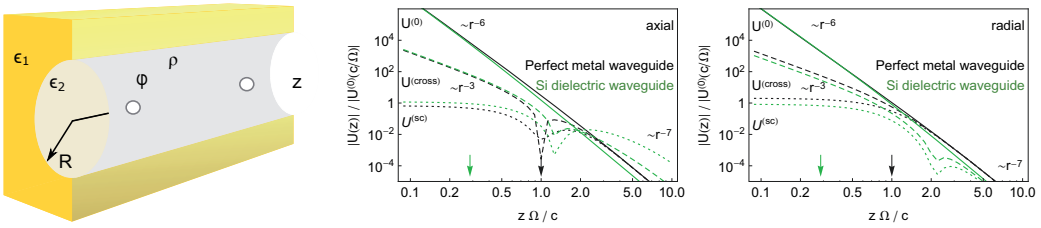

Fig. 2.8: Hollow-core fiber containing two polarisable particles on its cylinder axis, and contributions from free-space propagation and scattering contributions to the axial and radial components of the van der Waals potential. Taken from Ref. [14].

and a dielectric cylinder waveguide (green) for axial and radial dipole orientations, respectively. Guided modes that can be excited by resonant van der Waals interaction can potentially be used to tune the interaction strength between Rydberg atoms inside waveguides.

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2.1.4 Theoretical Quantum Optics

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General Outline of the Field of Research

The focus of our research is on the effects of quantized radiation fields, their propagation in media and interaction with matter. We derive observable nonclassicality conditions to characterize multimode quantum-correlated systems. For the detection of quantum effects, measurement schemes have been proposed and rigorously analyzed. Beyond the theoretical identification of quantum effects, we collaborate with experimental groups to implement our methods and we quantify the strength of the quantumness with novel techniques.

Entanglement Detection

In the growing field of quantum information and communication technologies, entanglement is a key resource. The detection of this nonlocal and nonclassical correlation between two or more quantum systems is, thus, of great interest. We focus on finding entanglement criteria for general systems.

In Ref. [1], we have introduced a new method to construct optimal witnesses. This technique allows one to confirm entanglement in any quantum system, if present. For certain quantum systems, such as the renowned Gaussian states, analytical solutions have been found. We have applied this theory to data from the experimental group of C. Fabre and N. Treps in Paris [2]. The results, depicted in Fig. 2.9, verify the entanglement signature in every combination of subsystems.

Nonclassicality Quasiprobabilities

Nonclassicality quasiprobabilities provide a universal method to visualize nonclassicality through negativities of non-singular phase-space functions. The underlying idea is the regularization of the Glauber-Sudarshan P function by means of so-called nonclassicality filters. We have identified optimal filters, which minimize the number of required data points to certify nonclassical effects with high statistical

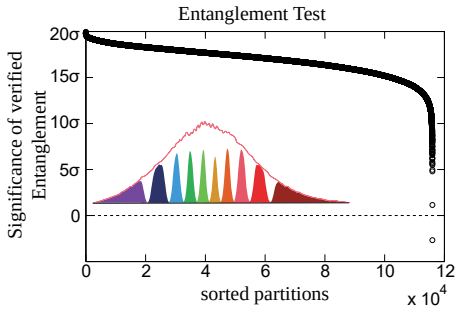

Fig. 2.9: Statistical significance of an entanglement test applied to a 10-mode Gaussian state. The inset shows the spectral structure of Gaussian states for ten bands of equal energy. These bands can be combined in 115 975 possible ways and for each of these possibilities an entanglement test has been performed. The circles represent the values certifying entanglement in terms of standard deviations σ for a certain partition. The circle below the dashed line indicates no certification of entanglement for the trivial decomposition of the system.

significance [3]. This includes the construction of an analytic filter which preserves the full information on the quantum state.

Using this powerful method, the characterization of multimode correlations can be done beyond other notions of quantum correlations. Furthermore, improvements on traditional measurement procedures have been advised [4]. In particular, we have proposed a continuous-in-phase sampling technique, in contrast to standard discrete phase-locked measurements. Our approach allows an unconditional verification of nonclassicality without interpolation errors.

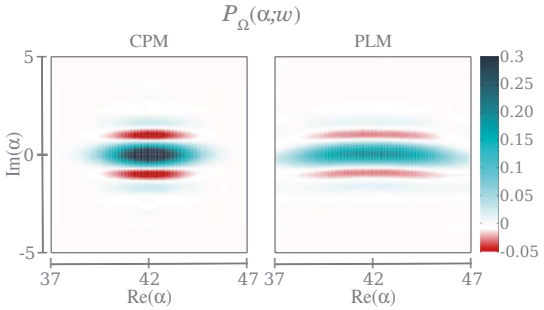

Fig. 2.10: Regularized P_Ω functions. The squeezed state is reconstructed via continuous phase measurements (CPM) and phase-locked measurements (PLM).

The nonclassicality quasiprobability for both measurement strategies is given in Fig. 2.10. On the left side one sees the correctly reconstructed state with our proposal, whereas the right-side plot in Fig. 2.10 is distorted due to the phase-locking technique. Experimental data obtained from the group of B. Hage (Sec. 2.1.2) have been analyzed and the regularized P function has been directly reconstructed. The sampling of nonclassicality quasiprobabilities is a powerful and universal method to

visualize quantum effects within arbitrary quantum states of light.

Click Statistics

In order to verify quantum effects, it is required to formulate a measurement theory and the corresponding quantumness (nonclassicality) tests. For the so-called click-counting detectors, we have derived such methods in close collaboration with G. S. Agarwal, Oklahoma State University. The theoretical foundation for the identification of all orders of nonclassical correlations with these detection devices has been formulated in our work [5]. Based on this approach, we also have studied phase-sensitive measurements and reconstructions of phase-space distributions in other recent contributions.

In collaboration with the experimental group of C. Silberhorn, Universität Paderborn, we have applied our method to uncover quantum correlations [6]. We have demonstrated nonclassical correlations between the two modes of the generated light field, see Fig. 2.11. With our technique, this has been achieved despite high losses and high pump-powers. This renders it possible to access the quantum features of radiations fields for many applications in noisy environments.

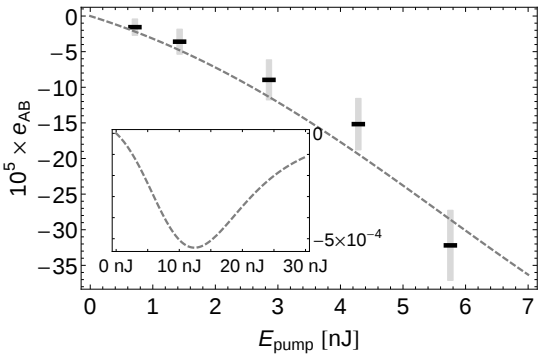

Fig. 2.11: The theoretical model (dashed lines) and the experimental results (black bars; error bars: gray areas) for the verification of nonclassical correlations, $e_{\mathrm{AB}} < 0$, is shown as a function of the pump energy E_{pump}, which drives a nonlinear interaction to generate two correlated beams of light.

Quantification of Quantumness

A question of fundamental importance is: How strong are the quantum properties of a given quantum system? The answer may be of relevance for applications of quantum effects in novel quantum technologies, for example, in the context of the enhancement of security in quantum communication. However, in our previous work we have shown that a quantification has very different aspects. We distinguish the quantification of the quantum properties of a given state from the quantification

of its usefulness for a particular application. The former is based on the convex structure of the quantum state, whereas the latter is merely an operational quantification for certain protocols. Our work concentrates on the universal quantification of quantumness.

In [7] we have unified the quantification of the nonclassicality of a single radiation mode with the quantification of entanglement. A nonclassical light field is combined with vacuum channels by a beam splitter, which yields entangled output beams in general. The quantum superposition principle, which is fundamental for the structure of quantum theory, is the key for our unified quantification of nonclassicality and entanglement. We have proven that the number of superpositions of coherent states needed for the representation of the single-mode input state is exactly the same as the number of superposition of separable states in the output fields. This unifies the quantification of nonclassicality and multimode entanglement.

Multimode quantum states have a complex structure, see, for example, the experimental results for frequency-comb entangled states in section *Entanglement Detection* [2]. It is of interest to combine the quantification of multipartite entanglement with the problem of uncovering the entanglement structure. The first attempt to combine these two aspects has been developed in [8]. For this purpose, we have derived a modified version of the separability eigenvalue problem to unify the identification of the structuring with the quantification of the entanglement. This paves the way to a more detailed understanding of complex entangled quantum states.

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2.2 Atoms, Molecules, Clusters and Plasmas

2.2.1 Quantum Theory and Many-Particle Systems

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General Outline of the Field of Research

The focus of the group is on the theory of nonperturbative laser-matter interaction, in particular strong-field ionization processes and time-dependent many-body quantum physics. Both topics are not only interesting because of possible applications such as particle acceleration, short-wavelength sources, or dynamical self-imaging, but also from a methodological point-of-view because all practicable "traditional" textbook approaches fail.

Strong-field ionization and laser-driven correlated dynamics

The complex structures in strong-field photoelectron spectra contain information about the laser pulse and the target. Hence, a deep understanding of the processes involved potentially allows the imaging of structure and internal dynamics as well as the manipulation of the emission of electrons and light. In close collaboration with the experimental "Clusters and Nanostructures" group, see Sec. 2.2.5, we developed a sensitive tool for the investigation of strong-field ionization dynamics based on two-color (ω-2ω) laser pulses, the so-called "phase-of-the-phase

spectroscopy" [1]. For the analysis of such strong-field laser experiments, *ab initio* solutions of the time-dependent Schrödinger equation (TDSE) are valuable but yield little understanding. For this reason we continued to develop semi-analytical methods based on the strong-field approximation and the so-called quantum orbits [2].

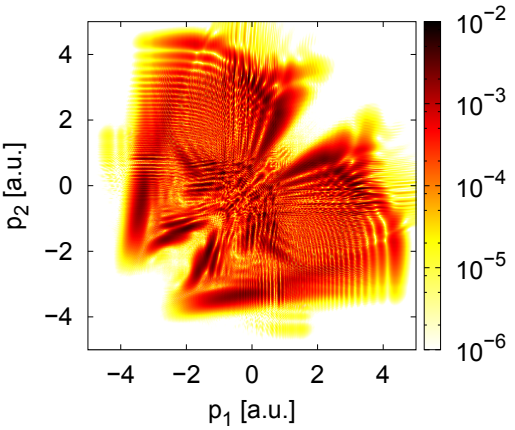

Fig. 2.12: Two-electron photoelectron momentum spectrum for helium.

Systems with more than a single active electron need to be treated by a nonperturbative many-body quantum method. Simple approaches such as time-dependent density functional theory (TDDFT) do not capture resonant or correlated processes of interest (e.g., Rabi floppings, nonsequential ionization, see Fig. 2.12, autoionization, Fano lineshapes etc.). Therefore we have developed a time-dependent theory based on natural orbitals (NOs) as basic variables, i.e., eigenfunctions of the one-body reduced density matrix. The challenge then is to express the time-dependent two-body reduced density matrix in terms of these NOs. An analytical solution exists for two-body systems so that we benchmarked our theory using a model helium atom for which the TDSE can be solved numerically exactly [3].

Laser-plasma and particle acceleration

The ionization dynamics in helium droplets during the interaction with intense laser radiation was studied using three-dimensional, relativistic particle-in-cell (PIC) simulations [4]. The field penetration causes ionization inside the droplet, mainly confined to the polarization plane (see Fig. 2.13). In Ref. [5] it was shown that the interaction of a laser-boosted solid-density parabolic relativistic "mirror" with a super-intense, counter-propagating laser pulse generates carrier-envelope-phase-tunable few-cycle pulses of multijoule energy and peak intensities exceeding $10^{23}\,\mathrm{W/cm^2}$. A new research direction in the group is aiming at the analytical modeling and kinetic simulation of ion-acoustic shocks, which play a role in the

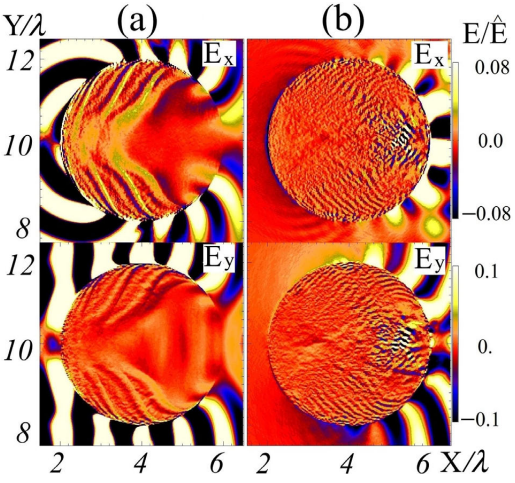

Fig. 2.13: Electric fields in the polarization plane inside and in the vicinity of the He-droplet during (a) and after (b) the interaction with the laser pulse.

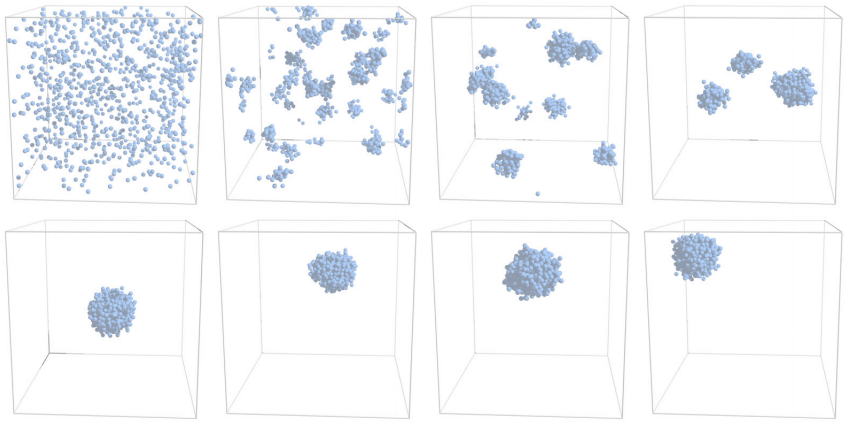

Fig. 2.14: Markov chain sampling of the coordinated wavefunction proposed in Ref. [7]. With 1000 helium atoms in a very large simulation cell, the system spontaneously forms an inhomogeneous phase.

generation of ultra-energetic cosmic rays. The reflection efficiency, the velocity distribution of reflected particles, and the shock's electrostatic structure are studied [6].

Monte-Carlo simulations

The ground-state and low-temperature properties of liquid and solid helium-4 were investigated by first-principles and Monte Carlo methods. An improved wavefunction for the ground state of solid helium enabled the calculation of the complete set of elastic constants of hexagonal close packed solid helium, relevant to experiments. A new exchange-symmetrical wavefunction for the solid state describes a phase transition between the liquid and solid phases of helium at zero temperature. A new ansatz for liquid helium allows one to study inhomogeneous states such as surfaces or helium droplets [7] (see Fig. 2.14). As quantum Monte Carlo methods are computationally intensive, a significant effort went into developing efficient, parallel methods, also for GPUs [8].

Dielectric response and optical properties

The understanding of optical properties in highly excited matter is central for diagnostic purposes. Starting from a consistently applied quantum-statistical many-particle approach within linear response theory, the dynamical collision frequency is calculated to include scattering processes in the dielectric function. We resolved the controversy with respect to the role of electron-electron collisions in calculating the dynamical conductivity in the warm dense matter region [9]. For highly resolved measurements of the Thomson spectrum in an ultrafast heated aluminum solid [10], the plasmon damping is treated by electron-ion collision models beyond the Born approximation to determine the electrical conductivity of warm dense aluminum. For ionized metal clusters, investigated at high temperatures using MD simulations,

a relation between the cluster charge and cluster size as well as temperature was derived. Further points of investigation have been spectral line profiles, in particular of inner shell transitions in mid-Z elements and the equation of state of partially ionized plasmas treated with a consistent cluster virial expansion [11]. Starting from a quantum master equation, line profiles and transition rates for Rydberg atoms are calculated introducing robust wave-packet states.

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2.2.2 Theoretical Cluster Physics and Nanophotonics

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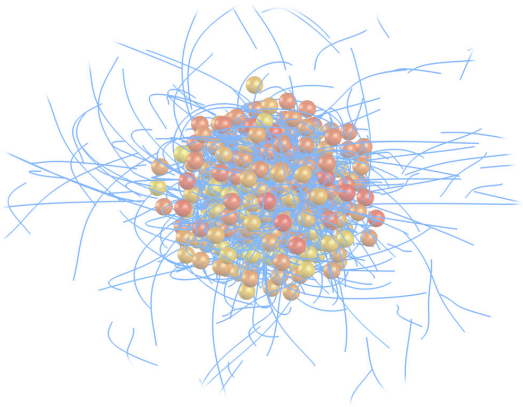
General Outline of the Field of Research

Since the invention of the laser in 1960, a particularly vibrant research field has developed around ultrashort intense laser pulses. Today, laser light flashes can be produced that last only a few tens of attoseconds, marking the shortest manmade events. Pulses can further be strong enough to drive highly non-linear dynamics. Most importantly, well-controlled laser fields now enable us to resolve and steer ultrafast light-matter interactions on their natural spatial and temporal scales.

Understanding the electron dynamics in strongly excited quantum systems and plasmas at solid density is important for virtually all applications of intense laser-matter science. Strong fields make it possible to excite or remove electrons from matter before ionic (or sometimes even electronic) relaxation processes begin. However, a solid density material under intense laser fields will be strongly excited and/or ionized, leading to a highly nonlinear response and transient physical and optical properties, the formation of matter states far from equilibrium, and complex ultrafast relaxation processes. The resulting quest for a tractable microscopic theoretical description of the relevant ultrafast laser-matter dynamics is a major challenge in strong-field science and defines the mission of our research.



Atomic clusters and nanoparticles are ideal nanolaboratories to study ultrafast strong-field induced many-particle dynamics in complex systems. First, clusters and nanoparticles are easier accessible in experiment and theory than, e.g., solids. Further, they are easily scalable regarding size and material, offering systematic routes to test the competition of surface and volume effects, the different responses of metallic and insulating material, the impact of electromagnetic field propagation and near fields, and the characteristic evolution of the matter response from the molecular phase all the way up to the bulk.

Attosecond electron dynamics in strong near-fields

The collective material polarization in laser driven nanostructures generates near-fields that are localized on the subwavelength scale, i.e., beyond the diffraction limit, and can be enhanced substantially with respect to the incident field. These features are ideal to extent the possibilities to drive, probe, and control coherent strong-field dynamics via waveform-controlled laser pulses from atoms and molecules to nanostructures. One possible route for control is offered by varying the carrier-envelope phase (CEP) of few-cycle laser fields. The optical response of the nanostructure itself depends on several parameters including material composition, shape, geometric configuration, and size, opening up a rich toolbox for tailoring the nanolocalized fields.

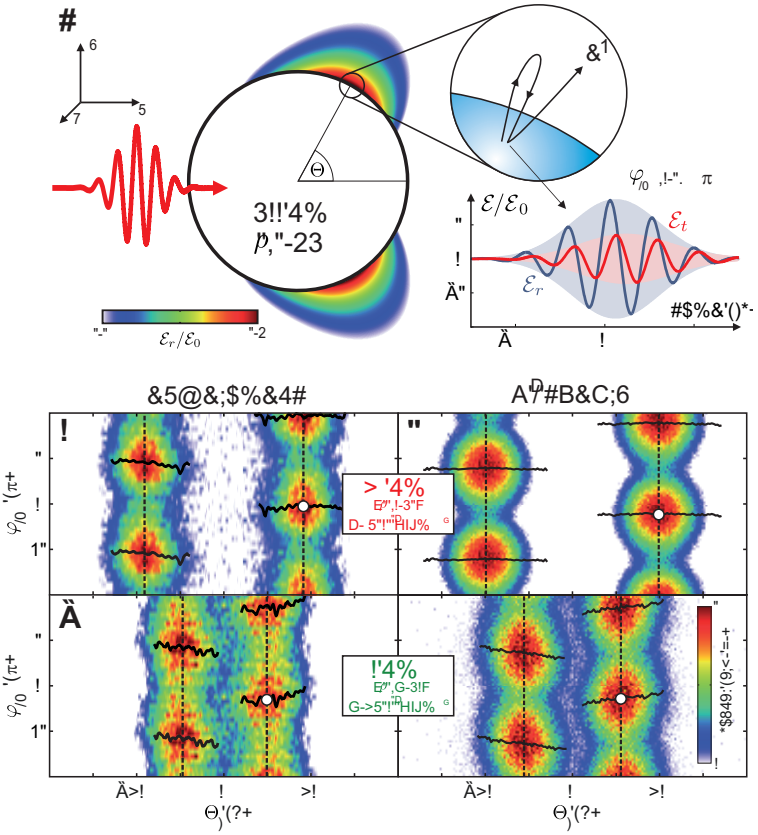


Fig. 2.15: Nanofocusing-induced photoemission from nanospheres. **(a)** Hot spots of the radial near-field in the propagation plane ($z = 0$) predicted by Mie's solution for $d = 400\,\mathrm{nm}$ and schematic illustration of the electron recollision process. **(b,c)** Measured angle and CEP-resolved electron yields $Y(\Theta, \varphi_{\mathrm{CE}})$ of near cut-off electrons with $E_{\mathrm{th}} = 0.5E_{\mathrm{cutoff}}$; sphere sizes and laser intensities as indicated. **(d,e)** same as (b,c) as predicted from M^{3}C simulations for the experimental parameters. Adapted from Ref. [1].

A particularly interesting possibility for control of the electron dynamics arises from electromagnetic field propagation. In a proof-of-principle study we could demonstrate the potential of this scheme, see Fig. 2.15, and found that strong-field induced recollision electrons can be guided by the field propagation-induced nanofocusing in large dielectric nanospheres. For such spheres, the linear near-fields are well described by the Mie solution and depend on the dimensionless scale parameter $\rho = \pi d/\lambda$, where d is the sphere diameter and λ the central wavelength. While maximal enhancement occurs at the poles for small spheres ($\rho \ll 1$), field propagation

becomes significant if $\rho > 1$ and shifts the hot spots in the propagation direction, see Fig. 2.15a. An example of the waveform control of the resulting strong-field photoemission without and with nanofocusing is shown in Fig. 2.15b and Fig. 2.15c, respectively, where the high-energy electron yield obtained experimentally is depicted as a function of projected emission angle and CEP. A comparison of the emission maps for small ($d = 100\,\mathrm{nm}, \rho = 0.4$) and large ($d = 550\,\mathrm{nm}, \rho = 2.4$) spheres shows that the emission is tilted by about 45° towards the laser propagation direction. The phase dependence of the signal under the respective critical angle (peak signal for emission into upper half space) is similar, giving evidence for robust attosecond control. To model the photoemission from dielectric nanospheres, we have developed a mean-field Monte-Carlo simulation model that allowed us to unravel the physics underlying the measured asymmetry features and cut-offs [1].

Cluster ionization dynamics in IR, XUV, and X-ray fields

A key issue for many applications of short wavelength free electron laser (FEL) light is how the nature and dynamics of intense laser-matter interactions develop as a function of wavelength. For corresponding exploratory studies on finite targets atomic clusters are promising prototypes, as great experience in their experimental and theoretical investigation is available from the vast amount of IR studies. Early experiments on small Ar_N clusters in intense XUV laser fields have shown strong evidence for the presence of a multistep ionization process and the disappearance of collisional plasma heating. Note that the highly efficient heating via resonant plasmon excitation, as is well-known from the IR regime [2], is not possible in the XUV spectral range.

Motivated by the first XUV pump-probe experiment on the ion emission from Xe clusters, we studied the transient ionization and relaxation dynamics in such pump-probe scenarios in more detail. Our theory analysis via molecular dynamics simulations supports that the increasing ion charge states measured with increasing delay in the experiments reflect the decreasing recombination efficiency in clusters that are probe-excited in later stages of expansion [3].

More recently, Schütte *et* al. investigated rare-gas clusters under intense XUV fields using a lab-based high-harmonics generation experiment for which we provided the corresponding modeling. This joint experimental and theoretical study [4] clearly confirmed the multistep ionization picture from the former FEL experiments. In follow up studies of this collaboration, we identified a new cluster ionization mechanism via correlated electronic decay [5] and found evidence for the strong sensitivity of electron-ion recombination during cluster expansion to weak external electric fields [6]. The latter one is key to explaining the final charge states in laser-cluster experiments.

Three-dimensional and dynamic cluster characterization via X-ray coherent diffractive imaging

A key challenge in single-shot X-ray imaging is the unique identification of three-dimensional structures. In joint work with colleagues from the University of Rostock, TU Berlin, and SLAC we have been able to demonstrate for the first time the simultaneous identification of both particle orientation and shape of free-flying nanoparticles from single scattering images. The corresponding soft X-ray wide-angle scattering experiment by I. Barke *et* al., for which we provided the theoretical analysis, was performed on large free silver clusters at FLASH [7]. A clear signature for the fact that 3D information is encoded in the single-shot scattering images is the absence of point symmetry, see example in Fig. 2.16. In order to adequately describe the scattering process at longer wavelengths, absorption in the target and multiple scattering must be taken into account, as these effects are typically non-negligible. A convenient method is the reconstruction via a forward fit of the measured scattering pattern with numerically simulated diffraction patterns of parameterized model shapes. The experimental example in Fig. 2.16 shows excellent agreement with our corresponding finite-difference time-domain (FDTD) simulation result for an octahedral cluster shape. In a follow-up theory study using the discrete-dipole approximation (DDA) we showed that the extraction of 3D information is feasible even for single-shot attosecond diffractive imaging [8].

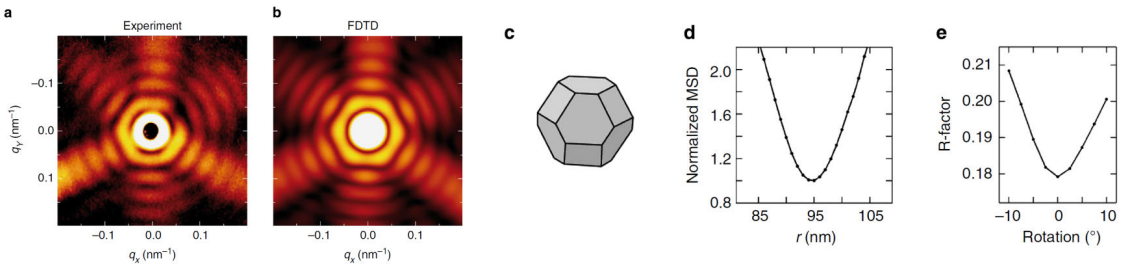


Fig. 2.16: Measured scattering image (a) from a single silver cluster at 13.5 nm wavelength and simulated pattern (b) from FDTD simulations for an octahedral cluster (c). The mean-square displacement (MSD) of the two images as a function of radius supports accurate size-determination. The R-factor evolution for a rotation of the shape around the horizontal axis demonstrates sensitivity on the 3D cluster orientation (e). From Ref. [7].

Time-resolved X-ray imaging may allow the direct visualization of femtosecond or even attosecond dynamics of matter with nanometer resolution. Such capability would have a large impact on several scientific fields. Applied to finite solid-density plasmas, this approach promises a substantial improvement over existing real-time plasma imaging techniques. To develop and test retrieval methods, complete knowledge of both the pump dynamics and the XFEL probe process is needed. This requires a self-consistent first-principle description of plasma dynamics and electromagnetic field evolution, including elastic and inelastic classical X-ray scattering.

In order to meet the above requirements, we have developed the microscopic particle-in-cell (MicPIC) technique. With this tool, many-particle correlations and plasma microfields can be resolved. Using MicPIC we were able to perform the first complete time-resolved X-ray imaging simulation [9]. We considered a near-infrared (NIR) pump X-ray probe scenario for a spherical hydrogen cluster, see Fig. 2.17. A short and intense NIR few-cycle pulse leads to complete (inner) ionization, strong heating, and subsequent expansion of the system. The simulated time-delayed X-ray scattering traces contain both elastic and inelastic contributions, where the latter contain Raman peaks induced by thermal plasma fluctuations (e,f). Note that inelastic X-ray scattering is a powerful diagnostic tool in plasma physics as it allows one to infer the plasma density and temperature. However, here we concentrated on the elastic scattering signal. We were able to connect its time evolution (e) with an anisotropic cluster expansion and suggested a scheme to extract the nanoplasma evolution from the scattering images with nanometer spatial and femtosecond temporal resolution.

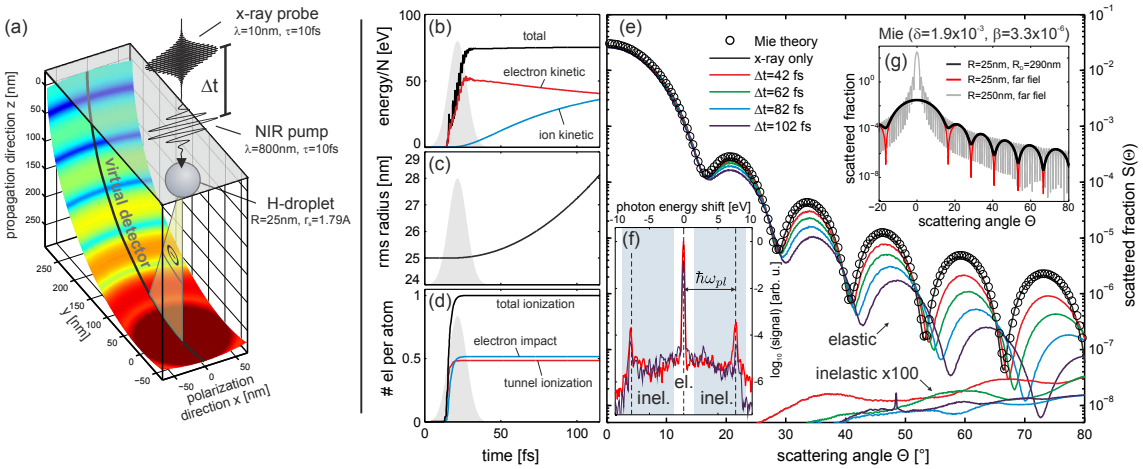


Fig. 2.17: Complete MicPIC simulation of an NIR pump X-ray probe scenario for an R=25 nm Hydrogen droplet. (a) Schematic setup of the simulation arena and the virtual detector. (b-d) Time evolution of selected observables after pump excitation. (e) Lineouts of the elastic and inelastic scattering from the probe pulse. (f) Spectrum of the scattered radiation including elastic and inelastic contributions. (g) Mie simulations of the near-field and far-field scattering pattern of Hydrogen spheres. Adapted from Ref. [9].

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2.2.3 Molecular Quantum Dynamics

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General Outline of the Field of Research

The research agenda includes four topics: Non-reactive and reactive dynamics of nuclear degrees of freedom, Photophysics and Photochemistry of elementary processes, dynamics after X-ray core hole excitation, and Environmental Physics. The dynamics of nuclei is studied in the context of linear and non-linear vibrational spectroscopy as a means to unravel the relation between molecular structure, dynamics, and function. The arsenal of methods comprises those from quantum, semiclassical, and classical theory. Applications are concerned with liquid water or ionic liquids. Photo-induced processes in electronically excited molecular states are investigated with various electronic structure and dynamics methods. Particular emphasis is put on systems relevant for photocatalysis and solar energy conversion. With the advent of novel X-ray sources core-level spectroscopy has experienced a revival as a means to unravel, for instance, details of electronic structure and dynamics *in situ*. We focus on transition metals in various environments, which are studied using first principles methods. Finally, an interdisciplinary effort is devoted to the introduction of atomistic simulation techniques into the field of soil science. Targets are organic pollutants and phosphates and their interaction with soil components such as organic compounds or mineral surfaces.

This research has been supported by: DFG (Sfb 652, Ku952/10-1, Ku952/6-1, IV 171/2-1), BMBF (Light2Hydrogen, InnoSoilPhos), Qatar National Research Fund, King Abdulaziz University Jeddah, LL&M (Sec. 4), and COST (Perspect-H_2O).

Nuclear Dynamics

The working horse here is classical molecular dynamics (MD), which provides a handy tool to zoom into the peculiarities of microscopic processes. The MD method

has proven itself as an extremely robust technique that can also serve as a basis for various semi- and quasi-classical extensions. In particular, Feynman's path integral (PI) formalism provides an elegant way to obtain quantum thermodynamic properties of the system in question numerically exactly by means of genuinely classical techniques, here classical MD. We utilized this approach to extend metadynamics, which is one of the most successful techniques to simulate free energy profiles, to incorporate nuclear quantum effects into simulations of reaction barriers and thus reaction rates without relying on harmonic corrections [1]. Further, using *ab initio* MD and its extension to approximate PI dynamics allowed us to fully explain intricate infrared spectra of protonated methane, which is often considered to be the most prominent member of the class of floppy or fluxional molecules, and its isotopologues, see Fig. 2.18 for a sketch of a molecule in a PI representation [2].

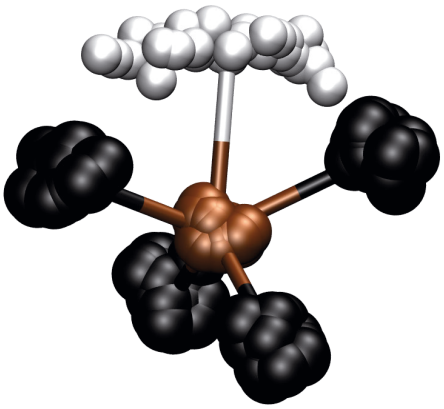

Fig. 2.18: One of the CH_5^+ isotopologues (CHD_4^+) in the PI representation.

Finally, combining quantum-classical MD with CARS spectroscopy (joint effort with the groups of S. Lochbrunner, Sec. 2.2.4, and R. Ludwig from the Chemistry Institute in the framework of SFB 652), pure dephasing rates in an aprotic IL were shown to depend on the pattern of hydrogen bonds linking ion pairs [3].

Often the description of the process under study can be reduced to a few parameters, which can not only ease the interpretation, but enable the identification of key properties. In condensed phase dynamics the Caldeira-Leggett model, based on representing the surrounding via a spectral density of a harmonic bath, bilinearly coupled to the system, enjoyed popularity. We developed a robust and efficient parametrization scheme for spectral densities in the framework of vibrational spectroscopy. It turned out that the applicability of the model to cases with anharmonic system potentials, as it is required for the description of realistic systems in solution, is questionable due to the presence of the so-called invertibility problem [4]. Another worrying result was that the conventional rigid bond method for parameterizing spectral densities yields qualitatively wrong results in the most important resonant region.

Photophysics

"Learning from Nature" is a common theme in the natural sciences. The ingenious machinery of photosynthesis is particularly attractive as it has evolved to efficiently convert the sun light into chemically usable energy. Can we mimic natural photosynthesis to open the door to an unlimited energy source? Do we need to copy just structural elements into man made supramolecular architectures? How impor-

tant is the interplay between structure and dynamics for the realization of function? Finally, did Nature restrict itself to the classical laws of Physics or did Quantum Mechanics provide some advantage? Questions like these have driven our research along two main directions: First, triggered by the BMBF project "Light2Hydrogen" theoretical investigations have been performed for a particular water splitting reaction involving iridium- and copper-containing photosensitizers as well as a series of iron carbonyls as water-reduction catalysts. Here, special attention was paid to the reliable description of the properties of charge-transfer electronic states. For this purpose, the optimally-tuned long-range corrected density functional theory has been shown to be promising due to its reasonable accuracy combined with computational efficiency [5].

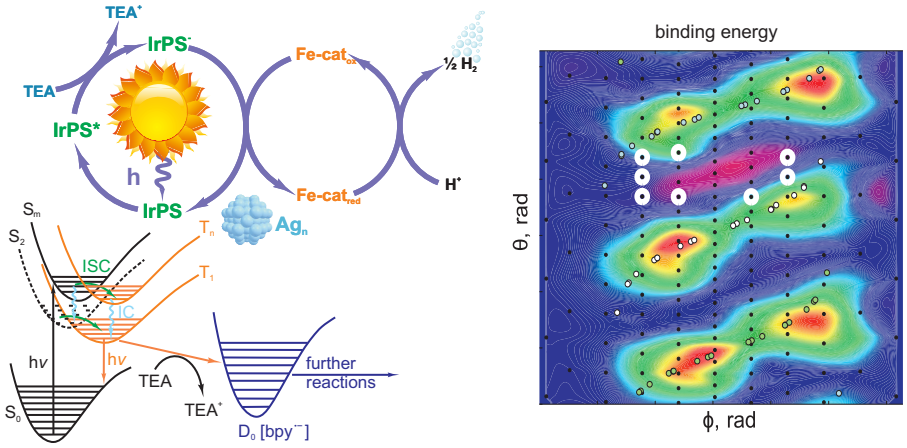

Fig. 2.19: Left: Photocatalytic water splitting cycle involving an iridium photosensitizer (IrPS), triethylamine (TEA) as a sacrificial reductant, and an iron catalyst (Fe-cat) to generate hydrogen. The efficiency is determined by elementary steps such as absorption, intersystem crossing (ISC), internal conversion (IC), and electron transfer. Right: Energy of binding between IrPS and TEA in dependence on their mutual position on a sphere. Dots denote configurations preferably for electron transfer. Their small overlap with regions of strong binding is a bottleneck for the efficiency of this reaction observed by the Lochbrunner group, Sec. 2.2.4 [5].

Second, Frenkel exciton dynamics in light-harvesting complexes, that is the energy transfer from the absorption site(s) to the photosynthetic reaction center, is one of the most efficient processes in nature. Understanding the mechanisms of this dynamics might help to improve artificial devices like organic solar cells. We applied wave-function and density matrix based approaches to study both, the coherent and dissipative exciton transfer in photosynthetic light-harvesting as well as in man-made molecular aggregates [6–8]. In particular we were interested in the dynamical and spectroscopic signatures of intra-molecular and environmental fluctuations (vibrations) For efficient determination of excitation energies, Coulomb couplings as well as their fluctuations, a density functional tight-binding protocol has been developed.

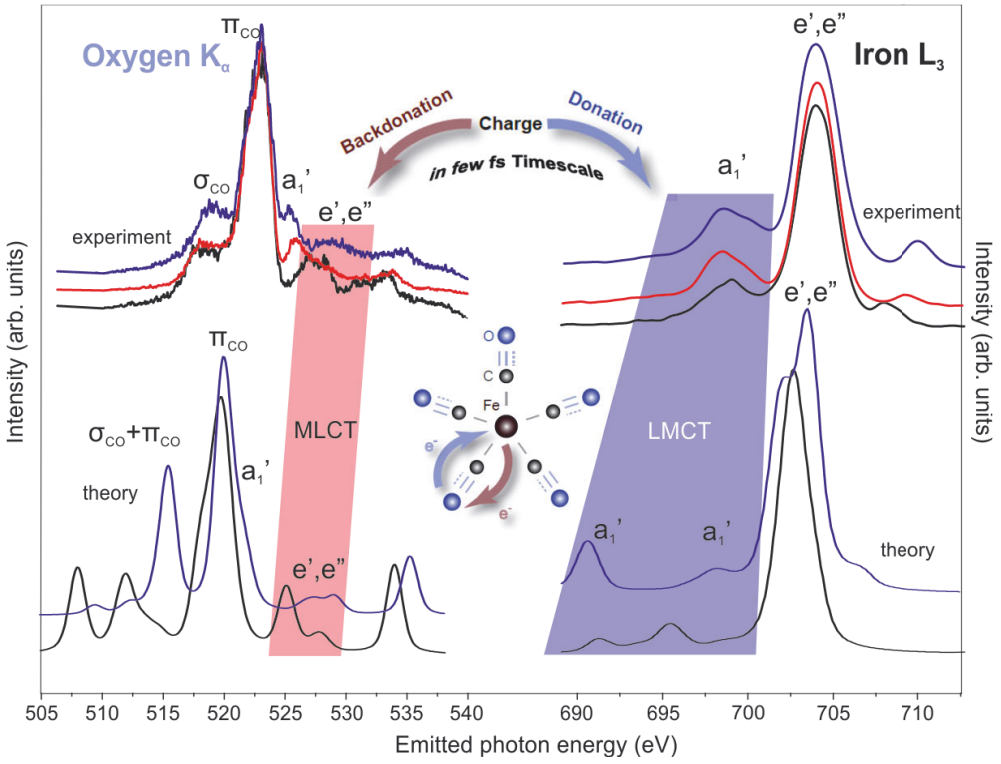

Fig. 2.20: Experimental and theoretical X-ray absorption and Resonant Inelastic X-ray Scattering spectra of the Fe L_3 edge (right) and the O K-edge (left) of $FeCO_5$. Charge transfer features characterizing chemical bonding are shaded [9].

X-ray Spectroscopy

Tracing atomic and molecular levels in course of various physical and chemical processes, X-ray spectroscopy is one of the most powerful tools to access structure and properties of matter in different states of aggregation. X-ray spectroscopic techniques probe the local electronic structure of a particular atom in its environment in contrast to UV/vis spectroscopy, where transitions generally occur between delocalized molecular orbitals. The combination of different absorption, emission as well as photo- and autoionization X-ray methods allows addressing various aspects of ultrafast dynamics and identification of short-lived intermediates of catalytic reactions. However, interpretation of complex experimental spectra and verification of experimental hypotheses is a non-trivial task and a powerful first principles theoretical approaches that allow for a systematic investigation of a broad class of compounds are needed. During the last years we have established an efficient and versatile

theoretical methodology for the treatment of X-ray spectra based on the multi-configurational self-consistent field electronic structure theory. This enabled us to quantify fundamental chemical concepts of bonding in metal-ligand complexes [9] and to address the role of electron delocalization at solute-solvent interfaces [10]. Besides the photon-in/photon-out light scattering processes, photon-in/electron out photoelectron spectroscopy has been developed to a point where electron correlation and spin-orbit coupling effects can be treated quantitatively [11].

Environmental Physics

Soil is a complex heterogeneous mixture of varying fractions of organic matter, mineral particles, water, and air. The interaction of substances introduced intentionally (fertilisers) or non-intentionally (pollutants) with soil determines their fate and thus the quality of our ecosystem. Microscopic models of soil can be obtained from experimental data giving statistical distributions of molecular compositions, which can be controlled in specifically prepared samples. This provides the basis for atomistic simulations using classical MD and electronic structure methods.

The focus of our research has been on two applications: First, the interaction of the different types of persistent organic pollutants with soil organic matter [12]. Second, in the frame of the Rostock Leibniz Science Campus "Phosphorous Research" we studied phosphate sorption at mineral surfaces in the presence of organic compounds and water [13].

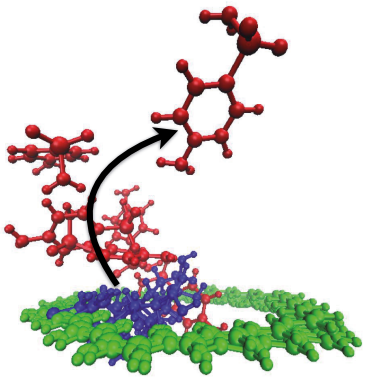

Fig. 2.21: Dissociation of a complex formed by the pollutant sulfanilamide (red) and (blue) from a cavity (green) in aqueous solution (not shown) as obtained from an MD trajectory. The situation mimics the interaction of hydrophilic pollutants and with a hydrophilic group of soil organic matter [12].

Highlights

- December 4, 2014, Marco Schröter receives the Faculty Award for the best master studies in Physics
- June 2015, Marco Schröter participates in the 65th Lindau Nobel Laureate Meeting
- December 3, 2015, Marie Preuße receives the Faculty Award for the best master studies in Physics

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2.2.4 Dynamics of Molecular Systems

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General Outline of the Field of Research

The group "Dynamics of Molecular Systems" performs research on photoinduced processes in molecules, supramolecular structures and organic materials. The goal is to observe and characterize the underlying fundamental steps and to elucidate the responsible mechanisms. Molecular systems exhibit a huge variety of properties and phenomena which can be explored in a broad spectrum of applications. This includes material design, organic electronics as well as nanotechnology, where implementing functions on a molecular scale is one of the ultimate goals. The rich behavior and variability result from the interplay of electronic and nuclear degrees of freedom. Understanding, controlling, and optimization of the respective molecular processes call for a microscopic and quantum-mechanical notion of the underlying mechanisms. We apply time resolved spectroscopy to achieve this goal. The focus is on ultrafast pump-probe techniques with a resolution down to 10 fs, which allow us to observe the processes in real time. Longer timescales are explored applying a streak camera to characterize the photoluminescence from the pico- to the microsecond time scale and an electronically triggered YAG laser system as excitation source to monitor absorption changes in the time range from nanoseconds to several hundred microseconds. The following topics summarize the main activities in the last three years.

Exciton Dynamics in Organic Systems

Intense research is going on to use organic materials in optoelectronic applications such as, e.g., solar cells. In this context the behavior of their fundamental electronic excitations, so-called Frenkel excitons, is crucial. The absorption of photons results typically in the formation of excitons and the associated energy is transported through the material if migration of the excitons takes place, see Fig. 2.22. The diffusion of excitons depends sensitively on the interaction between the molecular

chromophores and the degree of order in the system. We study these effects in a guest-host system consisting of a polymer doped with dye molecules as active sites. Thereby the density of the chromophores can be systematically varied and the spectral properties of the system are well defined. Ultrafast absorption measurements show that exciton-exciton annihilation contributes strongly to the exciton decay [1]. Analyzing the dynamics by taking diffusion-driven processes into account gives the local exciton mobility. We found that the Förster energy transfer theory in its conventional form overestimates the mobility, since it neglects energetic disorder. We extended the theory and derived an expression for the diffusion constant which contains the inhomogeneous line width of the optical spectra as a measure for energetic disorder [1]. In this way quantitative agreement with the data was achieved and one has now a tool to predict realistic exciton mobilities from measured absorption and fluorescence spectra.

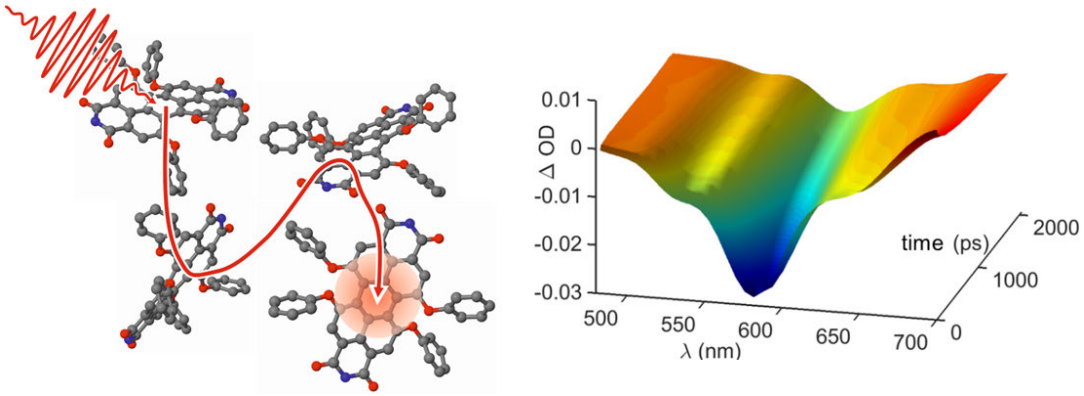

Fig. 2.22: Exciton migration between molecular chromophores (left) and transient absorption spectra showing decay dynamics due to exciton-exciton annihilation (right).

Excitons in Aggregates

Supramolecular structures of organic chromophores such as aggregates should result in a higher degree of order and might be also suitable to guide exciton migration. Hence, they are promising building blocks for photonic applications and are investigated by us within the SFB 652. Our femtosecond measurements performed in collaboration with scientists from Würzburg show that in the case of H-aggregates fast self-trapping can occur resulting in a negligible migration of excitons [2]. The formation of J-aggregates seems to be crucial for a high exciton mobility. Due to this we studied together with the Quantum Molecular Dynamics group, Sec. 2.2.3, the aggregation behavior of a specific perylene bisimide dye in detail. It turned out that the dye forms at first H-like dimers [3]. But the large aggregates appearing at higher concentrations exhibit a J-configuration. This results from the fact that due to steric reasons and contrary to the J-aggregates, the H-like dimers cannot be

extended by additional molecules. The excitons of the extended perylene bisimide aggregates exhibit a quite high mobility in accordance with the J-like character of the aggregates.

Fundamental Processes in Photocatalysis

The generation of hydrogen by light-induced water splitting with catalytic systems is a promising sun-powered energy source. The Leibniz Institute for Catalysis (LIKAT) is developing such systems and collaborating with our group, e.g., within the BMBF project Light2Hydrogen, to investigate the fundamental steps of the process. The results help to identify loss mechanisms and to optimize the catalytic system. The considered homogeneous systems are mixtures of solvent, water and an electron-donating compound in which a photosensitizer and a catalyst are dissolved with a low concentration. After photoexcitation a cascade of electron transfer processes shifts an electron from a donor molecule to a catalyst, where it is used to reduce protons resulting finally in molecular hydrogen, see Fig. 2.23.

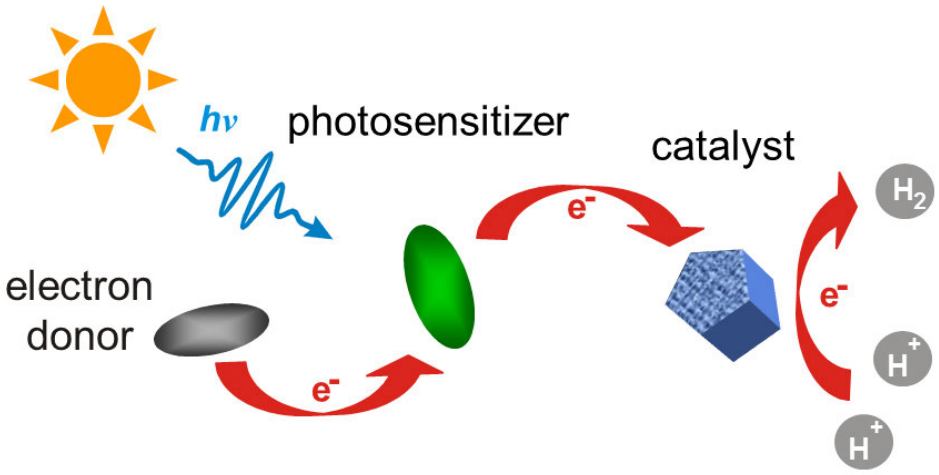

Fig. 2.23: Scheme of the light-induced electron transfer steps in the investigated photocatalytic system.

Our transient absorption measurements on iridium and copper complexes, used as photosensitizers, showed that after an absorption event an extremely fast intersystem crossing occurs [4]. Subsequent relaxation steps result within some picoseconds in the population of the lowest triplet state, which has a lifetime of a few hundred nanoseconds. In presence of an electron-donating compound fluorescence quenching takes place, indicating that an electron transfer onto the photosensitizer occurs, which is the first step in the catalytic process. However, our studies showed that the rate is much lower than the corresponding diffusion limit and a very high concentration of the electron donor is needed for quantitative quenching [5]. On the other hand the measurements indicate that the electron transfer from the sensitizer

to the catalyst is highly efficient. Since the catalytic system contains a high fraction of the donor compound, both electron transfer steps exhibit a yield of almost 100 % and thus do not present a bottleneck for the process. In collaboration with Wolfram Seidel from the Institute of Chemistry we also investigate complexes with two metal centers [6]. In this case one part of the molecule acts as a photosensitizer, while the other should play the role of the catalyst. The spectroscopic experiments indicate that also in some of these complexes fast photoinduced electron transfer occurs, which is the first step of the catalytic sequence.

Carbon nitride, a new polymeric semiconductor, is a promising candidate for heterogeneous photocatalysis. In collaboration with the TU Berlin and the LIKAT we investigate the photoinduced dynamics in this material. It turns out that light absorption results in extremely fast charge separation. The charge carriers are then migrating vertically to the layered structure of the material by statistical hopping steps [7]. Observed photoluminescence results from geminate recombination events and shows a characteristic non-exponential decay.

Ultrafast CARS Spectroscopy of Intermolecular Interactions

An ultrafast spectroscopic technique based on coherent anti-Stokes Raman scattering (CARS) was developed to gain better insight into complex vibrational spectra. The method makes use of ultrashort broadband Stokes pulses and narrowband picosecond pulses for Raman pumping and probing. In this way high temporal and spectral resolution are achieved simultaneously [8]. The theoretical description of CARS was adapted to our specific situation and reformulated such that it can be fitted to the measured time-dependent spectra. Parameters such as vibrational frequencies and dephasing times can be extracted with high accuracy even though interference effects lead in many cases to complex spectral signatures. In the case of congested Raman bands, information is now accessible which is hard to reveal by linear Raman spectroscopy. The introduced CARS technique was applied to study intermolecular interactions in acetic acid and ionic liquids. In the first case we were able to show that acetic acid molecules form in liquid phase not only chains but also in a large fraction dimers [9]. The properties of ionic liquids are determined by strong Coulomb forces and by hydrogen bonds. In a joint project of the SFB 652 we investigate together with the group of Ralf Ludwig from the Institute of Chemistry and the Quantum Molecular Dynamics group, Sec. 2.2.3, the intermolecular interactions in ionic liquids via the analysis of dephasing processes.

Highly Excited Dense Matter

During the last years a project was implemented which is dedicated to the interaction of intense laser radiation with condensed matter. This field attracts scientific interest for two reasons. First, femtosecond laser ablation is a promising approach for high precision machining. Second, one can generate in this way warm dense matter,

which is characterized by high densities in combination with high temperatures and which covers little explored regions of the phase diagrams of most materials. To observe the time-dependent response of materials to intense laser pulses, we have developed a pump-probe setup utilizing transmission and diffraction of an ultraviolet probe beam. Near infrared (NIR) pulses at 800 nm with a duration of 50 fs are used for excitation. A frequency-doubled fraction of the original NIR beam is focused collinearly with the excitation pulses onto a very thin foil serving as a sample and the transmitted light is monitored by a CCD camera. In first experiments a circular diffraction profile was observed which changes with time. An iterative algorithm was implemented to extract local changes of the index of refraction in the interaction region from the diffraction pattern. This provides information about the evolution of the electron density and the phase state of strongly excited matter. The work is performed in collaboration with the Theoretical Cluster Physics, Sec. 2.2.2, and Clusters and Nanostructures, Sec. 2.2.5, groups.

Photophysics of New Molecular Systems

Beside the main activities described above, several smaller projects are pursued, all of them in collaboration with other groups, for example with Martin Köckerling and Peter Langer from the Institute of Chemistry. The objective is to learn about the photophysics of new molecular systems like new rare earth compounds, substituted pyrazines, and indoles.

In collaboration with Udo Kragl, also from the Institute of Chemistry, and his group we have developed an approach to trigger optically the activation of enzymes [10, 11]. To this end a laser pulse induces a jump of the pH-value by exciting a compound which turns into an acid by a photoreaction. The original pH-value of the solution containing the enzyme and a substrate is chosen such that prior to the laser pulse the enzyme is more or less inactive but becomes active after the pH-jump. The activation of the enzyme after the laser pulse is monitored by measuring the consumption of the substrate and the rise of the product concentration.

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2.2.5 Clusters and Nanostructures

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General Outline of the Field of Research

Finite size, large surface fraction, limited capacity for heat and charge, and discrete electron states: these are the characteristics of clusters and nanoparticles. Our research is aimed at the remarkable consequences of nanoscale objects, many of which are accessible by spectroscopic means. Clusters in a molecular beam allow the investigation of electronic and optical properties ranging up to the strongly nonlinear regime. If clusters and nanostructures are in contact with surfaces, a number of additional effects can be observed, ranging from structural changes to unusual transport, doping, and catalytic properties. A large part of the research has been conducted within the SFB 652, HICE, REMEDES, Light2Hydrogen, and other BMBF projects like Nanoscopic Systems investigated at FLASH.

Laser Spectroscopy on Molecules, Clusters, and Nanoparticles

Ultracold helium nanodroplets provide an ultralow temperature nanolab for studies on the optical and electronical response of clusters within a weakly interacting environment. Experiments in the linear response regime have focused on a unique species that forms in the helium environment, i.e., a magnesium foam. In particular we concentrate on the photoemission by probing an intermediate foam state near the 3s-3p resonance. After the excitation the foam collapses and disintegrates. In the

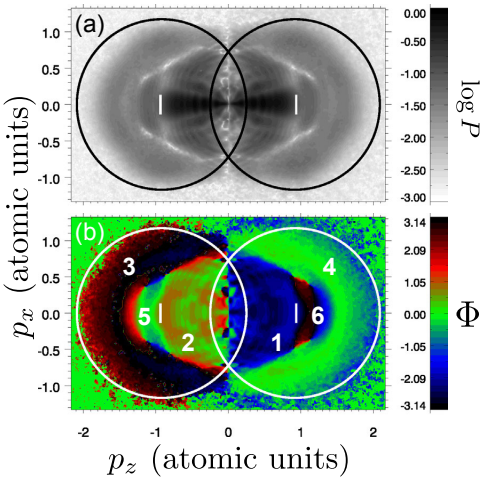

Fig. 2.24: Experimental relative-phase-contrast (top) and phase-of-the-phase (bottom) spectra for Ar, extracted from 66 Abel-projected VMI spectra per φ interval $[0 - 2\pi]$. The two-color components of the 100-fs pulse had intensities of 10^{14} and 10^{12} W/cm^2, respectively. Circles and vertical lines indicate $10U_P$ rescattering rings and $2U_p$ cutoffs, respectively. White numbers refer to special phase dependencies in the electron momentum spectra. Adapted from Ref. [6].

process a huge amount of binding energy is released and as a result high-lying states of the atom are populated. The resonant two-photon ionization electron spectra reveal that high-lying states including triplets are present, proving the hypothesis of a light-induced foam collapse. Similar results, but concentrating on the ions, have been obtained by using the femtosecond pump-probe technique [1]. In another study we have made an attempt to identify the onset of superfluidity in molecules surrounded by helium atoms by using the technique of impulsive alignment (together with group of von Heaften (Leicester, GB)) [2]. An interesting observable, also with respect to future technical applications in lithography in the extended ultraviolet, is soft X-ray emission from rare gas clusters. Studies have been conducted using optimized pulse envelopes in order to maximize the light emission. Beside studies on nanodroplets, experiments have been concentrated on the rapid heating of hydrogen microdroplets in intense 13 nm-light delivered by the free-electro-laser FLASH in Hamburg [3]. In another experiment we have characterized metastable nanoparticle structures by the single-shot wide-angle scattering of femtosecond soft X-ray pulses [4]. Photoemission is also studied at FLASH. We are interested in the size-dependent electronic properties of metal clusters with emphasis on core levels. Recently, we have rearranged the experimental setup, now using the radio-frequency technique. Clusters are accumulated in a Paul-type trap and extracted into the FEL interaction region.

The photoemission from atoms and molecules in intense two-color laser fields is studied to resolve the dynamics on a subcycle time scale. For this purpose we have built a velocity map imaging (VMI) electron spectrometer with an extended energy range [5]. To analyze the phase-dependent signals, spectra have been taken for various values of the relative phase between the fundamental and the second harmonic and post-processed via Fourier transformation (*Phase-of-the-phase spectroscopy*). In doing so we identified a new and target-independent universal structure. In collaboration with the groups of Bauer (Sec. 2.2.1) and Fennel (Sec. 2.2.2), we have been able to assign the signature to the so-called second-return [6].

Metal and rare gas clusters exposed to intense laser fields exhibit signatures of collective response and show evidence for effective electron acceleration. Experiments have demonstrated, that the temporal laser pulse structure plays a significant role. Atomic ions in charge states as high as $q = 24$ have been observed from xenon clusters at laser intensities close to the barrier suppression threshold. In order to study the impact of the pulse structure on the charge state and energy of the highly charged ions, we have developed a new Thomson-type spectrometer consisting of a magnetic deflection field and a position-sensitive detector. It features an increased transmission and a superior resolution in comparison to other instruments used in this field.

Clusters and Nanostructures at Surfaces

Formation of clusters in the gas phase and their deposition on crystal surfaces represent a versatile technique for the controlled production of nanosystems. Chemical properties of such deposited particles are topic of our research as well as self-organization phenomena at surfaces, including the possibility to induce phase transitions in atomic chains.

Nanoparticles at surfaces are model systems for studying catalytic processes. While large surface areas are naturally available in such systems, low activation energies are essential as well for efficient reactions, particularly in heterogeneous catalysis. For the case of oxidative dehydrogenation of cyclohexane, we have deposited cobalt oxide nanoparticles in a large size range on different substrates and investigated the evolution of particle shapes as a function of reaction temperature [7]. By combining various experimental methods including grazing-incidence X-ray absorption near edge structure (GIXANES), transmission electron microscopy (TEM), and reflection high-energy electron diffraction (RHEED) different compositions and morphologies become evident. These regimes strongly depend on the particle size, e.g., small particles below 7 nm diameter exhibit compact shapes, while at about 15 nm diameter hollow particles are observed that are formed by the nanoscale Kirkendall effect. We have applied a novel method based on RHEED for quantitative determination of activation energies of supported nanoparticles. The data reveal that not only the size of nanoparticles but also their detailed morphology can crucially affect reaction kinetics, as demonstrated for small oxidized cobalt clusters [8]. We have found unexpectedly small activation barriers for the reduction reaction of large particles, despite generally increasing barriers for growing sizes. We attribute these observations to the interplay of material transport and size-dependent inner particle morphology.

Scanning tunneling microscopy (STM) can also be used to manipulate surface structures. On the quasi one-dimensional Si(553)-Au reconstruction we have observed a reversible structural transition that is triggered by electrons injected by the STM tip. The periodicity of atomic chains temporarily switches from the 1×3 ground state to a 1×2 excited state [9], where the latter dominates at increasing

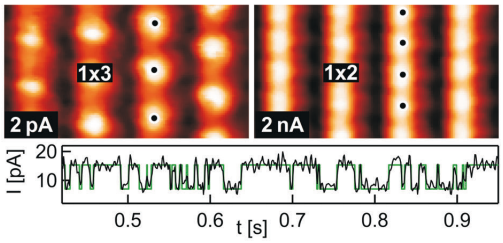

Fig. 2.25: Top: STM images showing the structural transition from a (1×3) to a (1×2) periodicity on Si(553)-Au upon increasing tunneling current. Bottom: Random switching between both structures results in a telegraph-type noise in the time-dependent tunneling current.

tunneling current. Surprisingly, this excitation is easier achieved at lower temperatures, i.e., lower average tunneling currents are sufficient for the phase transition. Density functional calculations reveal that upon charge injection the ground state becomes unstable, hence supporting the experimental findings. Subsequent experiments have enabled characterization of the structural transition as a function of temperature and tunneling current in detail [10]. They also have provided insight into the site dependence of the excitation efficiency and yielded quantitative data on the current-dependent occurrence probability for each of the contributing phases.

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2.2.6 Statistical Physics

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General Outline of the Field of Research

The research in the group *Statistical Physics* is focused on the theory of strongly correlated many-particle systems. In particular, we are interested in matter under extreme conditions of pressure and temperature and in the dynamics of the light-matter interaction on ultra-short time scales. We develop and apply methods of statistical and computational physics in order to treat quantum effects and strong correlations adequately. We collaborate with groups in Germany (European XFEL Hamburg, DESY Hamburg, DLR Berlin, BGI Bayreuth), USA (Livermore, Los Alamos, Sandia, Stanford), UK (U Oxford), France (CEA, U Paris), Russia (ICP Chernogolovka, IVTAN Moscow), and Kazakhstan (U Almaty). Our research is funded by the German Science Foundation within the SFB 652 *Strong Correlations in Radiation Fields*, the SPP 1385 *The first 10 Million Years of the Solar System*, the SPP 1488 *Planetary Magnetism*, and the BMBF within the FSP 302 *Free Electron Lasers*. We use computing resources at the HLRN and the FZ Jülich, and on the compute clusters Merkur, Venus, and Titan at the ITMZ of the U Rostock.

Warm Dense Matter and ab initio Molecular Dynamics Simulations

The behavior of the lightest elements, H and He, of molecular systems like CH_4, NH_3, H_2O, and of minerals like SiO_2, MgO, FeO (and their mixtures) under extreme conditions is of great interest in high pressure and planetary physics. In order to model the interior, evolution, and magnetic field of planets, the knowledge of thermodynamic, transport, and optical properties is needed for densities typical for

condensed matter and for temperatures of several 1000 K, i.e. for *warm dense matter* (WDM).

We have determined thermophysical properties of H-He and water-ammonia mixtures via molecular dynamics simulations which combine a classical treatment for the ions with a full quantum description of the electrons using density functional theory (DFT-MD). Besides the equation of state (EOS), transport coefficients such as the electrical conductivity and the diffusion coefficient, the pair correlation functions, and the opacity can be gained; see Refs. [2, 4, 5, 7]. A major goal is the calculation of the high-pressure phase diagram of WDM, especially with respect to insulator-to-metal transitions (IMT) and demixing phenomena.

As a prime example, shock-wave experiments performed at Sandia's Z machine on liquid deuterium have found strong evidence for an abrupt IMT as predicted by our DFT-MD simulations [9]. The corresponding high-pressure phase diagram is shown in Fig. 2.26. This simplest element undergoes a liquid-liquid (LL) transition at about 3 Mbar below 2000 K. Analysis of the EOS, the reflectivity, and the electrical conductivity indicates that the transition between a molecular non-conducting and an atomic conducting liquid is of first order.

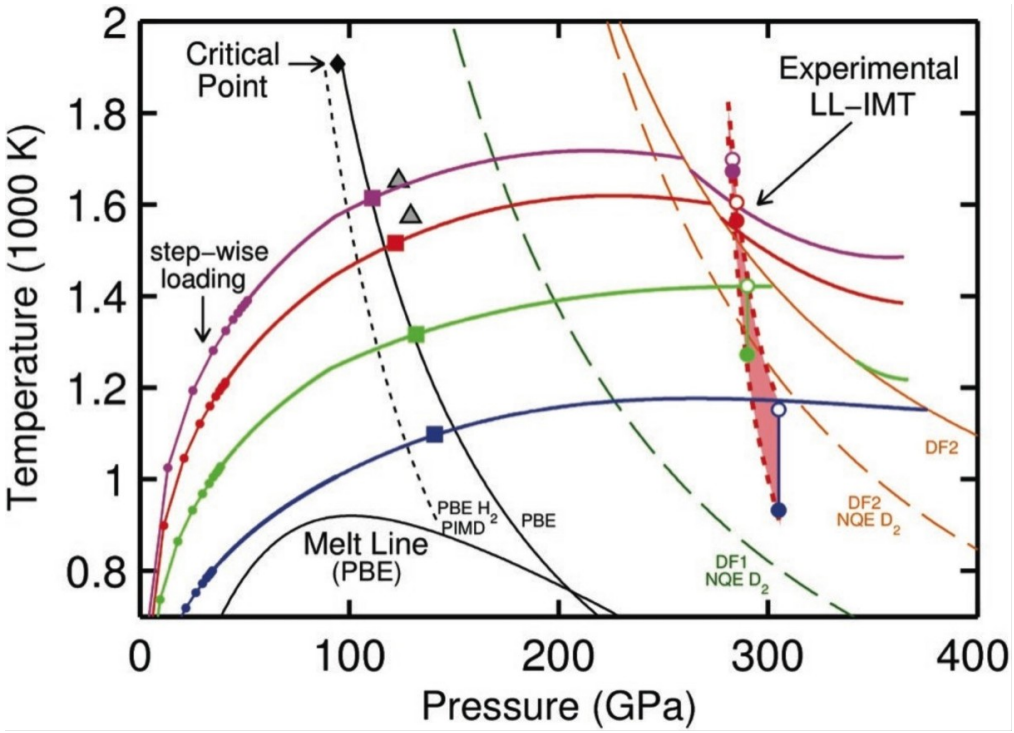

Fig. 2.26: Phase diagram of hydrogen/deuterium [9]: Theoretical predictions for the LL-IMT according to different exchange-correlation functionals (PBE, DF1, DF2) and the consideration of nuclear quantum effects (NQE). Four experimental compression paths and the region of the first-order LL-IMT are shown.

Planetary Physics

Planets are perfect laboratories to study WDM. Gas giants such as Jupiter and Saturn contain mainly H and He, while ice giants like Uranus and Neptune are composed of C-N-O-H-He mixtures. Super-Earths with up to 10 Earth masses might represent a substantial fraction of extrasolar planets so that the high-pressure behavior of minerals of the MgO-SiO_2-FeO complex is perhaps most important. Interior, evolution, and dynamo models for solar and extrasolar planets require accurate EOS data in order to narrow down the diversity of possible solutions.

We have used our DFT-MD EOS data for H, He, and water in order to construct interior models for Uranus and Neptune [1], see Fig. 2.27, Jupiter and Brown Dwarfs [6]. Similar models are currently calculated for Saturn and super-Earths. Our results for the material properties along Jupiter's isentrope were used by groups of the SPP 1488 as input in dynamo simulations that yield the magnetic field structure. Our water EOS data tables are employed by other groups for models of Neptune-like extrasolar planets.

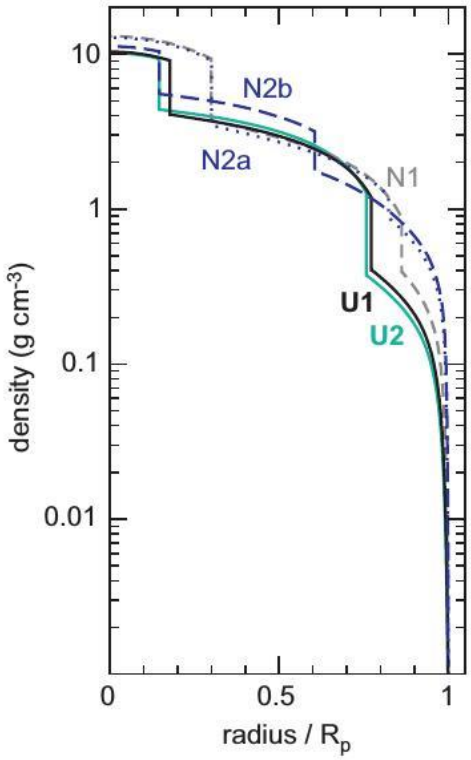

Fig. 2.27: Density profile along the normalized radius of Uranus (U) and Neptune (N) according to various models that all reproduce the observational constraints; see Ref. [1] for details. The ice giants are modeled within a three-layer model: a solid rocky core is surrounded by two water-H-He envelopes with different fractions of their constituents.

Interaction of Plasmas with Electromagnetic Fields

X-ray Thomson scattering (XRTS) has demonstrated its great capacity as a reliable and versatile tool for the diagnostics of dense plasmas [3, 10]. In particular, free

electron lasers (FELs) provide intense and ultra-short X-ray pulses that can probe matter under extreme conditions. The collective XRTS spectrum yields information on the density and temperature via the plasmon feature: its frequency position is directly related to the free electron density, and the temperature is derived from the detailed balance relation.

We have performed particle-in-cell as well as hydrodynamic simulations in order to characterize the target state during and shortly after illumination with intense optical or FEL light. Strong non-equilibrium states are generated by intense (optical) pump pulses, which influence the evolution of the target on fs-ps time scales. We have calculated the corresponding XRTS spectra and determined, e.g., the relaxation time into an equilibrium state with equal electron and ion temperatures, $T_\mathrm{e} = T_\mathrm{i}$, in H [3] and identified two-temperature states in the pump-probe experiments performed with Be [10]. Furthermore, the dynamic ion-ion structure factor has been calculated for the first time within the DFT-MD scheme [4]. The structural properties of multi-component two-temperature plasmas can also be gained from classical-map hypernetted chain calculations [8].

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2.2.7 Elementary Particles Physics

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The BABAR Experiment

Since summer 2000 the group participates in the BABAR-experiment [1] at the SLAC National Accelerator Laboratory in California (USA), supported by the BMBF. This experiment studies multi-particle final states produced in the electron-positron annihilation at a centre-of-mass energy of 10.58 GeV. At this energy, the $\Upsilon(4S)$-resonance is produced, an excited bound state of a b- and an anti-b-quark. It decays exclusively into a pair of B mesons, massive particles heavier than a helium nucleus. The data were taken between 1999 and 2008, and are analysed since 2000, with many analyses still ongoing and a continuous output of interesting results.

The main objective of the experiment is the investigation of a time-dependent CP asymmetry (particle-antiparticle asymmetry) in the decay of neutral B mesons. An important early achievement of BABAR was the first observation of this CP asymmetry in 2001. In the following years, subsequent studies have revealed CP asymmetries in more B decay channels, and improved the precision of the parameters of the Cabibbo-Kobayashi-Maskawa matrix which are responsible for this effect.

In addition to these key questions, the BABAR experiment offers an almost unlimited potential for studying charmed mesons, charmed baryons, tau leptons, and exclusive final states from radiative e^+e^- annihilation. Also, the 480 million collected $B\overline{B}$ pairs are used to study various effects apart from the CP asymmetries. The focus of our group's investigations is the production of baryons in B meson decays. Since B mesons are the heaviest weakly decaying mesons, they offer a unique possibility to study baryon production in meson decays. Our group has examined the features of new and established baryonic final states [2–5]. Many of these decays exhibit an enhancement of the decay rate at the threshold of the baryon-antibaryon mass. We have found a common pattern for this effect, which still puzzles the theorists working in this field, and also a counterexample supporting our ideas (see Fig. 2.28).

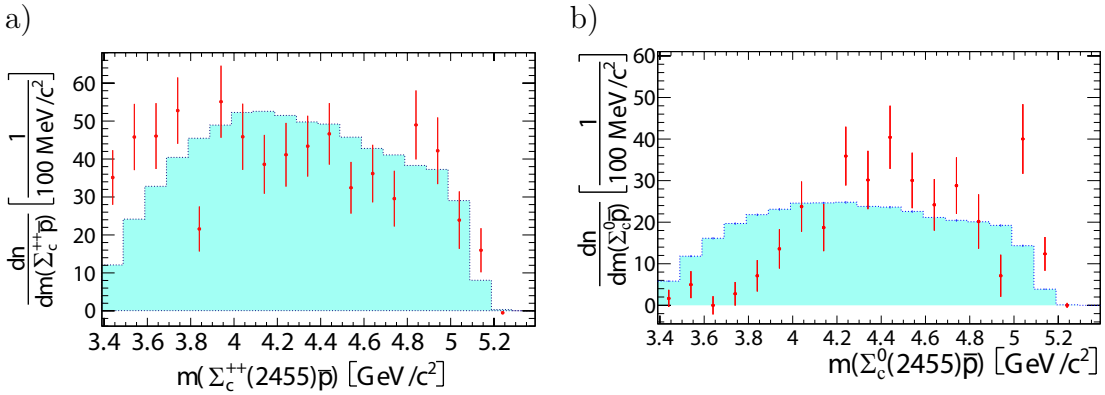

Fig. 2.28: An analysis of data from the BABAR experiment [2] shows significantly different distributions in the invariant baryon antibaryon mass of the related decays (a) $\overline{B}^0 \to \Sigma_c^{++}\overline{p}\pi^-$ and (b) $\overline{B}^0 \to \Sigma_c^0\overline{p}\pi^+$ (points with error bars). Both are compared with a uniformly populated three-body phase space (filled histograms). The different behaviour can be explained via virtual intermediate meson-meson or diquark-antidiquark states.

The LHCb Experiment

In July 2011 our group joined the LHCb collaboration, an international group of physicists who operate the LHCb detector [6] at the CERN Large Hadron Collider (LHC) near Geneva. This project is also funded as BMBF-Forschungsschwerpunkt 105. The LHC at the European Research Laboratory CERN is providing proton proton collisions since March 2010, at centre-of-mass energies of 7 TeV (2011), 8 TeV (2012) and 13 TeV (2015). The LHCb detector is located close to the beams on one side of the proton proton interaction point, while the other experiments, ATLAS and CMS, are optimised for particles at large angles. In proton proton interactions, the heavy b and $\bar{b}$ quarks are preferentially emitted at small angles to the beams. Therefore, LHCb is ideally suited to study B mesons and baryons with b quarks [7–11], and can supplement the CP violation studies at BABAR.

The experimental environment is quite different from BABAR, with higher particle multiplicity and jets focused in forward direction, but a high precision vertex reconstruction makes good for the increased combinatorial backgrounds. Our group is investigating decays into baryons from B and B_s mesons and Λ_b baryons. These studies can supplement our results obtained with the BABAR detector, but the higher B production rate allows us also to study CP and T (time reversal) symmetries and their violation in these decays [10].

We also look for decays that violate the conservation of baryon and lepton number, but conserve the difference of these numbers, e.g., the decay of the baryon Λ_b^0 to a charged kaon and a μ-lepton. Such processes are predicted to be extremely rare (with probabilities around 10^{-30}) by the Standard Model but could explain the baryon-antibaryon asymmetry in our universe as proposed for the first time by the Russian physicist Andrei Sakharov. Astrophysical measurements (WMAP and Planck) set

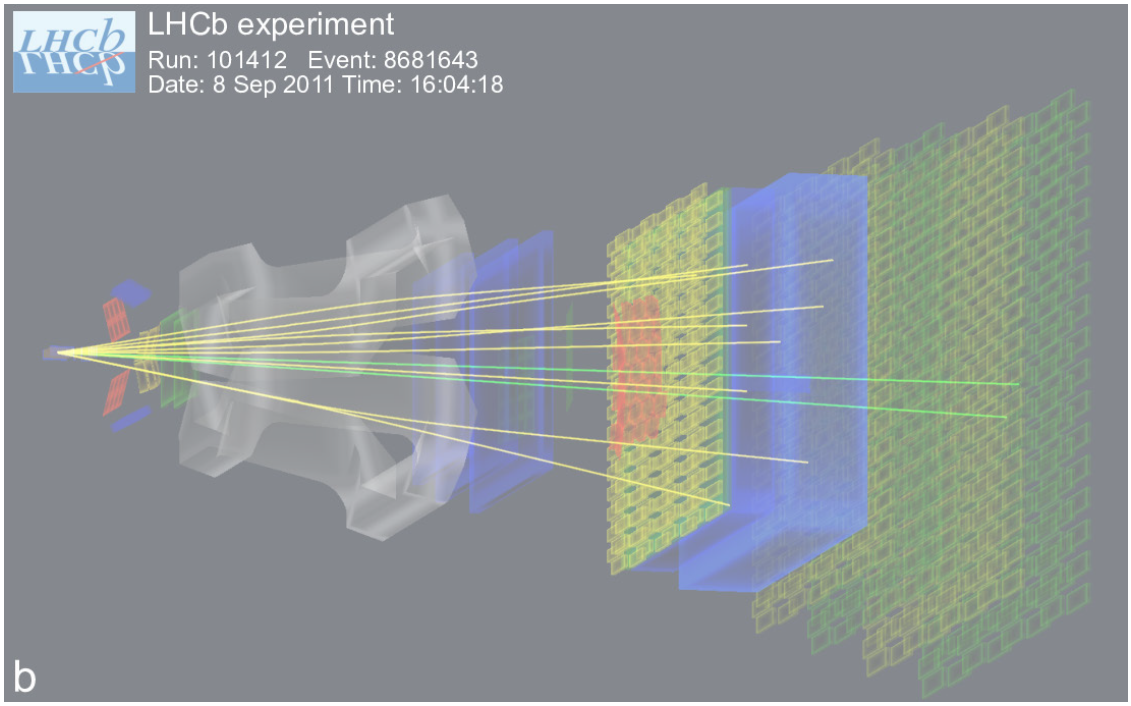

Fig. 2.29: One of a few very rare events observed in a recent analysis of data of the 2011/12 run of the LHCb experiment: The green tracks are two muons from the decay $B_s^0 \to \mu^+\mu^-$, which occurs once within 300 million B_s decays [12]. Some evidence for the even rarer decay $B^0 \to \mu^+\mu^-$, which occurs about once in 3 billion B^0 decays, has also been found.

the order of magnitude for such decays to 10^{-10}, a scale that is accessible by LHCb due to its unique production rate of $\sim 10^{11}$ b hadrons per year. The observation of such processes would prove physics beyond the Standard Model and would provide the missing link to understand the matter-antimatter asymmetry of our universe. A similarly rare decay, $B_s^0 \to \mu^+\mu^-$, has recently been observed at LHCb and CMS at a branching fraction of $3 \cdot 10^{-9}$ consistent with the Standard Model [12]. One event is shown in Fig. 2.29.

Publications

In the years 2013-15, we published 51 articles with the BABAR collaboration and 211 articles with the LHCb collaboration in refereed journals.

Among the more spectacular results are the observation of an unexplained high rate of semileptonic B decay to the heavy lepton tau [13, 14] and the observation of a pentaquark [15], a bound state of four quarks and an antiquark.

There were also two new books published [16, 17].

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2.3 Interfaces and New Materials

2.3.1 Physics of New Materials

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General Outline of the Field of Research

The main interests of the group *Physics of New Materials* are focused on synthesis and investigation of static and dynamic physical properties of novel advanced functional materials. These materials include magnetic nanoparticles [1], quasicrystals, carbides and nitrates, novel implant materials [2–7], catalysts [8, 9], glasses [10–12] as well as nanostructured carbon materials [13, 14]. The synthesis of functional materials is performed applying, e.g., sol-gel method, electric arc melting, mechanical alloying and non-equilibrium hybrid synthesis methods like field-assisted sintering (FAST) or microwave sintering. Physical properties are studied using different scattering techniques with X-rays, synchrotron radiation or neutrons, Mößbauer spectroscopy, differential scanning calorimetry, atomic/magnetic force microscopy, impedance spectroscopy, physisorption and chemisorption analysis or micro- and nanoindentation.

Metals and ceramics for biomedical applications

Pure titanium and titanium-based alloys are nowadays the most attractive metallic biomaterials for orthopedic implants in load bearing sites, as dental and orthopedic implants and heart valves, due to their excellent mechanical properties, biocompatibility and good corrosion resistance. As long-term load-bearing implants in clinic, the incorporation of porous structures into titanium and its alloys may lead to a reliable anchoring of host tissue into the porous structure, and allow mechanical interlocking between bone and implant. Because of their stable surface, oxide film (TiO_2), the Ti alloys are difficult to sinter by traditional sintering techniques. The FAST method gives the opportunity to densify titanium and were used to prepare

the Ti alloys and study their structural and mechanical properties as well as biocompatibility [2–5].

A functional gradient material composed of a dental ceramics and titanium was successfully consolidated using FAST in a two-step sintering process [6]. High energy X-ray diffraction studies on the gradient were performed at High Energy Material Science beamline at DESY in Hamburg. Phase composition, crystal unit edges and lattice mismatch along the gradient were determined from diffractograms, Fig. 2.30, applying Rietveld refinement procedure. These studies showed that a stable transition between titanium and the dental ceramics had been achieved.

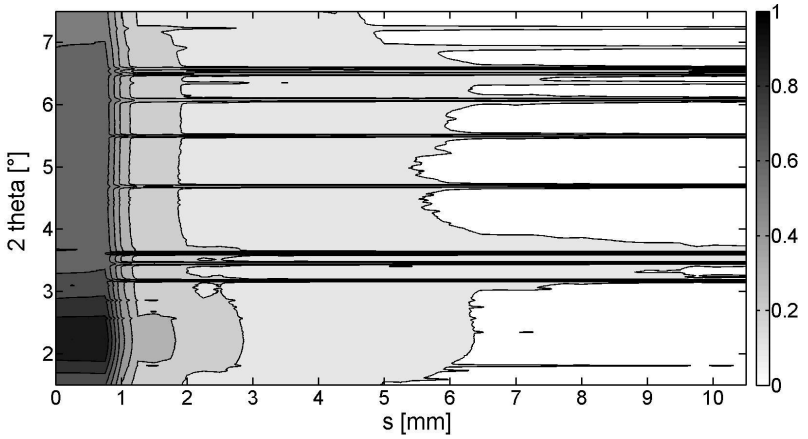

Fig. 2.30: Evolution of the high energy diffraction pattern along the whole gradient sample [6].

Calcium titanate is a potential electrically active implant material [7]. However, in a typical bulk form, it does not show the piezoelectric effect. Studies on nanostructured $CaTiO_3$ confirmed that the reduction of the crystallite and grain sizes results in a piezoelectric-like effect comparable to the one observed in a bone tissue, which can lead to much better interaction between the implant and the bone itself.

TiO_2 as catalyst

It is generally accepted that the theoretical model of photocatalysis on a TiO_2 surface consists of different consecutive steps, where each one is essential for the activity and the efficiency of the photocatalyst [8, 9]. In the initial step of the photocatalytic process, electron-hole pairs are generated upon irradiation of the material with photons of energies that are at least equal to those of the band gap values. In the second step, the formed electron-hole pairs can either recombine in the bulk or diffuse to the surface, where they can participate in chemical reactions. In this step, the lifetime and the velocity of the electron-hole recombination is crucial. Charge carrier traps are used to promote the trapping of electrons and holes at the surface leading to recombination suppressing and to more efficient charge transfer processes. The next step is the creation of $H^{\bullet\star}$ and $OH^{\bullet\star}$ radicals as a result of the

electron-hole interaction with water and, finally, a probable multiple step reaction of organic compounds with active radicals. The electron transfer process is more efficient if the species are pre-adsorbed on the surface. However, so far, the influences of the different stages of this model on the final efficiency of the photocatalysts were not well determined.

The photocatalytic activities of Degussa P25 powders annealed at various temperatures in vacuum and air were studied. Their compositions, crystal structure and specific surface areas were determined by XPS, XRD and BET, respectively. It was shown that the photocatalytic activity of P25 powders is significantly enhanced after annealing in vacuum [9]. The kinetic coefficient can be raised by 75 % during annealing at 400°C.

Structures of glasses

Diffraction studies for clarifying the atomic structure of oxide glasses are more and more concerned with materials that are formed of three or more oxides. The analysis of the short-range order is made by determination of parameters of the first-neighbour peaks. The overlap of the peaks of different pairs of atoms often does not allow determining the pair distances and coordination numbers. But sometimes, the peaks of the different pairs exhibit different distances and reliable coordination numbers can be obtained [10, 11]. The combination of X-ray and neutron diffraction helps in special cases [10, 11] where only few peaks overlap and a change of contrast is available for different radiation sources. Moreover, the large range of scattering vectors helps to avoid the broadening of pair peaks due to the termination effect of Fourier transformations.

An important result was obtained for the behaviour of the distortions of NbO_6 polyhedra in dependence on the Nb_2O_5 content [10]. Glassy materials that contain Nb_2O_5 are interesting for applications due to their strong non-linear optical indices. The strange distortions of the NbO_6 octahedra in case of small Nb_2O_5 content are explained with the special distributions of the bond valencies in the Nb-O-P bridges with the neighbouring PO_4 tetrahedra. The investigation of the Na_2O-GeO_2-P_2O_5 glasses was aimed at demonstrating the formation of a majority of GeO_6 octahedra in the glasses studied. The fractions of the GeO_6 and GeO_4 units change continuously in dependence on the GeO_2 content. The available number of oxygen atoms for Ge-O-P bridges determines the GeO_6 fraction.

Iron phosphate glasses are presently being considered as matrices for the storage of radioactive waste, even of that which cannot be vitrified using conventional borosilicate waste glass. Phosphate glass with a composition $60P_2O_5$-$40Fe_2O_3$ was investigated and a structural model was proposed [12]. The model is based on the crystal structure of $FePO_4$, which is composed of $[FeO_4][PO_4]$ tetrahedral rings. The rings were optimized using the DFT method and the obtained theoretical FTIR and Raman spectra were compared with their experimental counterparts. Moreover, the proposed model is in good agreement with X-ray absorption fine structure spec-

troscopy and Mössbauer spectroscopy measurements. According to the calculations, the Fe^{3+} is in tetrahedral and five-fold coordination. The maximal predicted load of waste constituents into the glass without rebuilding of the structure was 30 mol %. Below this content, waste constituents balance the charge of $[FeO_4]$–tetrahedra, which leads to their strong bonding to the glass resulting in an increase of the density, chemical durability or transformation and melting temperatures.

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2.3.2 Polymer Physics

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General Outline of the Field of Research

The Polymer Physics group is highly specialized in advanced calorimetry and thermodynamic modelling of glass transition and nucleation. The activities are in conjunction with the competence center Calorimetry and Thermal Analysis, Rostock (CALOR), Department Life, Light & Matter (LL&M), Interdisciplinary Faculty, University of Rostock. Calorimeters covering a dynamic range from $10^{-5}\,\mathrm{Ks}^{-1}$ up to $10^{7}\,\mathrm{Ks}^{-1}$ in cooling and heating are available and are used to study solidification, melting as well as vaporization of different materials [1–6]. Modeling by thermodynamics of irreversible processes and a generalization of the classical Gibbs approach is applied to the description of glass transition [7, 8] and crystal nucleation [9].

Crystal nucleation in polymers and metals

Nature gives numerous examples of materials whose performance is based on ordered arrangements of different submicron phases. Combined properties of bones or wood are still unsurpassed by synthetic matter in numerous applications. Low density, strength, biocompatibility and cost-efficiency often exclude each other in plastics or metal alloys. One possible solution for tailoring such properties is through different pathways of ordering during solidification from the melt. For example, crystal nucleation as well as the growth and reordering processes ultimately determine the internal structure and thus the properties of the final solid.

In order to shed light on this circle of problems we are studying homogeneous crystal nucleation by our fast scanning calorimetric methods [2, 6]. By overcritical quenching we did not only succeed to avoid crystallization and to reach the amorphous state for most fast crystallizing polymers. We have demonstrated that often a second critical cooling rate exists, which defines the limit for homogeneous nucleation [10]. Having samples at hand not containing nuclei created during cooling, gives us the opportunity to study homogeneous nucleation in detail.

Beside, thermodynamic modeling of glass transition and nucleation is successfully performed [9, 11, 12].

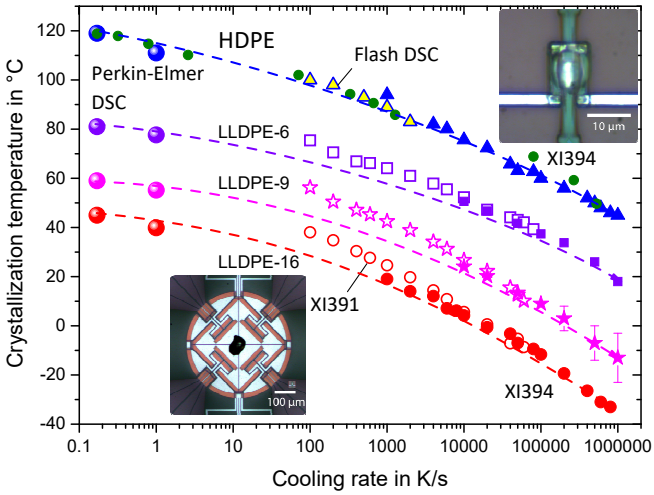

Fig. 2.31: Crystallization peak maximum temperature of high density polyethylene (HDPE) and linear low density polyethylene (LLDPE) with different content on 1-octene, as is indicated in the legend, as a function of the cooling rate. The use of different devices is indicated.

Ultra-stable Glasses

It was recently discovered that highly stable glasses of organic molecules can be prepared by means of physical vapor deposition (PVD) at substrate temperatures near $0.85T_g$. The vapor-deposited glassy films can exhibit extraordinary features relative to ordinary liquid-cooled glasses, which include higher kinetic stability, lower enthalpy, lower heat capacity, higher density, and reduced inert gas permeation. The basis of the increased stability of a glass is attributed to enhanced surface mobility, with newly deposited molecules having the ability to efficiently sample different minima of the potential energy landscape before being buried by other molecules during the deposition process.

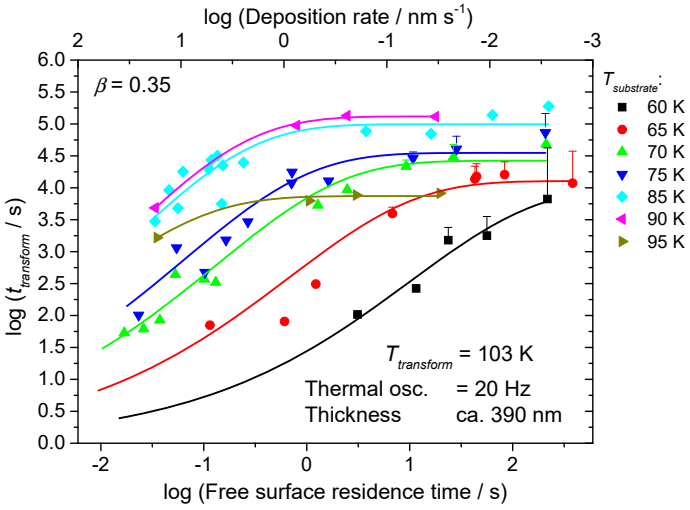

Fig. 2.32: The time needed for the isothermal transformation of ethylcyclohexane from the stable glass to the supercooled liquid as a function of free surface residence time, which is the time needed to deposit one monolayer. The free surface residence time is calculated from the deposition rate, which is given on the top axis.

We use PVD to prepare glasses of toluene [13], ethylbenzene [13], ethylcyclohexane [5] and tetrachloromethane, a simple organic molecule with a nearly isotropic molecular structure. *In situ* AC nanocalorimetry was used to characterize the vapor-deposited glasses. Glasses of high kinetic stability were produced by deposition near $0.8T_g$. The isothermal transformation of the vapor-deposited glasses into the supercooled liquid state gave further evidence that tetrachloromethane forms glasses with high kinetic stability, with the transformation time exceeding the structural relaxation time of the supercooled liquid by a factor of 10^3. The successful formation of PVD glasses of tetrachloromethane which have high kinetic stability gives a strong indication that molecular asymmetry is not a prerequisite for stable glass formation.

Vapor pressure determination of extremely low volatile compounds, e.g., ionic liquids, is challenging and time-consuming using conventional techniques. Particularly, ionic liquids tend to decompose already at temperatures where the vapor pressure is still very low. Standard methods for the determination of evaporation rates are thus limited to temperatures below the decomposition temperature, where evaporation proceeds very slowly. We were able to overcome this limitation using differential fast scanning calorimetry on very short time scales in inert atmospheres [3]. The method is based on the relatively fast evaporation of nanogram samples, exhibiting a significantly enhanced (up to a factor of 10^4) surface-to-volume ratio compared to conventional thermogravimetric samples. Due to extremely high heating rates, the sample is exposed to the thermal stress only for milliseconds. In these conditions the evaporation dominates in the mass loss even at temperatures above the possible onset of the decomposition process. In addition, since the method allows very high scanning rates (up to $10^6\,\mathrm{Ks}^{-1}$), evaporation of the samples on the way to and from the evaporation temperature is avoided and thus much higher temperatures can be reached in the measurement of the mass loss rate as compared to conventional methods. The absolute vapor pressures of several aprotic and protic ionic liquids were measured [3, 14].

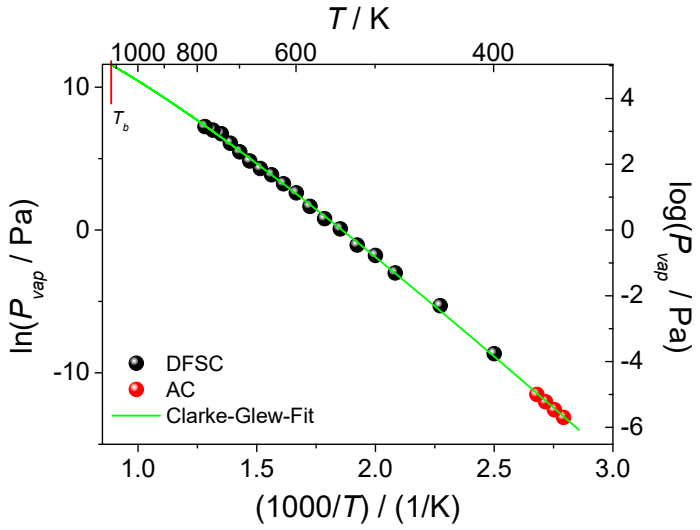

Fig. 2.33: Comparison of the vapor pressure data for [EMIm][NTf2] determined by AC calorimetry (red points) and DFSC (black points). The green solid line represents the Clarke-Glew-fit corresponding to the measured vapor pressures. It permits a reliable estimate of the boiling temperature $T_b = (1120 \pm 50)\,\mathrm{K}$.

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2.3.3 Physics of Nano- and Biomaterials

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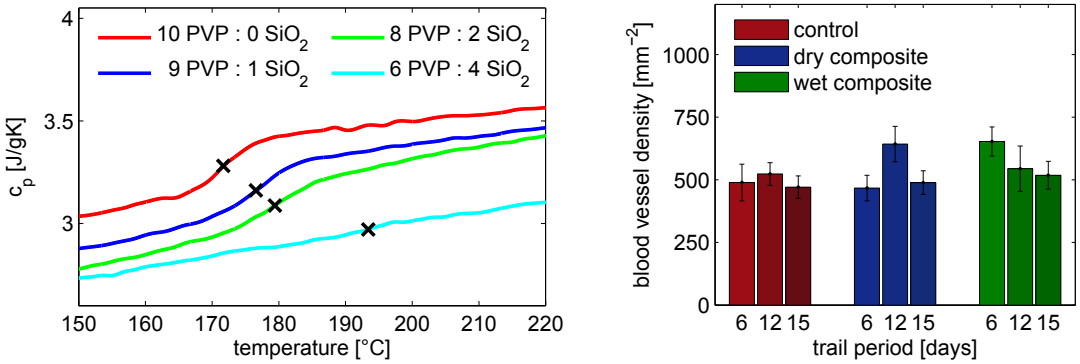
General Outline of the Field of Research

The main topic of our research is the structure analysis and development of nanoscaled materials. The investigations are performed using X-ray tomography, X-ray diffraction (SAXS and WAXS), scanning and transmission electron microscopy including spectroscopy (EDX and EELS) and electron diffraction. The sol-gel process is the key technique for manufacturing nanostructured materials. The improvement of the acceptance of a synthetic material in living tissue is of great importance. Therefore, we developed a synthetic nanostructured biomaterial with special properties. The interaction between the synthetic material and autological proteins is achieved by using a synthetic matrix of defined porosity. The special properties of the matrix are the reason for a high bioactivity. This activity stimulates the differentiation of adult stem cells and the formation of various tissues [1–6]. The cross-disciplinary research projects are cross-disciplinary efforts that draw together working groups of our faculty and the faculty of medicine, including physicists, chemists, biologists and physicians.

Polymer-silica nanocomposites for wound dressing

Nanostructured silica is essential for tissue growth and regeneration. Therefore we developed a nanocomposite from PVP (polyvinylpyrrolidone) and silica nanoparticles for soft tissue regeneration. The silica nanoparticles are derived from sodium silicate solution and are 1.3 - 1.6 nm in size. Fig. 2.34a shows the specific heat capacity over temperature of the composite with different silica content. The rise of the glass transition temperature with higher silica content points to a cross-linking between the polymer chains by the silica nanoparticles. The decreasing step in specific heat capacity is not only due to decreasing PVP content, but also caused by a formation of a rigid amorphous fraction of the PVP around the silica nanoparticles. Two wound dressings made from the polymer-silica nanocomposite were tested in a skin-defect model on mice. Fig. 2.34b shows the blood vessel density in dermal wounds on different days. The growth of the blood vessels at early wound heal-



(a) Differential scanning calorimetry of differently composed polymer-silica composites with the glass transition temperature (×).

(b) Blood vessel density in dermal wounds of mice on different days and with different wound dressing materials.

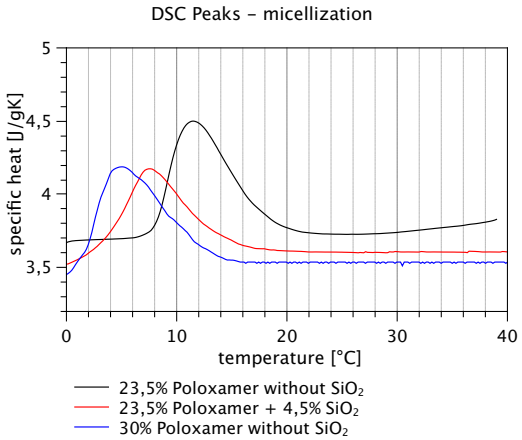
Fig. 2.34: Calorimetry and animal studies on a polymer-silica nanocomposite.

ing stages is accelerated in wounds, which were treated with wet composite wound dressings. Also the size of the remaining scar was significantly smaller.

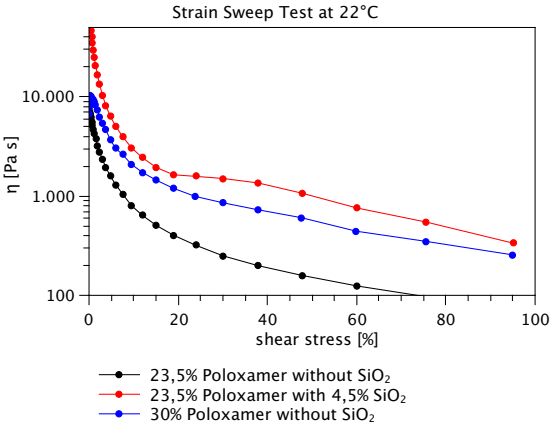
Polymer-based carrier material for improved application of bone substitutes

NanoBone S39 (NBS) granules are difficult to handle, to contour into desired shapes, and to keep in the defects. Inert polymers such as poloxamer are suitable for binding the granules and hence improving their handling characteristics [7, 8]. Poloxamer 407 is a nonionic triblock copolymer with many pharmaceutical applications, as it is nontoxic and biocompatible with cells and body fluid. The Poloxamer consists of a central hydrophobic block of polypropylene glycol flanked by two hydrophilic blocks of polyethylene glycol. The stability of the Poloxamer at various temperatures can be detected by Differential Scanning Calorimetry (DSC). The plot of the specific heat as a function of temperature shows an endothermic peak at the temperature of gel formation. In Fig. 2.35a, the red curve corresponds to the Poloxamer concentration of 23.5 % with the addition of 4.5 % SiO_2. The gel formation temperature is 7.5°C, which in the favored temperature range. A Poloxamer gel without SiO_2 requires a higher Poloxamer concentration to form a gel (blue curve), or the gel transition temperature moves to higher values (black curve). So a Poloxamer-SiO_2 gel has improved handling properties, while the polymer concentration is minimized.

The following viscoelastic measurements demonstrate that some particular addition of SiO_2 to Poloxamer increases the viscosity of the gel. This ensures that better handling properties are achieved with a smaller amount of Poloxamer. In Fig. 2.35b, the viscosity, η, is plotted as a function of shear stress. It can be seen that the viscosity is greatly increased with addition of SiO_2 to the Poloxamer gel. A 23.5 % Poloxamer gel with the addition of 4.5 % SiO_2 has approximately the same viscosity as a 30 % Poloxamer gel and significantly greater viscosity than a 23.5 %



(a) Differential scanning calorimetry of different Poloxamer solutions



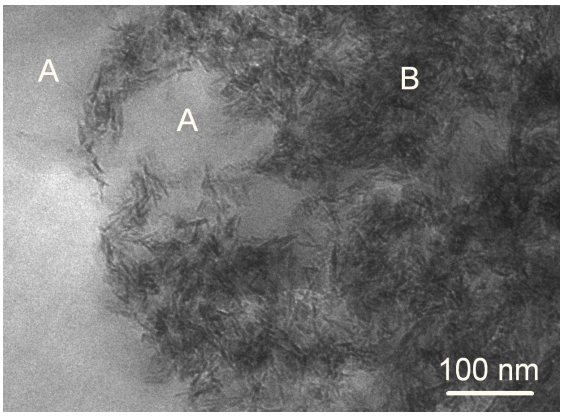
(b) Strain sweep test of the viscosity of gels at a temperature of 22°C.

Fig. 2.35: Mechanical properties of Poloxamer solutions with and without SiO_2.

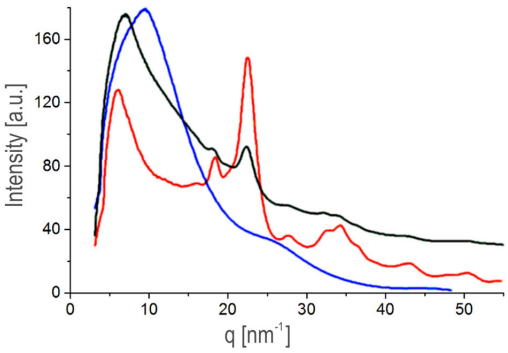
one. For a clinical application this means that the biomaterial is more mechanically stable and defects can be more completely filled.

Nanostructured coating on PEEK surfaces

PEEK (polyether ether ketone) as a semi-crystalline biomaterial is characterized by its very good mechanical and thermal properties. It has a bio-inert character due to its chemical stability. As a result, a bad bone-implant contact occurs in orthopedic



(a) Transmission electron micrograph of the interface between layer and implant (A – PEEK; B – silica hydroxyapatite).



(b) Electron diffraction curves of the PEEK surface after short melting and fast cooling (blue), the silica-hydroxyapatite layer (red) and the interface (black).

Fig. 2.36: Nanostructure of a PEEK silica-hydroxyapatite interface.

implants, which prevents a permanent bone integration. For this reason the aim of

this work was a bioactive coating on PEEK implants [9]. The spin-spray technique produces a nanoporous SiO_2 layer in which hydroxyapatite crystallites are embedded. It is now essential to create an interface between the layer and the PEEK surface. The polymer must penetrate the nanopores and thus form a composite of PEEK, SiO_2 and hydroxyapatite. The development of this interface is documented with transmission electron microscopy and electron diffraction. Figure 2.36a reveals that the PEEK penetrates into the nanopores of the material. The electron diffraction, Fig. 2.36b, documents that the PEEK surface is a pure glass, since no Bragg reflexes are detectable. Instead the curve shows an amorphous maximum at $12\,\mathrm{nm}^{-1}$. The electron diffraction curve of the interface is not a superposition of the PEEK curve and the curve of the layer. The diffraction peak at $12\,\mathrm{nm}^{-1}$ is no longer detectable. Obviously the mobility of the polymer chains in the nanopores is restricted, so that the relaxation is not possible.

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2.3.4 Physics of Surfaces and Interfaces

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MSc Graduates:	Kevin Oldenburg	Vents Valle
	Tamam Bohamud	Björn Vogler
MSc Staatsexam:	Lukas Rathje	
BSc Graduates:	Björn Vogler	Kai Wardelmann
	Heinrich Behle	Hanna Kolkmann
	Clemens Schindler	Christian Zietlow
	Christian Völkner	Hannes Wernicke
	Miriam Marsch	

* at Radboud U Nijmegen

General Outline of the Field of Research

The research program of the group is dedicated to unravel mechanisms and processes in the coupling of physical, chemical, and biologic structures on the nanometer scale. This includes excitation and transport in composite structures at surfaces made up of metal nanoparticles, molecule aggregates and proteins. We seek to elucidate the influence of the local environment on the respective processes underlying energy transfer, chemical reactions, and biophysical interactions. The studies require local probing approaches, such as scanning probe microscopy, adapted for the specific system and environment of the process under study.

Scanning Probe and Correlative Microscopy

Scanning probe microscopy methods provide the opportunity to study and modify nanoscopic landscapes down to molecular or atomic scale. Our studies range from wave function mapping with atomic precision at low-temperatures and ultra-high vacuum to transport measurements and manipulation in liquids, with conditions similar to those in living cells. Key issues concern spatial resolution, probing specificity, structuring, and adaptation to special environmental conditions [1–5]. Accessing different information channels from the very same region or structure on the surface enables exploration of complex mechanisms and interplays. This is pursued by the so-called correlative microscopy, which merges morphological, optical, and spectroscopic data, e.g., from scanning probe, photoelectron, and luminescence maps, (Fig. 2.37). At nanoscopic dimensions this approach requires proper navigation and setting of landmarks.

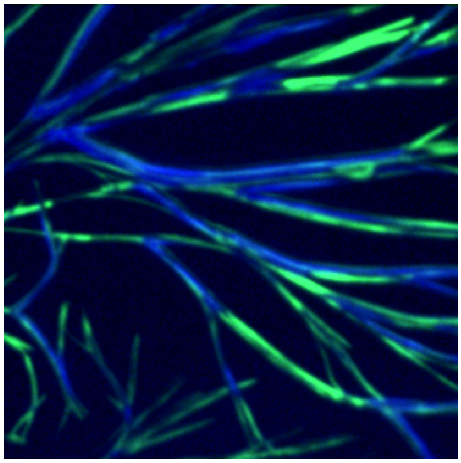

Fig. 2.37: Composite image of porphyrin aggregates showing the total electron yield from photoemission electron microscopy in the green color channel, and the optical fluorescence yield in the blue channel. Green areas indicate the presence of dark states which do not decay via luminescence. Image size: $30 \times 30\,\mu\mathrm{m}^2$.

Transport of Excitations in Molecular Aggregates

Light-matter interaction can result in a variety of phenomena, such as collective electron oscillations in metals, excitons in molecules, or electron-hole pairs in semiconductors. We are interested in effects arising from the coupling among these phenomena and their interaction with inhomogeneities of the surrounding system. We aim at real-space visualization of exciton transport in molecular aggregates by means of photoemission electron microscopy (PEEM). Metal nanostructures serve as well-defined local excitation sources for excitons in adjoining molecular aggregates. In comparison to fluorescence microscopy, PEEM directly detects the electron occupation rather than deexcitation channels from excited states. This provides an additional, complementary information enabling direct comparison of state occupation and deexcitation (see Fig. 2.37).

Nanostructuring Molecular Layers

Self-assembly of molecular aggregates is a convenient approach to arrive at nano- or mesoscopic structures. However, control over the aggregation is limited. To address questions how anisotropy, electronic properties, structure motifs, and geometric restrictions affect exciton propagation, creation of well-defined molecular nanostructure landscapes is important. We aim at combining long-range ordering by self-assembly and modification by nanolithography techniques, potentially enabling landscapes for controlled confinement and guidance of charges, light, and excitations. Local excitation can be achieved by plasmonic structures, such as arrays of nanotriangles prepared by nanosphere lithography (Fig. 2.38, left). An indication

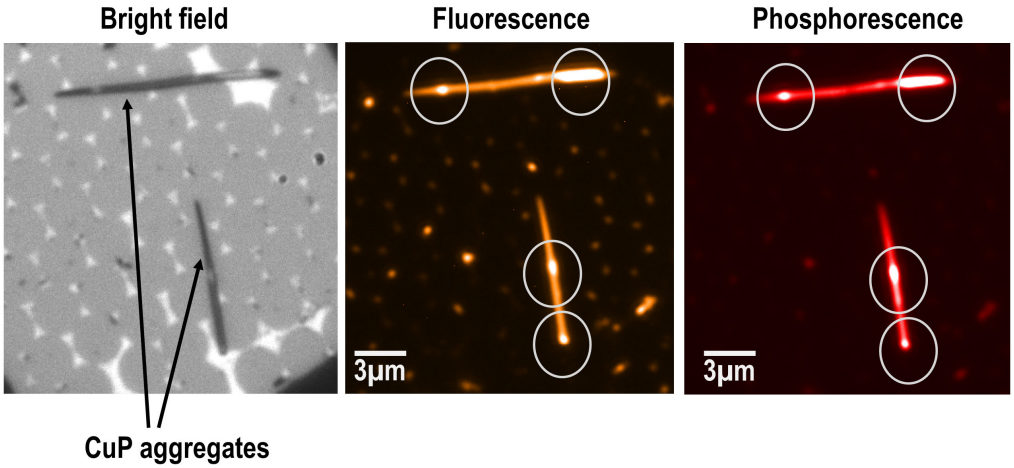

Fig. 2.38: Left: Optical bright-field image of metal structures prepared by nanosphere lithography with dye aggregate whiskers on top. Center, right: Fluorescence and phosphorescence images, respectively, from the same sample location.

of plasmon-exciton coupling is enhanced fluorescence of the molecule aggregate at the sites of plasmonic near fields. Using spatially-resolved fluorescence detection, different local configurations can be compared to each other, enabling identification of active sites and extraction of enhancement factors within a single measurement (Fig. 2.38, center). Triplet states are particularly promising candidates for long-range exciton mobility beyond the Förster mechanism. Hence, phosphorescence at larger wavelengths, in comparison to shorter-wavelength fluorescence, is suited to select potential molecule species and configurations for exciton transport (Fig. 2.38, right). Such data serve as a basis for studying the interplay of spatially-dependent excitation, exciton transport, and optical guidance in nano- and microstructured molecule assemblies.

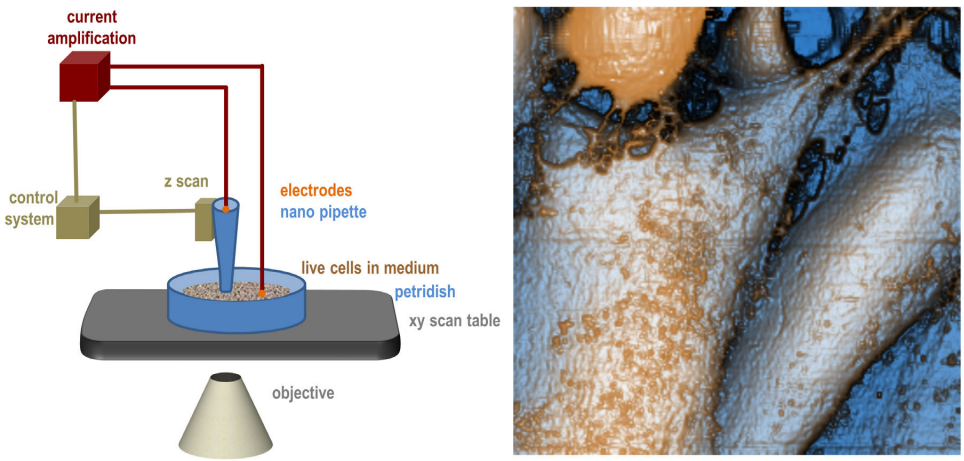

Fig. 2.39: Left: Experimental setup of SICM. Right: Topography ($45 \times 45 \times 3\,\mu m^3$) of live osteoblasts exhibiting characteristic features on the cell surface and in the intercellular region.

Interaction of Live Cells at Surfaces

Ion flow through nanopipettes represents an extremely gentle type of local interaction suitable for nanoprobing on very soft material surfaces, i.e., on live cells. Unlike atomic force microscopy, in Scanning Ion Conductance Microscopy (SICM) hardly any appreciable forces are applied. This means that the measured nanomorphology and functional maps reflect the undistorted situation of the live cell in the medium (Fig. 2.39). The ion current through the nanopipettes depends on the distance from insulating objects and on the local ion concentration. The spatial resolution is determined by the diameter of the nanopipettes, which are prepared from borosilicate in a laser-based puller. Osteoblasts are seeded and cultured on a surface in a Petri dish. We study morphological changes at migration fronts of osteoblasts on the nanoscale in response to triggers such as geometric, molecular, and electric field landscapes.

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2.4 Institute of Atmospheric Physics Kühlungsborn

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Dr. Axel Gabriel	Dr. Almut Gaßmann	Dr. Michael Gerding
Dr. Mykhaylo Grygalashvyly	Dr. Jens Hildebrand	Dr. Josef Höffner
Dieter Keuer	Dr. Johannes Kiliani	Dr. Rahel Knöpfel
Dr. Fazlul Laskar	Dr. Ralph Latteck	Dr. Jens Lautenbach
Dr. Qiang Li	Dr. Vivien Matthias	PD Dr. Dieter Peters
Dr. Manja Placke	Dr. Toralf Renkwitz	Dr. Urs Schaefer-Rolffs
Dr. Andrea Schneidereit	Dr. Gunter Stober	Dr. Boris Strelnikov
Dr. Irina Strelnikova	Dr. Marius Zecha	Dr. Christoph Zülicke

plus 22 PhD students and 19 master/bachelor students

General Outline of the Field of Research

The main task of the Institute of Atmospheric Physics (IAP) at the Rostock University is to conduct research in the field of atmospheric physics. The atmosphere is a multi-faceted and often quite variable medium of complex behavior. Its great complexity gives us the opportunity to seek niches in international research activity where even comparatively small investments can yield distinctive and interesting contributions to a deeper understanding of the atmosphere. The IAP emphasizes research in the areas of (a) the mesosphere and lower thermosphere, in particular at polar latitudes, (b) the dynamical coupling between the troposphere, stratosphere, and mesosphere, and (c) long-term changes of the thermal and dynamical structure in the middle atmosphere (∼10–120 km).

The main building of IAP being located in Kühlungsborn provides modern offices, laboratories, high speed computer facilities, and administrative and technical infrastructure (see Fig. 2.40). Field measurements are performed primarily here and at the institute's field station in Juliusruh (on the island Rügen) as well as at the ALOMAR observatory in Northern Norway. ALOMAR hosts instruments from several international institutes and is located close to the Andøya Space Center (69°N,16°E), poleward of the Arctic circle. The IAP also operates a mobile lidar[1] in a container which was stationed at various locations, more recently in Davis (69°S,78°E), Antarctica. The instrumentation at IAP mainly consists of lidars at various frequencies from the infrared to the ultraviolet range of the electromagnetic spectrum and several radars with frequencies between 100 kHz and 1 GHz. Furthermore, instruments

[1] Lidar: laser induced detection and ranging

Fig. 2.40: The main building of the IAP headquarter in Kühlungsborn showing laser beams of various lidars.

are installed on sounding rockets to measure neutral and plasma number densities in the mesosphere and lower thermosphere. Balloon borne measurements of turbulence in the stratosphere are performed at various field stations. The IAP performs model calculations and theoretical studies for a better physical understanding in the aforementioned areas of research, with emphasis on the interpretation of local phenomena in a global context. This includes the development of specially designed numerical models and cooperation with the experimental investigations. The scientists at IAP cooperate with several international research institutes and universities both on experimental and theoretical aspects of atmospheric physics. Typically 90 individuals were employed at the IAP, amongst them 22–26 scientists and 28–35 students.

In the following we provide some examples of typical research results in the three departments of the IAP. More details can be found on the website of the institute (www.iap-kborn.de) and in 130 scientific papers published by IAP scientists in the period 2013–2015.

Optical sounding of the Atmosphere (Prof. Dr. Franz-Josef Lübken)

The main areas of research in this department are the exploration of (a) the Arctic middle atmosphere at approximately 10 to 120 km altitude, (b) the thermal structure of the mesopause region at various latitudes,[2] (c) ice clouds in the mesopause region known as "noctilucent clouds" (NLC), and (d) turbulence in the lower stratosphere. Field measurements are performed by a number of lidars and by instruments

[2]Mesopause: pronounced temperature minimum near 90–100 km altitude.

mounted on balloons. New developments in lidar technology have allowed us for the first time to measure temperatures and winds in the middle atmosphere simultaneously [1]. In recent years we have established a new technique to measure turbulence in the stratosphere by *in situ* observations on balloons [2]. A global scale model called LIMA (Leibniz Institute Model of the Atmosphere) is used to interpret ice cloud measurements, their connection to background conditions, and long term trends [3].

As an example of capabilities of modern lidars we present in the following some results from our mobile iron resonance lidar which was located at Davis, Antarctica, from November 2010 until the beginning of 2013. These observations provided unprecedented details about the thermal structure of the middle atmosphere and the morphology of the iron layer. Here we concentrate on temperatures in the mesopause region, in particular during the summer season when daylight conditions prevail at polar latitudes. There are only very few lidars worldwide which are capable of making measurements under these conditions. In total we now have 2900 hours of unique temperature data from Antarctica.

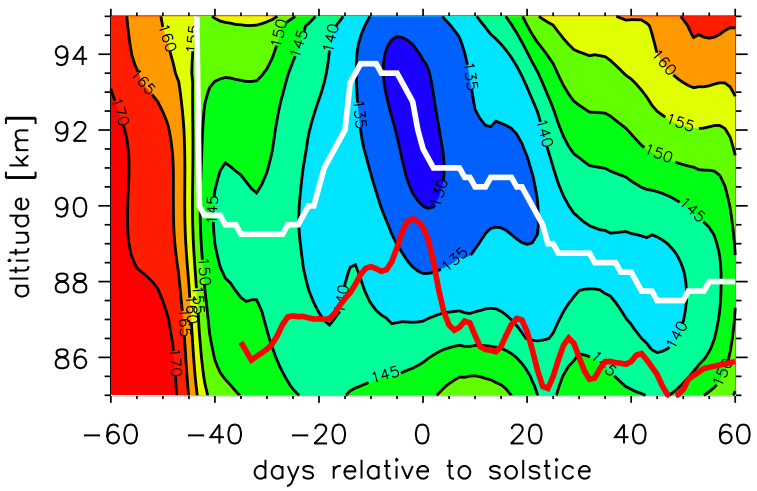

Fig. 2.41: Seasonal variation of lidar temperatures at Davis (69°S), Antarctica, during the winter/summer transition 2011/2012. White line: mesopause altitude, red line: peak height of the PMSE layer (see text for more details). From *L*übken et al., Geophys. Res. Lett., 2014.

In Fig. 2.41 smoothed lidar temperatures during the winter/summer transition in 2011/2012 at mesopause altitudes are shown [4]. At first, this region gets colder as is expected from similar measurements in the northern hemisphere. Note that at polar latitudes the mesopause is generally cold in summer and 'warm' in winter. Around solstice, however, the mesopause height increases abruptly ('jumps') to approximately 93 km and temperatures decrease below 130 K. In this period the

mesopause is located at unusually large altitudes ('elevated mesopause'). At the same time the mean altitude of strong radar echoes known as 'polar mesosphere summer echoes' (PMSE) increases. PMSE are linked to charged ice particles which can only exist in the middle atmosphere at temperatures below $\sim 150\,\mathrm{K}$. This allows one to study the temporal development of the thermal structure also in years when lidar observations are not available. Mesopause jumps as described above have never been observed before.

In the meantime we have collected more information, e.g., wind measurements in the mesosphere from an MF radar at Davis, and have performed model simulations to explain this unique behavior [5]. It turns out that the circulation in the stratosphere plays a crucial role in this context because it controls which part of the gravity wave spectrum from the troposphere can reach higher altitudes. Gravity waves are excited in the troposphere, propagate to higher altitudes where they finally deposit momentum and energy. In Antarctica and in a period around solstice gravity waves sometimes encounter special wind conditions, not only in the stratosphere but also in the mesosphere. This lets waves with relatively high phase speeds pass the stratosphere. Since mesospheric winds are rather low, the intrinsic wavelength is large which supports undisturbed propagation of gravity waves into the lower thermosphere. These gravity waves therefore break at extraordinary high altitudes and produce the mesopause jump observed by our lidar. The unique combination of stratospheric/mesospheric winds and the associated mesopause jump has never been observed in the northern hemisphere.

The overall relevance of these observations is their importance in studying the role of gravity waves in the dynamical coupling mechanism of the lower and middle atmosphere. This process is crucial for our understanding of the atmosphere. Note that during summer gravity waves drive the mesopause region away from radiatively controlled conditions by more than 120 Kelvin. Our observations have several implications. For example, comparisons of satellite measurements in the northern and southern hemisphere must be taken with care and should consider the special situation described above. For example, a comparison of NLC altitudes in both hemispheres is severely biased if periods of an elevated mesopause are not properly taken into account.

Radar and Rocket Borne Soundings of the Atmosphere (Prof. Dr. Jorge Chau)

The main research areas of the department are: (a) exploration and understanding of the Mesosphere and Lower Thermosphere (MLT) dynamics, (b) understanding of the microphysics of MLT layering phenomena associated to meteoric input, (c) MLT coupling with the lower and the upper atmosphere, (d) turbulence in the upper troposphere and lower stratosphere as well as in the mesosphere, (e) long-term changes of the observed dynamical features, and (f) studies of meteor radar echoes from an atmospheric and an astronomical point of view. The measurements needed to carry

out these activities are obtained from a variety of specialized radars and by instruments on board rockets. The temporal and spatial coverage of our research have a wide range, going from small scales (micrometers, few seconds) to large scales (few thousands of kilometers, years). In the case of large scale processes, our studies are complemented with satellite observations, reanalysis data, and modeling data.

Radars play an integral part in the studies of the dynamics of the MLT region at IAP. They observe not only the altitudes of interest, but also can operate under all sky conditions (i.e., with or without clouds). IAP radars are a combination of commercially available systems that allow continuous and long-term measurements, and are specialized one-of-a-kind systems that permit unique measurements of the MLT worldwide. Examples of the latter systems are (1) MAARSY, that is currently the most modern and versatile radar to study the polar middle atmosphere, and (2) MMARIA (Multi-static Multi-frequency Agile Radar for Investigations of the Atmosphere), which has provided for the first time horizontally-resolved MLT winds over regional scales instead of mean point measurements.

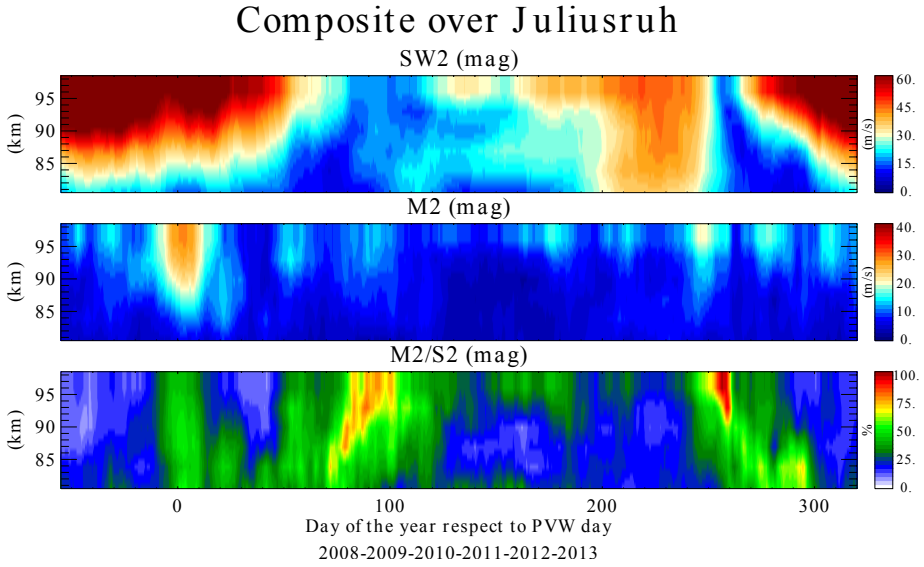

Fig. 2.42: Composite values from observations between 2008 to 2013 over Juliusruh, obtained with respect to the PVW day of each year for (top) Solar semidiurnal tide (SW2), (middle) semidiurnal lunar tide (M2), and (bottom) the ratio of M2/SW2. Note that the color distribution is not the same for SW2 and M2 results. From [6].

One of our most recent research result that takes advantage of our continuous and multi-site measurements has been the identification of the semidiurnal tide signature at MLT altitudes. Such signatures have been observed previously by other research groups, but its relevance has been neglected since on an annual basis its amplitude is much smaller than other tidal contributions. However, from six years of observations at a mid latitude and at a high latitude station, we have found that the semidiurnal

lunar tide at MLT altitudes reaches sometimes amplitudes comparable to the well-known solar semidiurnal tide, predominant at the latitudes of interest [6].

Besides the identification, we have found that the observed lunar tide enhanced amplitudes are highly correlated to the timing of the stratospheric polar vortex weakening (PVW), which in turn is related to the large vertical coupling phenomenon called sudden stratospheric warming (SSW). The lunar tidal signature is always present, modulated by the phases of the Moon. However, strong wind changes in the stratosphere, particularly in the northern hemispheric winter, shift the so-called Pekeris resonance peak of the atmosphere to 12.42 hours, which is the Moon period, causing the observed amplification. Figure 2.42 shows the composite values of six years over Juliusruh (Northern Germany) for: (a) the solar semidiurnal tide, (b) the semidiurnal lunar tide, and (c) their ratio. Note that the lunar signature is the strongest around PVW times. Around transition times it is small but comparable to the observed solar tide amplitudes.

Lunar tides being amplified in the MLT are important in the observed ionospheric and thermospheric changes (electron density, electric fields, composition) at low and mid latitudes [7]. Such changes could be more than 50–100 % than the expected variability around polar vortex weakening events, i.e., around SSW. More recently, the lunar tide signature has also been identified in reanalysis data, starting at sea-surface levels and increasing exponentially in altitude starting around 10 km. Our lunar tide research is an example of atmospheric coupling, connecting altitudes (from the sea surface up to ionospheric altitudes) and latitudes (polar to equatorial).

Theory and Modeling (Prof. Dr. Erich Becker)

The main research topic of this department is the dynamical coupling between the lower atmosphere (troposphere, 0–10 km) and the middle atmosphere (stratosphere, 10–50 km, and mesosphere, 50–100 km) with emphasis on long-term variability and small-scale dynamical processes. The dynamical coupling of atmospheric layers is controlled by waves of different temporal and spatial scales. These waves originate mostly in the troposphere; they propagate upward and dissipate at higher altitudes, giving rise to the so-called wave-mean flow interactions and feedbacks on the troposphere. In addition, the atmosphere is vertically coupled by the transport and mixing of chemically and radiatively active minor constituents, as well as by radiative transfer. IAP develops its own global and regional circulation models that are equipped with specific theoretical and numerical features in order to address scientific questions that are in the focus of IAP. For example, we need to simulate the general circulation of the atmosphere from the surface to the lower thermosphere (about 130 km altitude) and thereby cover a huge range of spatial temporal scales, i.e., from the planetary scale down to small-scale gravity waves (about 100 km horizontally and a few 100 m vertically). This demand includes special descriptions of unresolved dynamical scales, radiative transfer, photo-chemistry, and other relevant processes [8].

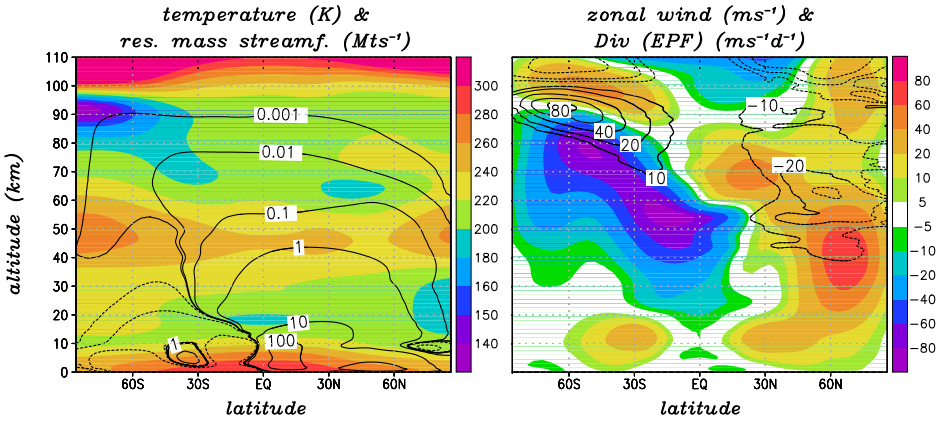

Fig. 2.43: Temporally and zonally averaged fields during January as simulated with the new version of the KMCM with resolved gravity waves. (a) Temperature (colors, unit K) and residual mass streamfunction (contours drawn for -10, -1, -0.1, 0.001, 0.01, 0.1, 1, 10, 100 $\times$ 10^9 kg s^{-1}). (b) Zonal wind (colors, unit m s^{-1}) and generalized Eliassen-Palm flux divergence (contours drawn for -40, -20, -10, 10, 20, 40, 60, 80 m s^{-1} d^{-1}).

In complex climate models, the general circulation up to the lower thermosphere can only be simulated in a realistic way when resorting to some parametrization of gravity waves. Corresponding methods are also used or developed at IAP for application in long-term simulations, e.g., in order to study mechanism and modes of long-term variability. However, gravity-wave parameterizations are questionable due to several oversimplifications that must be made. Up to date, there exist only two global circulation models worldwide that simulate a realistic general circulation up to 100 km altitude while describing gravity waves and their effects explicitly. The Kühlungsborn Mechanistic general Circulation Model (KMCM) is one of those. In recent years, this model has been further developed such as to include also explicit computations of radiative transfer and the tropospheric moisture cycle including the full surface energy budget and a simple ocean model [5]. In addition, a new non-hydrostatic model (abbreviated as ICON-IAP) has been developed that can be run with very high spatial resolution in regional geometry [9]. Such a model is suitable to simulate various details of the generation of gravity waves in the troposphere and their breakdown in the middle atmosphere.

As an example from the KMCM, Fig. 2.43 shows the general circulation averaged during January with regard to temperatures and zonal winds (wind in eastward direction). These fields are completed by the residual mass stream-function (which corresponds to the averaged trajectories of air parcels) and the so-called wave drag which is equivalent to the divergence of the Eliassen-Palm flux (EPF) being made up by all waves resolved in the model. The wave drag in the upper mesosphere is realistic, i.e., comparable to expectations from observations. This is a consequence of the fact that gravity waves are generated intrinsically in the troposphere and are damped in the upper mesosphere by an advanced parameterization of turbulent

diffusion that adjusts to dynamic instability of these waves. Also the summer-to-winter-pole circulation in the mesosphere is quantitatively realistic and gives rise to a cold summer mesopause (around 90 km over the southern polar cap) and a warm winter stratopause (around 50 km over the northern polar cap). Note that these features deviate by about 100 Kelvin from a hypothetical temperature distribution that would result without atmospheric waves. This new model version will be used in several projects where we intend to analyze the role of gravity waves in, for example, long-term changes or the three-dimensional mixing of minor constituents in the mesosphere.

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2.5 Leibniz-Institute for Baltic Sea Research Warnemünde – Department of Physical Oceanography and Instrumentation

Head: Prof. Dr. Ulrich Bathmann

The Leibniz Institute for Baltic Sea Research (Leibniz-Institut für Ostseeforschung Warnemünde, IOW) was founded in 1992 on the recommendation of the German Council of Science and Humanities. It succeeded the Institute for Oceanography, Warnemünde, which was the premiere oceanographic research institute of the German Democratic Republic's German Academy of Sciences. Today, the institute is a member of the Leibniz Association (Leibniz-Gemeinschaft, WGL). The institute's facilities are financed by the German Federal Ministry of Education and Research, and the Mecklenburg-Vorpommern Ministry of Education. IOW's research program focuses on coastal oceans and marginal seas, with a particular emphasis on the ecosystem of the Baltic Sea.

Fig. 2.44: IOW's research vessel Elisabeth Mann Borgese in the Central Baltic Sea.

IOW consists of four departments, which are the Marine Geology, the Marine Chemistry, the Biological Oceanography and the Physical Oceanography and Instrumentation. In the following, the working groups of the latter department are briefly introduced.

Coastal Ocean Process Modelling

Head: Prof. Dr. Hans Burchard

Staff:	Dr. Berkay Basdurak Dr. Knut Klingbeil	Dr. Johannes Becherer Dr. Kaveh Purkiani	Dr. Ulf Gräwe Dr. Elisabeth Schulz
Ph.D. Graduates:	Johannes Becherer Mahdi Mohammadi-Aragh Merten Siegfried	Knut Klingbeil Kaveh Purkiani	Xaver Lange Elisabeth Schulz
MSc Graduates:	Xaver Lange		

General Outline of the Field of Research The dynamics of the coastal ocean depends critically on hydrodynamic processes which interact with each other in a complex way. Our approach to understand these processes and their impacts on the coastal environment is to combine dedicated process observations, see, e.g., Ref. [1] with numerical process studies using full hydrodynamics ranging from simple geometries to complex multi-decadal system simulations with realistic forcing. Applications include estuarine [2], coastal [3] and shelf sea studies [4], see Fig. 2.45. The major model tools are the one-dimensional General Ocean Turbulence Model (www.gotm.net) and the three-dimensional General Estuarine Transport Model (www.getm.eu). These Public Domain community models are further improved by developing new numerical methods and analysis tools [5].

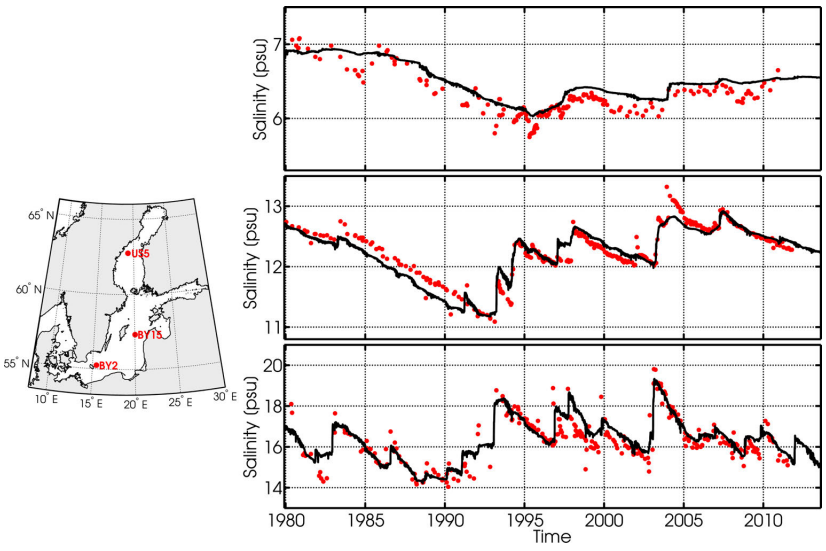

Fig. 2.45: Comparison of observed (dots) and simulated (lines) bottom salinity time series for three stations in the Baltic Sea marked on the map in the left panel: upper panel: Bothnian Sea; middle panel: Gotland Sea; lower panel: Bornholm Basin. The effect of the 1993 and 2003 major Baltic inflow events is clearly seen at all stations as sudden increases in bottom salinity, see Ref. [4] for details.

Scientific highlight: Thermohaline overturning circulation of the Wadden Sea The Wadden Sea of the German Bight is a natural laboratory for studying processes of estuarine exchange in tidally energetic environments. In a series of papers, e.g., [1–3], conducting field experiments, numerical model simulations as well as developing new theoretical concepts, we could elucidate the role of horizontal density gradients on the hydrodynamics and sediment dynamics of the Wadden Sea and similar coastal environments. The major findings were: (i) The Wadden Sea is less dense than the adjacent North Sea most of the time due to differential effects of precipitation and warming; (ii) This establishes an estuarine circulation, which is driven by density gradients due to temperature and salinity differences, such that this circulation is truly thermohaline; (iii) This longitudinal estuarine circulation is strongly modified by lateral (cross-channel) density gradients; (iv) Quarterdiurnal tides have a significant seasonality, which might trigger a strong seasonality in sediment import; (v) Tidal asymmetries driven by estuarine circulation may substantially contribute to sediment import into the Wadden Sea.

Regional Oceanography

Head: Dr. Volker Mohrholz, Dr. Martin Schmidt

Staff:	Dr. Anja Eggert	Dr. Tim Junker	Dr. Michael Naumann
	Dr. Annethea Muller	Dr. David Meyer	
	Dipl. Ing. Dietmar Rüß	Dipl. Ing. Toralf Heene	Sebastian Beier
Ph.D. Graduates:	Lydia Siegfried	Sarah Quandt	
MSc Graduates:	Tom Lange	Martin Mohrmann	Michael Thurm

General Outline of the Field of Research The focus of the working group is on processes occurring on various time and spatial scales comprising micro-structure and turbulence, mesoscale processes such as upwelling [6], filament dynamics [7], and Baltic Sea inflow dynamics [8], as well as large scale processes like the circulation in the South-Atlantic eastern boundary currents [9]. The themes span from physical oceanography to biogeochemistry, the variability of the productivity in an upwelling system, or the analysis of the coupling of the nitrogen and carbon cycle within the Baltic Sea, see, e.g., Ref. [10]. The work comprehend ship-based field studies and long-term investigations with moored devices. It includes the development of new measurement techniques, the application and development of analytical process models and syntheses with coupled numerical biogeochemical models.

Scientific highlight: Dynamics of a filament in the Benguela upwelling system Off-shore spreading filaments of cool water are common to all major upwelling systems in eastern boundary currents. Filament surface structures are well known from remote sensing data of sea surface temperature (SST) and water colour, but field

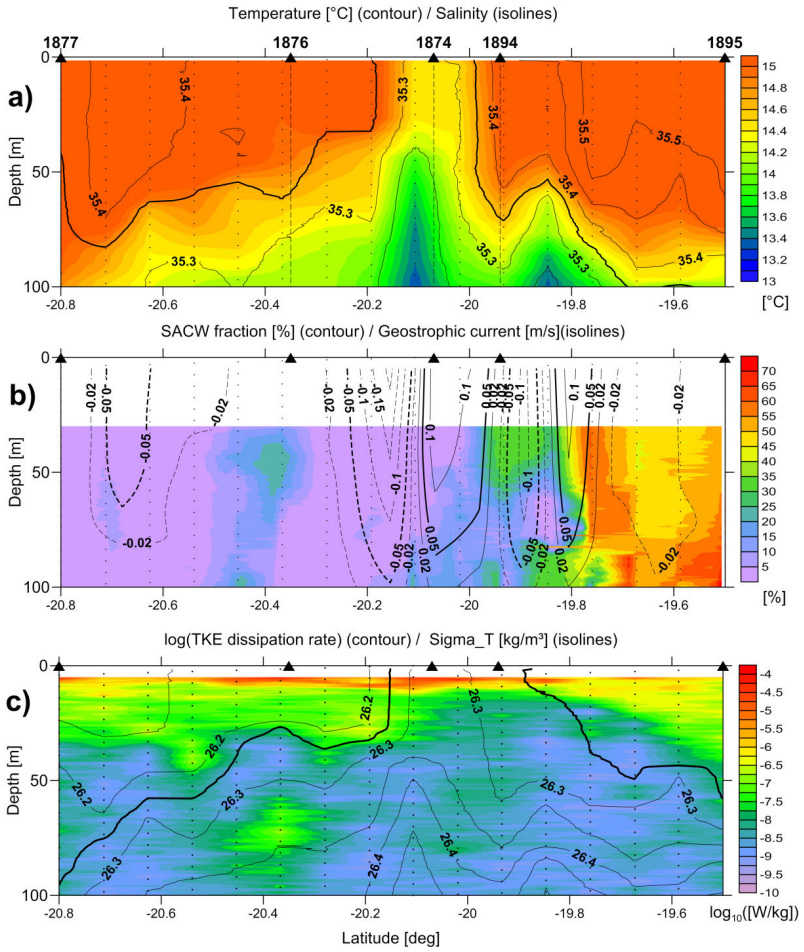

Fig. 2.46: Section through a filament in the northern Benguela (September 2013). Temperature and salinity (a). Watermass distribution and geostrophic currents (b). Distribution of density and dissipation of turbulent kinetic energy (c).

studies are rare because of the transient character of the filaments. During a multi-disciplinary field experiment in the northern Benguela system an upwelling filament was studied to obtain information about its vertical structure [7]. The observed filament covered the upper 100 m of the water column and was found stable for a period of nearly one month. Because of the long lifetime of the filament geostrophic adjustment was observed. The resulting off-shore and on-shore transports exceeded the wind-driven Ekman transport. inside the filament the surface water layer was oxygen depleted, whereas methane and CO_2 concentrations were enhanced.

At its location near the Angola-Benguela frontal Zone, the filament separated two different types of central water and served as a mesoscale pattern extending the interface between these water bodies. The impact of filaments on the ecosystem is highlighted by the observed high phytoplankton biomass and high measured primary productivity at the front between filament and ocean waters.

Systems Dynamics of the Baltic Sea

Head: Dr. Thomas Neumann, Dr. Torsten Seifert

Staff:	Dr. Hagen Radtke	Dr. Rene Friedland
MSc Graduates:	David Faro	

General Outline of the Field of Research The aim of the research is to develop a comprehensive understanding of the Baltic Sea's ecosystem response to external forcing. For this purpose we develop and apply spatially highly resolved, coupled hydrodynamic and biogeochemical models. The research is not primarily focused on single processes; instead we are looking for their complex interplay.

Since the response time of the Baltic Sea hydrodynamics is on the order of 30 years and even longer for the biogeochemistry, we perform our investigations on longer time scales. In particular, we looked into the impact of climate change on the biogeochemistry and the food web of the Baltic Sea [11], as well as on the carbon cycle [12]. To understand possible future changes the understanding of past changes is essential [13]. The confidence in model simulations relies on the predictive capacity of the model systems. Therefore, we continuously improve the process formulations in the used models, especially in the biogeochemical part [14, 15].

Scientific highlight: Advanced time integration scheme In marine ecosystem models, biogeochemical processes are described in the form of differential equations. The local biogeochemistry can be represented by a set of ordinary differential equations (ODEs), which describe the temporal evolution of "state variables", e.g., nitrate concentration or nitrogen in cyanobacteria. The ODEs become partial differential equations if physical processes such as passive advection, turbulent diffusion and sinking of organic matter are included. In a three-dimensional ecosystem model, these equations need to be discretized and solved numerically. While typically much effort is put into elaborate numerical schemes for advection/diffusion processes, for the solution of the biogeochemical equations often even a simple Euler-Forward discretization is used. A good time-stepping scheme for biogeochemical models should possess, however, a list of desirable properties:

- The scheme should be conservative, that is, the total amount of chemical elements like nitrogen should not be changed numerically. In state-of-the-art ecosystem models, the conservation of several elements is required at the same time.
- The concentrations calculated during a time step should be non-negative.
- A high order of accuracy is desirable, as this implies a good approximation to the exact solution.
- The scheme should be computationally fast, here explicit schemes mostly have advantages over implicit ones.

- If possible, the scheme should support stiff problems, that is, such where a production/consumption time scale is faster than the model time step.

In Ref. [14], a new time-stepping scheme was developed, which possesses all of these desirable properties. It is based on a modified Patankar scheme, but has been improved in two essential points: Both the restriction that only one chemical element could be conserved and the implicitness were overcome, while we were able to keep the favorable properties (second-order accuracy, non-negativity, possibility to solve stiff problems). The use of a higher-order numerical scheme, especially with the possibility of solving stiff problems, means that the same degree of accuracy can be achieved by using larger model time steps, which in turn yields a speedup in model calculations and savings in the computation time.

Remote Sensing and Marine Optics

Head: Dr. Herbert Siegel

Staff: Dr. Thomas Ohde, Dr. Juliane Brust-Möbius, Dipl. Geo. Iris Stottmeister, Dipl. Phys. Monika Gerth

General Outline of the Field of Research The group is focused on applications of satellite data in the infrared and visible spectral range closely coupled with bio-optical *in situ* measurements. The application of satellite data includes the annual development of the SST in the Baltic Sea and its climatology, dynamic processes, coastal runoff, and phytoplankton blooms. Optical studies concentrate on optically active water constituents (chlorophyll, suspended matter and yellow substance), their absorption and scattering properties and the influence on spectral reflectance (water colour) and radiative transfer in the water column. The results contribute to the annual hydrographic-hydrochemical and biological assessments of the state of the Baltic and to an HELCOM environment fact sheet. Daily observation of cyanobacteria along the German coast in summer and information about potentially affected regions support local authorities (LUNG, LAGuS, LLUR and Tourism). The main bio-optical study has been a new optical model for the Baltic ecosystem model ERGOM developed in IOW, see, e.g., Ref. [15]. Besides the Baltic Sea, the upwelling systems along the western coast of Africa build another regional focus of our group [16, 17].

Scientific highlight: 2014, the warmest year since 1990 in the Baltic Sea Investigations on satellite derived SST of the Baltic Sea showed that 2014 was the warmest year since 1990. The annual mean value was about 1.2 K above the average for 1990-2014 and 0.4 K higher than 2008, formerly the warmest year, see Fig. 2.47. Except for February and June, all other months, and especially July and August in the northern Baltic Sea, contributed to that value. After a mild start of the year, a strong cooling started around January 20 and lasted until the beginning

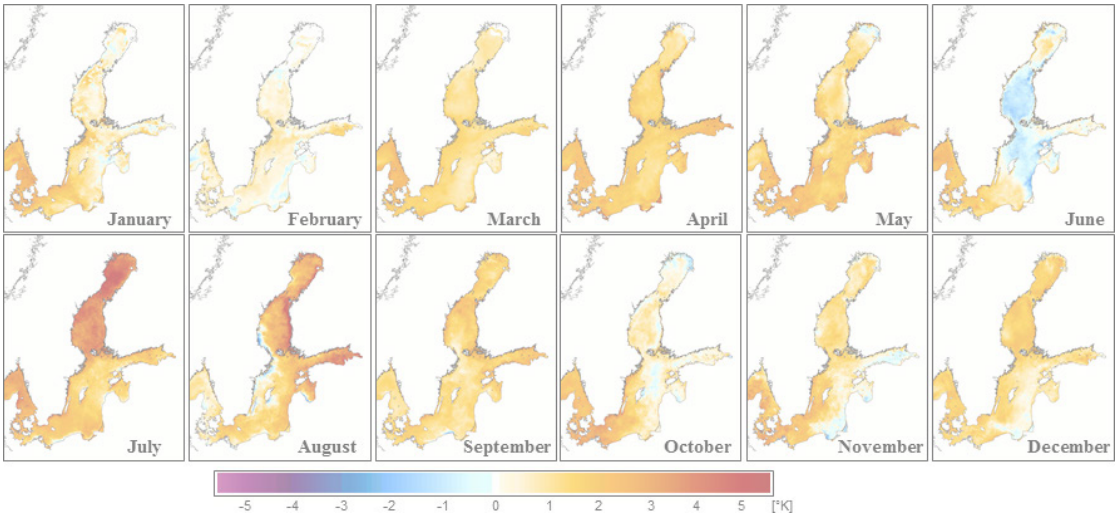

Fig. 2.47: SST-anomalies of monthly averages of the Baltic Sea in 2014 referring to long-term means (1990-2014). Results are taken from: Siegel, H. and M. Gerth (2015). Development of sea surface temperature in the Baltic Sea in 2014. HELCOM Baltic Sea Environ. Fact Sheets Hydrography: http://helcom.fi/baltic-sea-trends/environment-fact-sheets/hydrography/development-of-sea-surface-temperature-in-the-baltic-sea/

of February. The monthly average of January exceeded the long-term averages for 1990-2014 by +2 K. January was the second-warmest month in the western Baltic after 2007. February was the coldest month of the year in the Arkona Sea and Gulf of Bothnia, and March in the Gotland Sea. From March to May, anomalies of +1 to +3 K were recorded throughout the Baltic Sea and even from March to December in the western part. June was the only month with basin-wide negative anomalies of -1 to −2 K in the central and northern Baltic Sea. August was the warmest month in most areas. The warmest day was 28 July with temperatures of 21-25 °C. Atypical uniform SST distribution in the entire Baltic Sea in July and August led to high anomalies of up to +5 K in July in the northern part, where July was the warmest month since 1990. October and November were with anomalies of up to +3 K warmest months in the western part in the last 25 years.

Small-scale Processes and Mixing

Head: PD Dr. Lars Umlauf

Staff:	Dr. Peter Holtermann		
Ph.D. Graduates:	Chris Lappe	Kirstin Schulz	
MSc Graduates:	Ronja Ebner	Robert Kemsies	Jan-Torben Witte
BSc Graduates:	Jan-Torben Witte		

General Outline of the Field of Research Our group focuses on small-scale physical processes in the ocean, that we analyze using a combination of field work, theory, and numerical methods. Recent examples include studies of turbulence and mixing in the bottom boundary layer [18], in the surface layer affected by surface waves [19], and in tidally-driven coastal areas [20]. In a recent modeling study [21], we could also show that deep-water mixing processes in the Baltic Sea are reproduced with good accuracy with the latest generation of three-dimensional circulation models. Finally, as an interdisciplinary side-line of our research during the last years, we have also collaborated with colleagues from Japan to investigate the interaction of turbulence and vertically propagating plankton species [22].

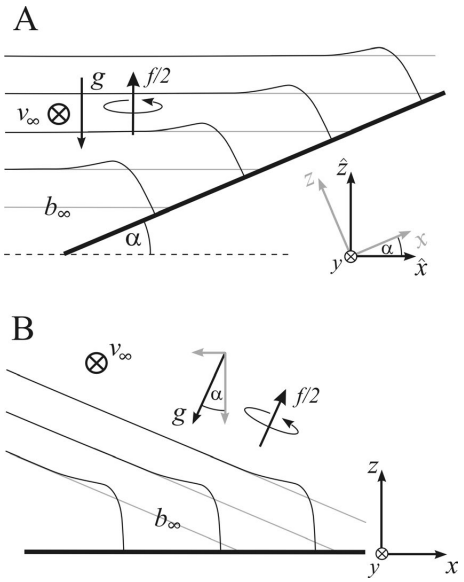

Fig. 2.48: Schematic view of the density field near a rotating uniform slope with slope angle α for (a) geopotential and (b) rotated coordinate systems. Thin lines indicate isopycnals (lines of constant density) in the actual (black) and equilibrium configuations. For details, see Ref. [18].

Research Highlight Turbulent bottom Ekman layers are among the most important energy conversion sites in the ocean. Their energetics are notoriously complex,

in particular near sloping topography, where the feedback between cross-slope Ekman transports, buoyancy forcing, and mixing affects the energy budget in ways that are not well understood. We attempted to clarify the energy pathways and different routes to mixing, using a combined theoretical and modeling approach, see the geometry in Fig. 2.48. Our analysis was based on a newly developed energy flux diagram for turbulent Ekman layers near sloping topography that allows for an exact quantification of the energy conversion rates and energy pathways. We could show that mixing efficiencies increase with the slope angle and interior stratification, but do not exceed the threshold of $5\dot{\%}$ except for very steep slopes, where the canonical value of $20\dot{\%}$ may be reached. Available potential energy generated by the cross-slope advection may equal up to $70\dot{\%}$ of the energy lost to dissipation for upwelling-favorable flow, and up to $40\dot{\%}$ for downwelling-favorable flow [18].

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2.6 Physics Education

Head: PD Dr. Heidi Reinholz

Staff: Dr. Yultuz Omarbakiyeva, Dipl.-Des. Wiebke Loseries, Christine Prühs, Marion Pauer, Dr. Andrea Sengebusch, Christoph Gelzenleuchter, Robert Leppin, Lena Boldt, Dr. Viola von Oeynhausen, Matthias Hofstetter, Carmen Dilger, Kirsten Müller

The Goal

Our activities are multi-layered. Both sides of the teaching-learning interface are addressed and interrelated. While providing lectures and seminars for the future teacher generation is the primary focus, we also offer workshops for schools and their students as well as advanced vocational training for already experienced teachers. Further, we also want to reach out to the broader community by events such as the *Lange Nacht der Wissenschaft* (Long night of Sciences) and the *Physiktag* (Day of Physics). From the scientific point of view, we focus our activities on empirical research with respect to teaching methods and modern technology.

Teaching

The curriculum for the courses in physics education has been rewritten over the last few years in order to include new developments with respect to teaching methods and modern technology. Questions of motivation, diagnostics in teaching, and interdisciplinary teaching are discussed as well as practically oriented seminars and activities have been introduced. Units like "Physics and Technology" and "Applications of New Technology in Teaching and Learning Physics" have been established as popular modules. School-related lab work and first teaching experiences in schools are seen as particularly helpful to students and teaching staff. The ten-semester course that also includes units on pedagogy and psychology as well as studies on science and education of a second teaching subject is completed with a final state examination (*1. Staatsexamen*). This is followed by a teaching internship, which is possible in schools throughout the whole federal state and beyond.

Research

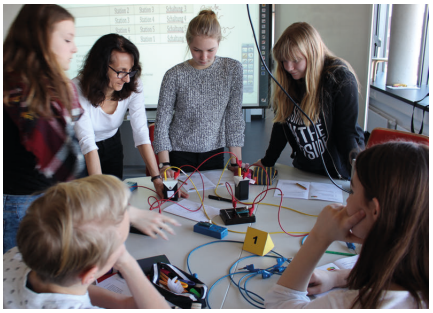
Aspiring teachers must have different explanation patterns at hand for the description of physical phenomena in order to individually address existing preconceptions of the students. A seminar in the context of the teacher education has been developed and evaluated by means of empirical social research. The explanation capabilities of future physics teachers should be developed by multiple contacts with groups of school students. Here, the focus is on the preparation of "good explanations" of experiments with respect to different student needs and an associated growth of diagnostic capabilities.

Working and learning with computers, tablets and smartphones is a part of the everyday life for students as well as for teachers. About 70 % of children and 98 % of teenagers in Germany own their personal, usually daily-used, smartphone. Possible use of these devices in schools involve not only search functions, but scientific explorations and investigations using multimedia applications. Moreover, a common smartphone or tablet can be treated as a 'hand-held laboratory' according to the amount of incorporated sensors. We are aiming at the implementation of new media in class, focusing on the investigation of implications on the exploration and explanation skills of students.

Another topic focuses on the connection of physics and sports, as an example for context-guided teaching. Close-to-life and socially relevant contexts form a meaningful framework to the subject. The embedding of professional knowledge in contexts has a positive effect on learning processes and can significantly increase the students interest in physics. Several concepts of learning units in the physical contexts of body and sports have been prepared throughout term-associated projects [1].

PhySch

The learning-teaching-lab PhySch (short for *Physik und Schule*) [2] is a project on the interface between science and schools. The recent years were characterized by re-arranging and improving the already available content as well as developing new content, which has been clustered in different branches of the PhySch lab not only with respect to the physical but also to the pedagogical goals. The different branches or labs show a broad range: e.g., elementary school projects (Kidslab), astronomical projects (Astrolab), learning-to-explain projects (Mechaniklab), learning-to-explore projects (Photonlab) as well as a teachers club and an explorers club to provide science-related platforms for social interactions. In general, university students who are trained to become science teachers are deeply involved in the labs. They design experiments which complement the school curriculum in two ways: on one hand by experiments which can not easily be done in schools, e.g., the Franck-Hertz or Miliken experiments; on the other hand by experiments which go beyond the school curriculum but contain various aspects that are already taught at school, e.g., intelligent glass, fuel cell vehicles or black boxes demonstrating the nature of science. Instructions for experiments are prepared at an appropriate level by the university students who are also responsible to lead the school students through the projects, which are offered at university venues or locally in the schools.



School students in our PhySch lab

Since 2003, the Institute of Physics has organized the annual **Lighthouse com-**

petition [3] for the schools of Mecklenburg-Vorpommern, which compete against each other for the Lighthouse Cup. After a pre-quiz about the main topic of the year (2013: *Viel Wind um Energie*, 2014: *Alltagsphysik*, 2015: *Lichtblicke*), the best teams have to find good scientific explanations for experiments which are presented on a stage. Meanwhile, the labs of the institute are opened to be visited and hands-on activities are available to be done. Last not least, a lecture with lots of impressive experiments repacked in a new story every year (2013: *Asterix und Obelix - et reformationes bononiae (und die Bologna-Reform)*, 2014: *Das Schneewittchen Mysterium. Geheimakte XY märchenhaft*, 2015: *Die Odyssee. Eine göttliche Intervention*) are prepared and presented by a group of physics students, including future teachers.

Fig. 2.49: The Lighthouse Cup

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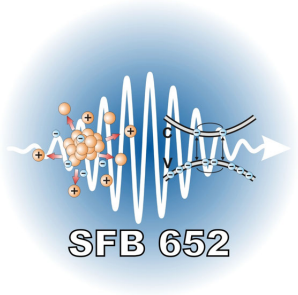
3 Collaborative Research

3.1 Collaborative Research Center (SFB 652) "Strong Correlations and Collective Effects in Radiation Fields: Coulomb Systems, Clusters and Particles"

Executive Board: Prof. Dr. Stefan Lochbrunner [a]
Prof. Dr. Karl-Heinz Meiwes-Broer [b]
Prof. Dr. Ronald Redmer
Prof. Dr. Heinrich Stolz



Homepage: http://web.physik.uni-rostock.de/sfb/

[a] leader of the intergrated graduate school
[b] spokesman

Collaborative Research Centers (Sonderforschungsbereiche) are long-term (up to 12 years) research centers at German universities devoted to topics at the frontier of science. The innovative and cross-disciplinary research program is treated in various projects in a coherent approach coordinated by the executive board. Funding is provided by the Deutsche Forschungsgemeinschaft (DFG).
The second funding period of the SFB 652 ended on June 30, 2013. The DFG has granted a third funding period that started on July 1, 2013 and ranges to June 30, 2017.

3.1.1 Projects and Project Leaders (status 31.12.2015)

A1	Matter exposed to VUV- and X-ray radiation	Prof. Dr. Karl-Heinz Meiwes-Broer Prof. Dr. Ronald Redmer PD Dr. Josef Tiggesbäumkker
A2	Thomson-scattering and correlations in warm dense matter	Prof. Dr. Ronald Redmer
A3	Correlated processes in laser-excited trapped cluster ions	Prof. Dr. Lutz Schweikhard[1] Dr. Gerrit Marx[1] Prof. Dr. Karl-Heinz Meiwes-Broer
A4	Optical properties and dielectric response of strong correlated Coulomb systems	PD Dr. Heidi Reinholz
A5	Controlled energy transfer of intensive laser pulses into clusters and particles	PD Dr. Josef Tiggesbäumker Prof. Dr. Karl-Heinz Meiwes-Broer
A8	Microscopic description of atomic clusters in intense laser fields	Dr. Thomas Fennel
A9	Simulation of quantum dynamics in strong laser fields using density functional theory	Prof. Dr. Dieter Bauer
A10	Influence of the local environment on the energy transfer dynamics in molecular aggregates	Prof. Dr. Sylvia Speller Dr. Ingo Barke
A11	Light-induced interaction between nanoparticles and molecules at surfaces	Prof. Dr. Stefan Scheel
B1	Excitonic Bose Einstein condensates in traps	Prof. Dr. Heinrich Stolz
B2	Non-classical light from semiconductor micro cavities and quantum films	Prof. Dr. Werner Vogel Prof. Dr. Heinrich Stolz
B5	Dynamics, quantum coherence and entanglement of strongly correlated excitonic systems	Prof. Dr. Holger Fehske[1]
B6	Radiation field-induced correlations in doped Helium droplets	Prof. Dr. Karl-Heinz Meiwes-Broer Prof. Dr. Stefan Scheel

[1] Physics Department, University of Greifswald

B9	Dynamics of correlated excitons in molecular aggregates	Prof. Dr. Stefan Lochbrunner
B10	Laser-driven multi exciton dynamics in molecular aggregates	Prof. Dr. Oliver Kühn
B11	Structural correlations in liquid Coulomb systems	Prof. Dr. Ralf Ludwig Prof. Dr. Oliver Kühn Prof. Dr. Stefan Lochbrunner
B12	Quantum correlations in light and matter: characterization and verification	Prof. Dr. Werner Vogel
B13	Preparation, characterization and application of quantum correlations in radiation fields	Prof. Dr. Boris Hage
B14	Non-equilibrium description of excitonic Bose Einstein condensation in traps	Prof. Dr. Heinrich Stolz Prof. Dr. Holger Fehske
MGK	Integrated Graduate School	Prof. Dr. Stefan Lochbrunner

3.1.2 Overview

The common goal of the research activities is to contribute to a deeper fundamental understanding of the role of strong correlations and collective phenomena for the interaction of radiation fields with matter. Characteristic for the SFB 652 are the joint experimental and theoretical efforts to investigate these issues in a broad spectrum of systems including ultracold quantum condensates, exciton clusters in semiconductor quantum films, atomic clusters and nanoparticles, as well as warm dense matter and molecular systems so that new frontiers in light-matter research are being explored. Along this line the centre connects topical issues from various subjects, including physics of correlated Coulomb systems, semiconductor physics, quantum and molecular optics, and cluster physics in an interdisciplinary manner. State-of-the art light sources, such as stabilized optical cw-lasers, ultra-intense femtosecond lasers, as well as the DESY VUV free-electron laser (FLASH) are used for the experimental investigations. In perspective, to attack new regimes regarding to the parameters of the radiation field, also the DESY X-ray free-electron laser (X-FEL) will be used for the experimental program. Some projects (A1, A2, A8) participate in first experimental campaigns at the LCLS X-ray free-electron laser in Stanford/USA.

3.1.3 Structure

Thematically the projects are classified in two research complexes. Project complex A is devoted to the investigation of optical excitations of existent strongly correlated Coulomb systems, while complex B addresses the generation of correlations by the radiation field itself. About 50 scientists collaborate on the above outlined topics, including several colleagues from the University of Greifswald. The central topic in the project complex A is the excitation and analysis of dense Coulomb systems, i.e. clusters and particles, warm dense matter, dense electron-ion systems, and particle-hole systems in semiconductors. The theoretical investigations in projects A1, A2, A4, A6, A8 and A9 are accomplished in close collaboration with the main three experimental topics, which are: (i) the excitations of clusters and particles by radiation from free-electron lasers (A1, A5), (ii) the controlled coupling of intense optical laser pulses to clusters and particles (A3, A5) and (iii) the study of energy transfer processes after optical excitation in a photoemission electron microscope. For the analysis of the systems as well as the exploration of new routes for future application of light-matter correlations, cutting-edge control techniques such as pulse optimization through genetic algorithms and pump-probe control schemes with phase-stabilized pulses are utilized. For the theoretical description state-of-the-art many-body techniques such as quantum particle-in-cell methods (A1, A8, A9), quantum kinetic equations (A6), linear response theory (A2, A4), density functional theory and quantum molecular dynamics simulations (A1, A2, A9) are applied.

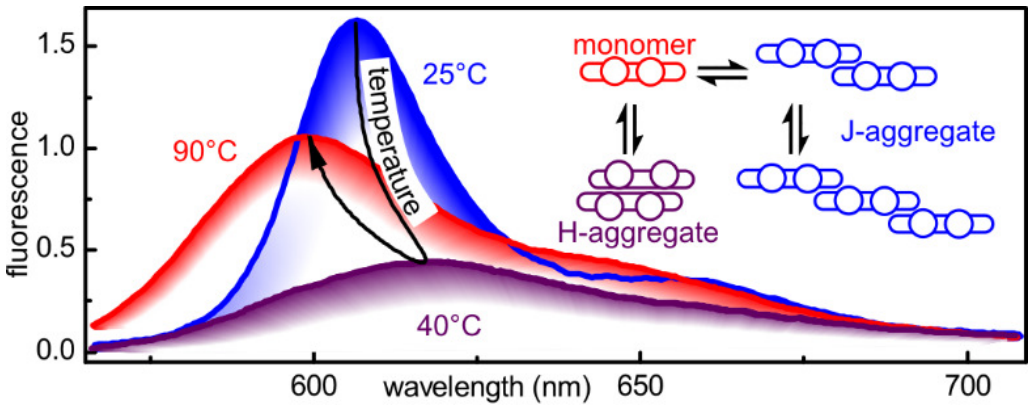


Fig. 3.1: The fluorescence of a perylene bisimide dye shows an unconventional temperature dependence. This is caused by two aggregation pathways, one leading to H-type dimers prevailing at intermediate temperatures, and the other to J-aggregates dominating at low temperatures.

Project complex B concentrates on the build-up of correlations in semiconductors, atom condensates, clusters, optical and molecular systems. Semiconductors and molecules represent ideal targets for the study of many-particle effects in a wide density range because of the well-controlled elementary excitation of the excitons. In semiconductors a limiting factor is the finite lifetime of the excitons which, how-

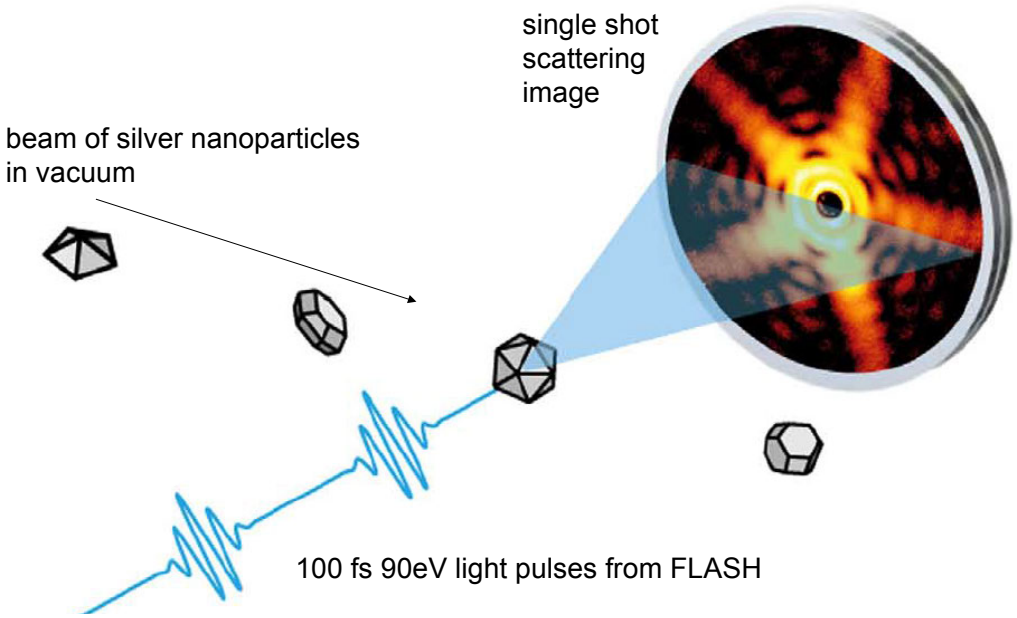


Fig. 3.2: Experiment on the single-shot scattering of individual free silver nanoparticles, obtained at the free electron laser FLASH. From a comparison with simulated results we conclude on the particle size and shape. Figure adapted from Barke et al., Nat. Comm. **6**, 6187 (2015).

ever, can be tuned by the choice of the material or a proper external confinement potential. Corresponding studies constitute a major issue within the projects B1-B2. Excitons in mesoscopic potential wells are investigated in project B1, being promising candidates in this context. Essential for the realization and the control of the light-induced correlations is the development of theoretical concepts that can provide a consistent connection of quantum optics with many-particle theory. This is the subject of the project B2. In the project B5 the formation of exciton-polariton quasiparticles through cooperative effects and the build-up of correlations at high pressures are investigated. Within the project B6 the light-field induced formation of novel metal atom condensates in exotic and ultracold environments, such as suprafluid helium droplets, is studied.

During the course of the 1st funding period it became possible to include the field of exciton dynamics in molecular systems, within the project B9. This comprises experimental as well as theoretical activity on molecules as an additional basis for the collaborative research centre. In the second funding period these activities had been extended within the projects B9 and B10. The projects B9-B11 emphasize the importance of correlation effects in the dynamics in molecular systems. In particular, it became possible to build a bridge to physical chemistry (B11) by including research on ionic liquids. The projects A8, A9 and B12 strengthen activities in many-particle and density functional theory as well as in quantum correlations between light and

matter. Experimental verification of such correlations are in the centre of B13.

Within the reporting period the SFB 652 could significantly be strengthened by the inclusion of several new aspects. 19 scientific projects and an integrated graduate school constitute an internationally high-ranked research centre with a lively academic service, which reaches out into the Faculty of Mathematics and Natural Sciences as well as into the whole university, especially via the Department of Life, Light and Matter of the Interdisciplinary Faculty. This interdisciplinary research platform was founded at the University of Rostock in 2007, also based on the SFB 652 with its scientific competence and its long-term missions.

The two results sketched in Fig. 3.1 and Fig. 3.2 give an impression of current collaborative activities in the SFB. The first example illustrates how subtle changes in the geometry of molecular nanostructures can cause drastic variations of their optical properties. The exciton dynamics in such structures is studied in the SFB projects B9 and B10 in collaboration with the University of Würzburg using an aggregating perylene bisimide dye. Its fluorescence changes from the typical spectrum of the monomer to the stronger and sharper emission of J-aggregates if the temperature of a warm cyclohexane solution is cooled down to room temperature. However, the transition occurs not monotonically but the fluorescence shows an unexpected decrease and red shift at intermediate temperatures, see Fig. 3.1. To explain this behavior a biphasic aggregation model was developed [Fennel et al., J. Am. Chem. Soc. **135** (2013), 18722]. It shows that the intermediate phase is dominated by dimers, which exhibit an H-type configuration and which cannot assemble to bigger aggregates due to steric reasons. The elongation to larger structures is only possible via a J-dimer, which occurs only in small numbers but serves as a condensation nucleus for the growth process.

The second example concerns the ultrafast scattering response of silver nanoparticles to extreme ultra-violet (EUV) femtosecond pulses. Several scientists of the SFB are involved in experiments at the free electron lasers FLASH (Hamburg), LCLS (Stanford), and FERMI (Trieste). Figure 3.2 depicts a corresponding experiment using FLASH pulses at 90 eV to explore the morphology of free clusters in the beam. We demonstrated that single-shot wide-angle scattering of femtosecond soft X-ray free-electron laser pulses allows three-dimensional characterization of the resulting metastable nanoparticle structures. For individual free silver particles, which can be considered frozen in space for the duration of photon exposure, both shape and orientation are uncovered from measured scattering images. We identify regular shapes, including species with fivefold symmetry and surprisingly large aspect ratio up to particle radii of the order of 100 nm. Scientists of A1, A5, A8, A10 and B6 have been involved, together with the ones from the Technical University in Berlin, and the FLASH team.

4 Department of Science and Technology of Life, Light and Matter

4.1 Overview

In a world which is becoming ever more complex, innovative or even revolutionary solutions primarily require two things: An extremely high specialization and a conceivably close interaction of various scientific areas. More than ever before, new ideas and technologies are being based on interdisciplinary thinking. On these grounds in 2007, the Department 'Science and Technology of Life, Light and Matter' (LL&M) has been founded within the Faculty of Interdisciplinary Research of the University of Rostock. Its activities search to connect scientific effort of the faculties of natural sciences and mathematics, agriculture, engineering sciences as well as medicine. Three further departments 'Maritime systems', 'Ageing of individuals and society' and 'Knowledge – Culture – Transformation' together with LL&M currently constitute the Interdisciplinary Faculty (INF), which is supported by the University and the state of Mecklenburg-Western Pomerania. The aim is to identify and strengthen fruitful research fields through an appointment policy that is consequently oriented towards profile and strategy in order to foster international competitiveness.

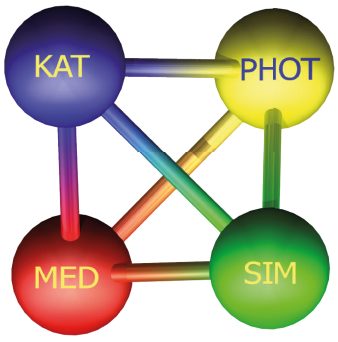


Fig. 4.1: Catalysis, Photonics, Medicine, and Simulation technology are in the core of the Department of Life, Light and Matter.

4.2 Program of the Department

The department LL&M aims at interdisciplinary research and training in the fields of photon sciences, engineering and catalysis, regenerative medicine and numerical simulations. The program comprises activities within several faculties and institutes of Rostock University. Among those are the basic sciences – chemistry, physics and mathematics – as well as the more applied mechanical and electronic engineering, informatics, and life sciences. In addition, the Leibniz-Institute for catalysis (LIKAT), the Leibniz-Institute for atmospheric research (IAP), the Leibniz-Institute for Plasma Science and Technology (INP-Greifswald) as well as the Gesellschaft für Schweißtechnik International (GSI) are significantly involved.

The scope of the investigations reaches from fundamental problems like the interaction of light with matter via the development of photocatalytic processes to fundamental mechanisms in the field of cell biology. Smart materials play an important role in all of these areas. One backbone of the Department LL&M is research on the impact of atomic and molecular properties onto macroscopic systems. Linked to this is the study of microscopic mechanisms that allow control by, e.g., light or molecular active substances. These operations on the atomic or nanometer scale can be used for the development and modification of new methods and materials. Potential applications in biomedical and technical areas are as numerous as fundamental insights into a highly interdisciplinary field.

4.3 Contribution of the Physics Institute to LL&M

Among the about 40 research groups within LL&M, 13 belong to the Physics institute. These are:

Prof. Dr. Thomas Gerber	Physics of Nano- and Biomaterials
Prof. Dr. Boris Hage	Experimental Quantum Optics
Prof. Dr. Oliver Kühn	Molecular Quantum Dynamics
Prof. Dr. Jürgen Kolb	Bioelectronics (INP Greifswald)
Prof. Dr. Stefan Lochbrunner	Dynamics of Molecular Systems
Prof. Dr. Franz-Josef Lübken	Leibniz Institute for Atmospheric Physics
Prof. Dr. Karl-Heinz Meiwes-Broer	Clusters and Nanostructures
Prof. Dr. Fedor Mitschke	Nonlinear Optics
Prof. Dr. Ronald Redmer	Statistical Physics
Prof. Dr. Christoph Schick	Polymer Physics
Prof. Dr. Sylvia Speller	Physics of Surfaces and Interfaces
Prof. Dr. Heinrich Stolz	Semiconductor Optics
PD Dr. Josef Tiggesbäumker	Clusters and Nanostructures

4.4 Current Activities

In the period under review one focal point of LL&M has been the enhanced networking among the workgroups in different scientific disciplines. At first, the members had to recognize their own benefits when participating in this interdisciplinary effort. With support by the University and the local government PhD scholarship funds could be granted to 14 students. All of them worked on interdisciplinary topics and were coached by two supervisors from separate institutes.

LL&M defines itself as a research department. Hence its main aim is the identification and establishment of topical research subjects in order to attract high-level scientists and enhanced third-party funding. In this respect the PhD scholarships serve as a glue money to strengthen initiatives setting up new research projects. In the meantime LL&M has established a graduate network with own workshops. Further on the master level, we started the International program "Physics of Life, Light an Matter" which is taught in English.

Some larger projects as well as few smaller ones could be either continued in the proximity of the department or be started. One major success has been the funding of a laboratory building specific for the Department LL&M. Approved by the German Council of Science and Humanities (Wissenschaftsrat) the scientific building will provide additional 2400 sqm of extensively equipped space. The topical focus of LL&M and the high standard of the contributing research groups made it possible to acquire beyond 20 Mio. EUR funding for the new building and for equipment. The additional capacity is mainly used to house five *Centers of Competence*, as well as laboratories for temporal projects. The *Centers of Competence* are (i) Surfaces/ Interfaces, (ii) Microscopy and Spectroscopy, (iii) Calorimetry,(iv) Nuclear Magnetic Ressonance (NMR), and (v) Mass Spectroscopy. Modern equipment in all areas facilitates research in this interdisciplinary field.

Several larger projects with the contribution of LL&M research groups include:

- Collaborative Research Center DFG-SFB 652 *Strong correlations and collective effects in radiation fields: Coulomb systems, clusters and particles*,

  see Sec. 3.1 for the overview. This project is centered at the Institute of Physics, with one project leader being from the Chemistry Department of the University of Rostock and three project leaders from the Institute of Physics of the University of Greifswald.
- The Graduate School *welisa - Analysis and Simulation of Electrical Interactions of Implants with Bio-Systems* increases the communication among the PhD students within weekly colloquia, workshops, and other social activities. The doctoral students have the possibility to do their doctorate at the interface among electrical engineering, materials science, medicine, biology, physics and scientific computing. Along with this, occupational perspectives in research and industry

Fig. 4.2: View of the scientific building LL&M.

of the medical technology are introduced to the young scientists through the high interdisciplinarity of their research topic.

- The Helmholtz Zentrum München has set up a *Virtual Institute for Complex Molecular Systems in Environmental Health* (HICE) together with the University of Rostock and additional research partners. The project is funded by the Initiative and Networking Fund of the Helmholtz Association. HICE examines the biological effects of aerosols from relevant anthropogenic sources. In the focus are health effects of aerosols from combustion processes (so-called *particulate matter*, i.e., emissions from car and/or truck traffic and heating) known from epidemiological studies. In addition to the exact chemical and physical analysis of aerosol composition, their biological effects are investigated using primarily innovative *in vitro* models of lung tissue.
- The combined research project *Ionische Flüssigkeiten als Abschreckmedien in der Wärmebehandlung metallischer Werkstoffe* is funded through the DFG and connects activities of physics, chemistry and engineering (Keßler, Kragl, Schick) within the Center of Competence Calorimetry.
- Several projects were supported by the German government through BMBF. Here, one focus is the behaviour of matter under the excitation with strong x-ray pulses.

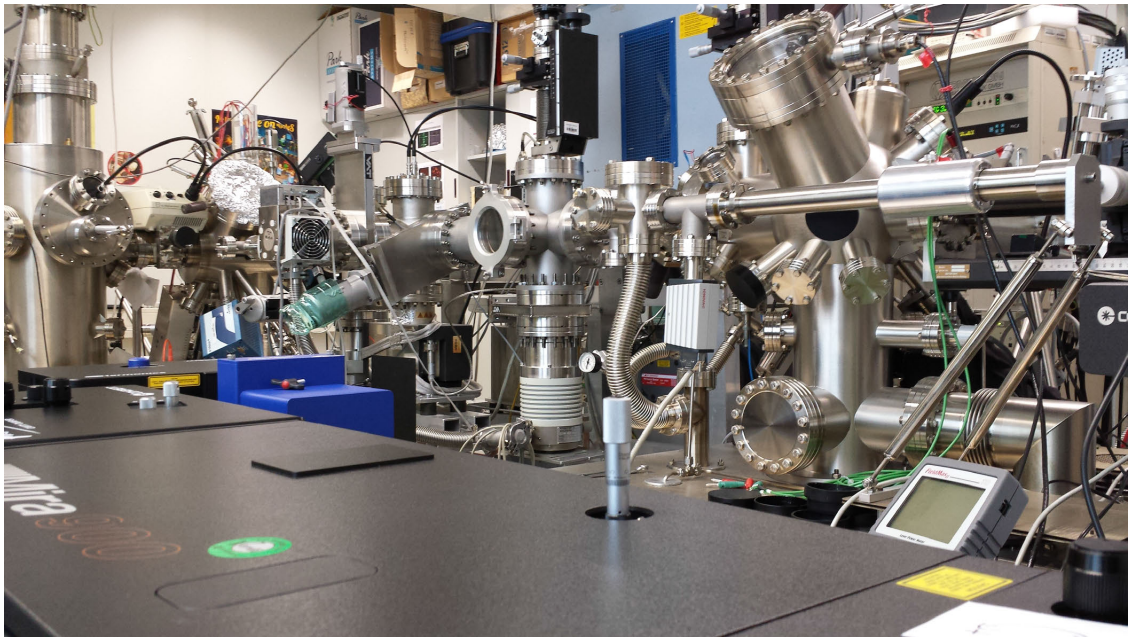


Fig. 4.3: Equipment of Center of Competence: Surfaces and Interfaces

Others deal with recent techniques in ion and electron acceleration.

Furthermore, physics research groups and members of the department have been involved in two cutting-edge Research and Innovation Projects in East Germany ('Spitzenforschung in den Neuen Ländern'):

- *Regionale Entwicklung durch Medizintechnische Innovation und Spitzenforschung* (REMEDIS). This collaborative project focuses onto the development of new implants for clinical applications. The consortium unites competence in the areas of the engineering sciences, medicine and natural sciences from the university. Other local, national and international institutes and companies are involved.
- *Light2Hydrogen - Energy for the Future.* This research project explores new ways for hydrogen generation, boosting efficiency using nanotechnology and other novel technologies for a post-oil society. The production of hydrogen with the sole use of solar power would be a magnificent contribution to the generation of energy, which will not access fossil resources and will not pollute the atmosphere. Co-funding by the state M-V has been provided through the project *Nano4Hydrogen.* In close connection and intensive exchange with the sister project Light2Hydrogen, a unique basis upon the research topic *photo-catalysis* has been established.

A variety of additional smaller and larger research projects constitute interdisciplinary work connecting the Physics Institute with other institutes and groups. The Department LL&M strives for increasing such concerted activities in order to strengthen the international competitiveness of the University of Rostock.

Fig. 4.4: Top view on the LL&M laboratory building, being attached to the new Physics Institute on the Campus Südstadt

5 Academic Qualifications, Colloquia, and Workshops

5.1 Habilitation and PhD Theses

Author	Date	Title of the Habilitation theses
Dr. Jan Sperling	16.07.2015	Quantum correlations and measurements

Author	Date	Title of the PhD theses
Tian-Min Yan	30.01.2013	Trajectory-Based Coulomb-Corrected Strong Field Approximation
Philipp Sperling	29.04.2013	Wechselwirkung intensiver Laserpulse mit dichten Plasmen - Ultrakurzzeitkinetik und Diagnostik
Mathias Ahrenberg	29.05.2013	In-situ investigation of vapor-deposited glasses of toluene and ethylbenzene via alternating current chip-nanocalorimetry
Sebastian Göde	08.07.2013	Strahlungsfeldinduzierte Korrelationen in Atom-aggregaten, Clustern und Mikrotropfen
Ulf Weber	12.07.2013	Calciumorthophosphate mit kontrollierter Kristallmorphologie und ein injizierbares, poröses Biomaterial: Materialentwicklung und Charakterisierung
Martin Adam	24.09.2013	Nanostrukturierte Beschichtung auf Implantaten zur Erhöhung der Osseointegration
Varun Kapoor	18.12.2013	Model atomic systems in intense laser fields: exact time-dependent density functional and Floquet theory
Knut Klingbeil	19.02.2014	Approaches for the improvement of physical transport processes in numerical models of coastal oceans
Manja Placke	21.02.2014	Gravity waves and momentum fluxes in the mesosphere and lower thermosphere region
Philipp Rohrmann	24.02.2014	Experimentelle Charakterisierung von Bindungszuständen aus drei Solitonen in dispersionsalternierenden Glasfasern

Bernd Kaifler	24.03.2014	Thermal Structure and Gravity Waves in the Antarctic Middle Atmosphere Observed by Lidar
Natalie Kaifler	25.03.2014	Noctilucent clouds and the dynamics of the mesopause region at high latitudes: Observations with the ALOMAR RMR lidar
Vivien Matthias	31.03.2014	The role of planetary waves in coupling processes of the middle atmosphere
Christian Schaal	02.04.2014	Energie- und ladungsaufgelöste Analyse von Ionen aus der Laser-induzierten Coulombexplosion von Clustern
Jens Hildebrand	04.04.2014	Wind and Temperature Measurements by Doppler Lidar in the Arctic Middle Atmosphere
Holger Keuer	08.07.2014	Verbesserung der Osseointegration orthopädischer Implantate
Johannes Becherer	11.07.2014	Estuarine Circulation in well-mixed tidal inlets
Peter Grünwald	14.07.2014	Nonclassical light from Semiconductor micro- and nanostructures
Stefan Polei	30.10.2014	Oberflächenpotential und elektroneninduzierte Manipulation niederdimensionaler Strukturen
Johannes Kiliani	07.11.2014	3-D Modeling of Noctilucent Cloud Evolution and Relationship to the Ambient Atmosphere
Yi-Ling Chen	12.11.2014	Plasma Diagnostics Applying K-Line Emission Profiles of Si an Ar
Qingqing Xu	26.11.2014	Materials for Carbon Dioxide Separation
Sonja Lorenzen	11.12.2014	Quantum-statistical approach to pressure broadening for Lyman lines from dense hydrogen and hydrogen-like plasmas
Elisabeth Schulz	16.12.2014	Residuelle Zirkulation in gezeitendominierten Ästuaren: Beiträge und Abhängigkeiten
Torsten Leddig	19.12.2014	Search for the decay $B \to \Lambda_c^+ \bar{p} l \bar{\nu}$ with the BABAR detector
Christoph Mahnke	14.01.2015	Optische Superkontinua in Glasfasern: Untersuchungen zu Mechanismen der Entstehung mit und ohne Rückkopplung
Bin Yang	09.02.2015	Crystal Nucleation of Single Tin Droplets Studied by Fast Scanning Calorimetry
Matthias Lütgens	08.04.2015	Ultraschnelle kohärente Raman-Spektroskopie an wasserstoffbrückenbildenden Flüssigkeiten
Kaveh Purkiani	28.04.2015	Numerical analysis of stratification and destratification process in tidally energetic inlets

Carmen Mihoc	06.05.2015	Phase evolution studies in Al-Cu-Fe quasicrystals to tailor the mechanical properties of quasicrystal-polymer composites prepared by spark plasma sintering
Kerstin Witte	11.05.2015	Hyperfine interactions in nanostructured iron oxide composites
Mathias Arbeite	22.06.2012	Mikroskopische Beschreibung der ultraschnellen Anregungs- und Relaxationsdynamik von Edelgasclustern in intensiven VUV-, XUV- und Röntgenlaserpulsen
Siegfried Sobkowiak	23.06.2015	Theoretische Beschreibung von Exzitonen in druckinduzierten Potentialfallen bei ultratiefen Temperaturen in Kupferoxydul
Sunipa Som	29.06.2015	Numerical Simulation of Exciton Dynamics in Cuprous Oxide at Ultra Low Temperatures
Franziska Fennel	15.07.2015	Einfluss der energetischen Unordnung auf die Exzitonenmigration in organischen Systemen
Mateusz Lisaj	22.07.2015	Laser Control and Spectroscopy of Molecular Vibrations and Reaction Dynamics
Andreas Becker	29.07.2015	Materie unter extremen Bedingungen: Strukturmodelle, Zustandsgleichungen und Materialeigenschaften für das Innere von Großen Planeten und Braunen Zwergen
Yujie Quan	28.08.2015	Optimization of Ti-6Al-4V and its foams for biomedical applications by field assisted sintering technique
Christian Peltz	02.10.2015	Fully microscopic analysis of laser-driven finite plasmas
Stephan Bartling	23.10.2015	Morphologie, Struktur und Aktivierungsenergie deponierter Cobalt-Nanopartikel unter reaktiven Bedingungen
Artur Szewczyk	16.11.2015	Mesospheric Turbulence: The Role in the Creation of Mesospheric Inversion Layers and Statistical Results
Andreas Schneider	11.12.2015	In-situ turbulence observations in the stratospheric wind and temperature field
Robert Püstow	18.12.2015	Evolution des Saturn auf der Basis von ab initio - Zustandsgleichungen

5.2 Physics and SFB Colloquia

Date	Speaker, Affiliation: *Title*
10.01.2013	Dr. Sergei D. Ivanov, Universität Rostock: *Quantum Dynamics*
17.01.2013	Dr. Wieland Schöllkopf, Fritz-Haber-Institut der MPG, Berlin: *Helium-Quantenreflexion*
07.03.2013	Dr. Lars Umlauf, Institut f. Ostseeforschung: *Struktur und Dynamik bodennaher Strömungen im Ozean*
21.03.2013	Prof. Dr. John R. Klauder, University of Florida Gainesville: *Completing Canonical Quantization*
11.04.2013	Dr. Faming Zhang, Universität Rostock: *Spark Plasma Sintering of Nanomaterials and Biomaterials*
18.04.2013	Prof. Dr. Andrey Vilesov, University of Southern California: *Vorticity and shapes of spinning superfluid helium droplets*
16.05.2013	Prof. Dr. Tilman Spohn, Deutsches Zentrum für Luft- und Raumfahrt, Institut für Planetenforschung: *Thermal History of Planetary Objects: From Asteroids to super-Earths, from plate-tectonics to life*
13.06.2013	Dr. Daniel Wegner, Westfälische Wilhelms-Universität Münster, Institut für Angewandte Physik: *Understanding and tuning molecule-substrate coupling for molecular electronics and magnetism*
20.06.2013	Prof. Dr. Hans-Dieter Meyer, Universität Heidelberg, Physikalisch-Chemisches Institut: *Molecular Quantum Dynamics studied with the Multi-Configuration Time-Dependent Hartree (MCTDH) approach*
27.06.2013	Prof. Dr. Bruno Ismer, FH Offenburg, Institut für Angewandte Forschung: *Herzschrittmacher, Defibrillatoren und Ablatoren – Physikalische Techniken zur Behandlung von Herzrhythmusstörungen*
04.07.2013	Prof. Dr. Uwe Kreibig, Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen: *Erweiterte Mie-Theorie: Auf dem Wege zu einer realistischen Theorie der Nanooptik*
11.07.2013	Prof. Dr. Cornelia Denz, Westfälische Wilhelms-Universität Münster, Institut für Angewandte Physik: *Structured light – complex photonic lattices for applications in information processing, material science, and biophotonics*
24.10.2013	Dr. Robert Löw, Universität Stuttgart - 5. Physikalisches Institut: *A single electron in a Bose-Einstein-Condensate*
07.11.2013	Prof. Dr. Oliver Kühn & PD Dr. Roland Waldi, Institut für Physik: *Nobelpreise für Theoretische Chemie und Physik 2013*
21.11.2013	Prof. Dr. Carsten Fallnich, Westfälische Wilhelms-Universität Münster - Institut für Angewandte Physik: *Lichtkontrolle in Glasfasern*
28.11.2013	Prof. Dr. Reinhard Dörner, Goethe-Universität Frankfurt am Main - Institut für Kernphysik: *The Power of Coincidence Imaging – Fundamental Physics with Small Molecules*

05.12.2013	Prof. Dr. Claude Fabre, Université Pierre et Marie Curie - Paris: *Entangled Quantum Frequency Combs: a New Tool for Scalable Quantum Computing?*
09.01.2014	Prof. Dr. Christian von Savigny, Ernst-Moritz-Arndt Universität - Institut für Physik: *Was macht eigentlich das Ozonloch? - Hintergründe und aktueller Kenntnisstand*
16.01.2014	PD Dr. Frank Meyer, zu Heringdorf Universität Duisburg-Essen: *Eine Super-Zeitlupe für Plasmonenwellen*
23.01.2014	Prof. Dr. Eberhard K. U. Gross, Max-Planck-Institut für Mikrostrukturphysik - Halle/Saale: *How to make the Born-Oppenheimer approximation exact: A fresh look at potential energy surfaces and Berry phases*
03.04.2014	PD Dr. Maren Voss, Leibniz-Institut für Ostseeforschung Warnemünde: *Von Prozessen zu Stoffbilanzen: Der Stickstoffkreislauf der Ostsee*
10.04.2014	Prof. Dr. Villy Sundström, Lund University - Chemical Physics, Sweden: *Solar light to electrons and fuel – the fundamental processes*
24.04.2014	Prof. Dr. Markus Münzenberg, Ernst-Moritz-Arndt Universität Greifswald - Institut für Physik: *Hot spins and organic spins for THz spin-electronics*
08.05.2014	Prof. Dr. Jorge L. Chau, Leibniz-Institut für Atmosphärenphysik Kühlungsborn: *Studies of the mesosphere and lower thermosphere with radars*
15.05.2014	Prof. Dr. Cornelia Denz, Westfälische Wilhelms-Universität Münster, Institut für Angewandte Physik: *Strukturierte Lichtfelder – Photonische Gitter für die Informationsverarbeitung und Biophotonik*
22.05.2014	Prof. Dr. Dirk O. Gericke, University of Warwick - Centre for Fusion, Space & Astrophysics, United Kingdom: *Warm Dense Matter – Complex Quantum States between Solids and Plasmas*
05.06.2014	Prof. Dr. Massimo Altarelli, European XFEL GmbH, Hamburg: *X-ray Free-Electron Lasers: Expanding the Frontiers of Crystallography*
19.06.2014	Prof. Dr. Ulf Saalmann, Max-Planck-Institut für Physik komplexer Systeme, Dresden: *X-ray driven electron and ion dynamics in atomic and molecular clusters*
26.06.2014	Prof. Dr. Regina de Vivie-Riedle, Ludwig-Maximilians-Universität München, Department Chemie: *The interplay of nuclear and electron wavepacket motion in the control of molecular processes: A theoretical perspective*
07.07.2014	Dr. Thomas Kalinowski, ehem. Institut für Mathematik: *Optimale Bestrahlungsplanung in der Krebstherapiestudie*
10.07.2014	Prof. Dr. Mikhail Ivanov, Max-Born-Institut Berlin: *Surprising strong-field physics in laser filaments*
16.10.2014	Dr. Kai Schlage, PETRA/DESY Hamburg: *New routes for magnetic nanostructure fabrication and characterization*

23.10.2014	Prof. Dr. Moritz Sokolowski, Universität Bonn: *Large π-conjugated molecules adsorbed on surfaces*
06.11.2014	Prof. Dr. Sylvia Speller, Instiut für Physik: *Smart couplings with small systems*
13.11.2014	Prof. Dr. Peter Heering, Universität Flensburg: *Historische Experimente im Nachvollzug analysieren*
20.11.2014	Prof. Dr. Dwayne Miller, CFEL und Universität Hamburg: *Mapping atomic motions with ultrabright electrons: The chemists' Gedanken Experiment enters the lab frame*
11.12.2014	Prof. Dr. Sybille Günther, Max-Planck-Institut für Plasmaphysik, Garching: *Physics basis of magnetic fusion power plants*
08.01.2015	Prof. Dr. Manfred Bayer, Technische Universität Dortmund: *Rydberg excitons in cuprous oxide*
15.01.2015	Prof. Dr. Eberhard Riedle, Ludwig-Maximilians-Universität, München: *From vacuum fluctuations of the electromagnetic field to ultrafast spectrometers for chemical processes with extreme spectral and temporal coverage*
22.01.2015	Prof. Dr. Hartmut Ruhl, Ludwig-Maximilians-Universität, München: *The interaction of ultra-thin foils with intense laser radiation*
09.04.2015	Dr. Jan Sperling, Universität Rostock: *Quantum correlations and measurements*
21.05.2015	Dr. Christian Rödel, Universität Jena: *Novel routes in relativistic surface high harmonic generation*
04.06.2015	Prof. Dr. John Plane, University of Leeds: *How large is the cosmic dust flux into the earth's atmosphere?*
11.06.2015	Prof. Dr. Hans-Jakob Wörner, ETH Zürich: *Controlled attosecond dynamics in molecules*
02.07.2015	Fakultätskolloquium, Wissenschaftshistorischer Rundgang: Abschied vom Physikalischen Institut
15.10.2015	Prof. Dr. Metin Tolan, Universität Dortmund: *Geschüttelt, nicht gerührt! James Bond im Visier der Physik*
29.10.2015	Prof. Dr. Caren Hagner, Universität Hamburg: *Warum müssen Neutrinos Masse haben – Hintergründe zum Nobelpreis 2015*
24.11.2015	Dr. Alexander Sorokin, Institute for Scintillation Materials of NAS of Ukraine: *Molecular Aggregates: Luminescence properties and exciton dynamics*
03.12.2015	Dr. Peter Wagner, Institut für Mathematik: *Zur Extremalen Graphentheorie*
10.12.2015	Prof. Dr. Kai Roßnagel und Prof. Dr. Michael Bonitz, Universität Kiel: *Kiel-Rostock-Kolloquium*
17.12.2015	Prof. Dr. Ralph Neuhäuser, Universität Jena: *Merkliche Sonnenflecken zur Vergnügung derer Anschauenden*

5.3 Scientific Meetings and Workshops

Date	*Title*
16.–19.06.13	Quantum Fluid Clusters, Regensburg
08.–13.09.13	XVII. International Conference on "Recent Progress in Many-Body Theories", Rostock
23.–25.10.13	2nd International Joint Workshop on "High Pressure, Planetary and Plasma Physics", Berlin
23.–24.05.14	9th Materials' Days, Rostock
14.–19.06.14	Lähnwitzseminar on Calorimetry
24.07.14	SFB 652 Summer Workshop on "Ultrafast Cluster Dynamics", Rostock
27.–28.08.14	3rd International Workshop on "Exciton Dynamics and Spectroscopy", Rostock
24.–26.09.14	3rd International Joint Workshop on "High Pressure, Planetary and Plasma Physics", Rostock
09.–10.10.14	SFB Workshop 2014 in Plau am See
01.-07.02.15	Winter School on "Matter in Extreme Conditions", Montgenevre/France
04.–05.06.15	10th Materials' Days, Rostock
13.–18.09.15	3rd International Conference on "Correlations in Radiation Fields" (CERF15), Rostock
20.–25.09.15	Cluster Meeting, Lindow
23.–25.09.15	4th International Joint Workshop on "High Pressure, Planetary and Plasma Physics", Bayreuth
10.12.15	Rostock-Kiel Colloquium, Rostock