

Institute of Physics  
Research Report  
2007-2009





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**Research Report  
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# Preface

In this research report the Institute of Physics at the University of Rostock presents its activities during the years 2007 - 2009. They are based on a long tradition in physical research at this place. The University was founded in 1419 and is the oldest in the Baltic area. One of its students has been the famous astronomer Tycho Brahe. The first chair of physics was set in place 1874 for Ludwig Matthiessen who investigated problems in optics which is still a very active research field of the institute. Later several well known physicists like Otto Stern, Pascual Jordan, Walter Schottky and Friedrich Hund joined for some time the University. The institute has meanwhile a high reputation in several of the most innovative research fields in physics like light-matter-interaction and nanomaterials. Due to the two adjunct external institutes Baltic Sea Research Institute and Leibniz Institute for Atmospheric Physics there is in addition strong expertise in maritime and atmospheric physics.

With respect to education and training the institute offers programs for all needs in the field of physics. They are highly attractive for students and were ranked twice as absolute top in the CHE reports. In accordance with the Bologna process the original diploma studies had to be transferred into bachelor and master programs. Still the traditionally strong scientific components of the studies are conserved. An additional master program is offered in English adapted to the special needs of students from abroad. Programs for teachers of all types of schools are provided as well as physics courses for other natural sciences and engineering. In addition there are outreach activities for pupils and the public. A new graduate school with the focus on light-matter-interaction was established beside the existing one 'Physics, Chemistry, and Technology of New Materials' and provides ideal conditions for PhD students with regard to supervision, extended training, visibility, and promotion of the ability to work on one's own.

During the last three years Professors Röpke, Henneberger, and Kranold retired. Oliver Kühn and Dieter Bauer were appointed as Professors for Theoretical Physics and Stefan Lochbrunner for Experimental Physics. Prof. Kühn works on the ultrafast dynamics of molecules and Prof. Bauer on the quantum dynamics in intense laser fields. Prof. Lochbrunner's research focuses on time resolved spectroscopy of molecular processes and organic materials. With these appointments the institute strengthened its competence in photo induced processes and electromagnetic interactions. At the same time the gap between atomic physics on one side and solid state physics and material sciences on the other side is closed by introducing research on molecular systems beside the established field of cluster physics.

The research is accompanied by extensive acquisition of third party funding. This



Institute of Physics (source: Prof. F. Mitschke)

holds for the individual groups and in particular for several collaborative initiatives. First of all, the collaborative research center SFB652 was prolonged for a second period of another four years. Ten groups of the institute, one of the Institute of Chemistry and three from the University of Greifswald are collaborating within the center. A more detailed description is found in section 3.1. Three other collaborative initiatives are based on the department “Science and Technology of Life, Light, and Matter” (LL&M) which is one of the four departments of the Interdisciplinary Faculty (see Chapter 4). For the department LL&M a team of physicists (Profs. Redmer, Meiwes-Broer, Lochbrunner) and chemists (Profs. Ludwig, Kragl, Zimmermann) wrote a successful proposal for a research building dedicated to complex molecular systems and worth 20 Mio. Euro. The building will provide laboratory space and facilities for interdisciplinary projects and construction will start at the end of 2010. Three groups (Profs. Meiwes-Broer, Kühn, Lochbrunner) of the Institute of Physics contribute to the initiative ‘Light to Hydrogen’ (L2H) which started at the end of 2009 and is dedicated to the development of efficient photocatalytic methods to split water into hydrogen and oxygen using solar energy. It is led by the Leibniz-Institute for Catalysis and funded by the BMBF via the program “Spitzenforschung und Innovation in den neuen Bundesländern”. Funded by the same program, the initiative ‘Regional Development of Medical Innovation and Research’ (REMEDIS) also started at the end of 2009. It has the goal to develop new micro implants and is headed by the Institute for Biomedical Technique of the University. Two groups of the Institute of Physics (Profs. Meiwes-Broer and Lochbrunner) participate in this collaborative project which again is a part of the research of the department LL&M. These activities demonstrate that the insti-



July 22nd, 2009: Physics leaves the main building of the university after 50 years.

tute plays an important role for the central research areas in Rostock and strongly contributes to the profile of the University.

The plans for a new physics building made crucial progress during the last years. An architecture competition was conducted and the detailed planning for the building is nearly completed. Construction will start at the end of 2010. More information will be given in section 1.2. Due to the major reconstruction of the main building of the University the groups of Profs. Kühn, Redmer, Röpke, and Schick had to move out and are located in the Wismarsche Straße until the new physics building will be opened.

In the following we present the activities of the institute with the help of some statistics and particularly by short descriptions of the main research projects performed in the individual groups. The reader will see that a lot of innovative and exciting science is going on and we encourage everyone to contact us in order to learn more about this attractive place, to start collaborations, to look for postdoc and PhD positions, or to find the optimal course of studies.

Prof. Dr. Stefan Lochbrunner  
Managing Director, Institute of Physics



# 1 Overview of the Institute

## 1.1 General

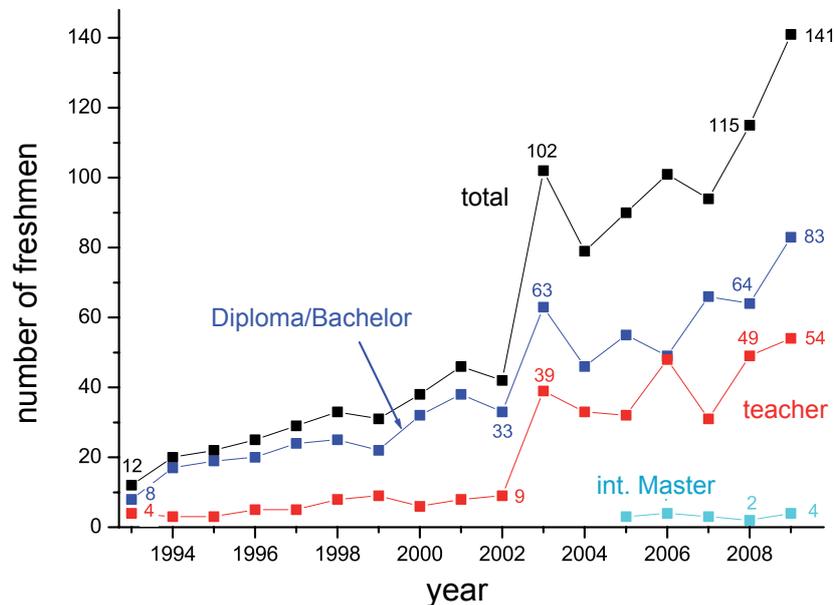
During the period of this report the number of **faculty members** could be kept on a constant level of 14 professors (without Leibniz institutes), with the newly introduced W2/W3 positions gradually replacing the traditional C3/C4 appointments. The scientific staff was completed by 5 lecturers (Privatdozenten). PD Dr. Heidi Reinholz has been appointed to a temporary professorship at the J. Kepler-University Linz, Austria (from 10/2009 on).

	2007	2008	2009
C4 professors	8	8	8
C3 professors	5	5	4
W3 professors	1	1	2
W2 professors	0	0	1

In the reporting period 23 students received their **Doctor's degree** and one **Habilitation** has been issued by the Faculty of Mathematics and Natural Sciences (see Section 5.1 for details).

Concerning the number of **freshmen** the favorable trend of the previous years continued, reaching a total of 141 students (Bachelor and teacher) in 2009 (see graphics on next page). While the majority of the students still comes from Mecklenburg-Vorpommern, we have witnessed an increase in the number of students from other states of Germany and from abroad. The attractiveness of Physics at the University of Rostock has been underpinned by the CHE ranking of the Zentrum für Hochschulentwicklung in 2009 where our institute has been among the top three in Germany.

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 (HBFÜG) and by industry. The major part of operational expenses of the institute was financed by these external financial sources. Here, the budget exceeded 3.5 Mio Euro in 2009.



Number of freshmen at the Institute of Physics. Note that in 2007 the Bachelor replaced the Diploma curriculum.

## 1.2 New Building for the Institute of Physics

Plans for a new building for the Institute of Physics have been made since 1950 but have never been realized in the former GDR (East Germany). These efforts were intensified after the German reunification in 1990. The current plans of the State Mecklenburg-Vorpommern schedule a begin of the construction by the end of 2010 so that the new institute should be finished by the end of 2012.

The new Institute of Physics will be built on the Campus *Südstadt* in the Albert-Einstein-Straße, see Fig. 1.1. The competition to design the new Institute was won by the company *Gerber Architekten GmbH* from Dortmund in October 2008. The new Institute consists of a laboratory building and a teaching complex with lecture halls and seminar rooms. Both buildings are connected by a bridge over the Campus Street in the first floor. The total floor space of the institute will be 6915 m<sup>2</sup>, among them 800 m<sup>2</sup> for the Collaborative Research Center SFB 652. The total costs for the project amount to 36.6 Mio. Euro.

The laboratory building will provide a state-of-the-art infrastructure for the research fields of the institute: Optics and Laser Physics, Nanomaterial Research, and Molecule, Cluster and Plasma Physics. The laboratories are equipped with complex systems for temperature control, vibration damping, and are screened against external electromagnetic sources. The interior and the offices will generate a friendly



**Fig. 1.1:** The locations of the new buildings of the Institute of Physics and the science building LLM on the Südstadt campus. A: physics institute, B: physics teaching building, C: research building of the department LLM (estimated locations).

atmosphere for scientists and students. The buildings are equipped with a high-speed computer net. The teaching complex houses three lecture halls of different size, seminar rooms, rooms for the student’s physical laboratory work as well as the permanent physical collection. Eventually, all facilities for research and teaching in Physics at the University of Rostock will be located in one complex, after the Institute has used various buildings spread over the whole city for more than 50 years.

Simultaneously, the laboratory building for the Department Life, Light and Matter (LLM) of the Interdisciplinary Faculty will be built in direct neighborhood of the new Physics Institute. The funding of the LLM building could be achieved within a German-wide competition led by the German Science Council (Wissenschaftsrat) in May 2009. The corresponding research program has been devoted to “Complex Molecular Systems” and is strongly driven by Physics and Chemistry, but it reaches



**Fig. 1.2:** Prof. T. Strothotte, Dr. O. Ebnet, H. Tesch (from left) on occasion of the first cut of the spade at the site of new Informatics/Physics campus on July, 18th 2008 (source: Prof. F. Mitschke).

out into topics of life sciences and engineering. The company *Gerber Architekten GmbH* has finished the plans in April 2010. The scheduled building has a total floor space of 2387 m<sup>2</sup> and will cost 15 Mio. Euro. It will house three core facilities for mass spectrometry, nuclear magnetic resonance, and a center for modeling and simulation.

The whole complex consisting of three buildings (laboratory building Physics, teaching complex Physics, laboratory building of the Department Life, Light and Matter) will be finished by the end of 2012 on the Campus *Südstadt*. It will have a strong impact on research and teaching in Physics in Rostock. We therefore anticipate that it will attract many scientists and students.

## 2 Research Activities

### 2.1 Optics and Laser Physics

#### 2.1.1 Nonlinear Optics

**Head:** Prof. Dr. Fedor Mitschke

**Staff:** Dr. Michael Böhm                      Dr. Adarsh Kumaran Nair Vasala Devi  
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Dipl.-Phys. Peter Keller              Dipl.-Phys. Christoph Mahnke  
Dipl.-Phys. Toralf Ziemis  
Hartmut Reichwagen                  Anja Gloede  
Helga Harder                              Theresa Kopplow

#### **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 light propagation is influenced. *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 inside they rely on nonlinear processes themselves.

Our focus during the report period has been on the nonlinear interactions which occur when a short pulse of light travels down an optical fiber. The group head published a review article in [7]; after his earlier textbook on fiber optics in the German language 2005 now also an English edition has come out [8].

Given the right conditions, very special pulses called solitons can arise. A quarter century after their first experimental demonstration solitons have found their way into commercial applications in optical telecommunication. One aspect of our work deals with the fundamental limitations of the data-carrying capacity of fibers, and with ways to extend that limit using soliton concepts. Another aspect is to use the nonlinear interactions in a fiber to generate broadband light; feedback is employed to enhance the process.

#### **Soliton Molecules**

Optical communication is all about robust pulse structures: Signal pulse shapes must be stable over long distances so that the message arrives intact. This makes solitons so valuable because they have the property of ‘self-healing’ after perturbation. We

kept pursuing the case of dispersion-managed fibers (a.k.a. dispersion-alternating fibers) because these have several technical advantages and are increasingly favored in applications.

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, may provide a viable means to further increase the data-carrying capacity of fibers, so that the impending capacity bottleneck (called the ‘capacity crunch’ by some) might be avoided.

The surprising discovery of stable soliton molecules prompted researchers elsewhere to pursue this concept further in theoretical studies. However, our experimental proof of existence was technically demanding, and has not been attempted elsewhere since. In the meantime we have refined the original demonstration:

The experiment was vastly improved by the incorporation of a new diagnostic tool, a method by which an unambiguous assessment of the complex (amplitude-and-phase) structure of the soliton molecules becomes possible. We could show in [5] that previously advocated techniques fail where this new method (dubbed ‘VAMPIRE’, for ‘very advanced method for phase and intensity retrieval of e-fields’) works flawlessly.

The insight provided with this method allowed a detailed understanding of the interaction mechanism that keeps the solitons bound together in the molecule. A theoretical model based on a perturbation ansatz corroborates the findings[4].

Recently it has been observed by several researchers that in the process of generation of supercontinuum in an optical fiber, there are occurrences of soliton pairs which maintain their mutual separation while they jointly slide in frequency due to the Raman shift. We modified our perturbation ansatz to this situation and could show that these pairs are not bound pairs in the precise meaning of the word, but rather that the attractive or repulsive interaction between them is strongly reduced by the Raman effect so that the separation quite naturally remains neutral[6].

### **Soliton Analysis**

Soliton radiation beat analysis is a mathematical, computer-assisted technique providing insight into soliton dynamics which is not subject to the severe restrictions of the ‘classical’ analytical technique, Inverse Scattering Transform. After the first demonstrations of this method in 2006 we have now applied it to several situations in which previously no direct insight was available.

The case of arbitrary, non-soliton-like pulse shapes was treated in [1]. The particularly intriguing case of a lossy fiber, with the eventual destruction of the soliton, was elucidated in [2]; it turned out that the literature contains some half-truths.

### Fourier Transform

We have introduced a discrete Fourier transform technique which extracts more spectral information from a given time series data set than conventional discrete Fourier transform. Valid information is obtained between the spectral bins of conventional discrete Fourier transform, scalloping error is greatly reduced, and amplitude and phase of Fourier components are more true to the process under study as with conventional discrete Fourier transform. The method was spelled out in a publication written jointly with M. Tasche of the Institute of Mathematics[3].

### Photonic Crystal Fiber

We have ventured into the possibility of guiding light in a photonic crystal fiber with hollow core, when the core is filled with a liquid. The liquid is intended to move particles into the fiber where they experience intense interaction with the guided mode.

### Optical Supercontinuum

We have investigated the generation of spatially coherent yet broadband light – now known as optical supercontinuum – in a highly nonlinear photonic crystal fiber. In our approach the nonlinearity was further enhanced by optical feedback.

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## 2.1.2 Quantum Optics

**Head:** Prof. Dr. W. Vogel

**Staff:** Dr. C. Di Fidio    Dr. A. Semenov    Dr. E. Shchukin  
Dr. Th. Richter    Dr. D. Vasylyev    Dr. S. Singh  
Dr. S. Mandal  
Ch. Gehrke    P. Grünwald    Th. Kiesel  
F. Töppel    J. Sperling    A. Mahdifar

### Nonclassicality

The characterization of nonclassical effects is of fundamental interest for the basic understanding of quantum physics, cf. e.g. [22, 20]. In addition, they can be useful for applications, such as highly sensitive measurements. We have shown that the nonclassical signatures of characteristic functions can be used for very sensitive measurements of damping effects [9].

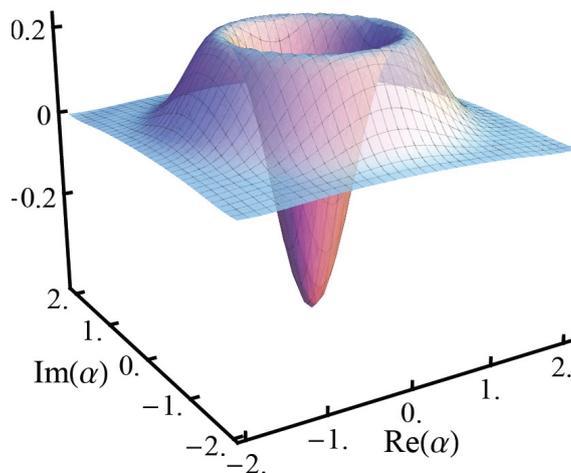
Nonclassicality criteria on the basis of observable moments, which have been developed by us, have been generalized for characterizing the nonclassical space-time dependent correlation properties of a radiation field [21]. This method allows to completely describe the quantum effects of multimode fields. In addition, also radiation properties of atomic sources can be characterized by these conditions.

We have analyzed the properties and the realization of some complex nonclassical states. The preparation of sphere-coherent states with trapped ions has been considered [8]. We have studied generalized squeezed states including the possibilities of their experimental preparation in the motion of trapped ions [13].

Of particular interest is the possibilities to identify quantum effects in experiments. Based on the experimental study of single-photon-added thermal states (SPATS), we have reconstructed the Glauber-Sudarshan  $P$  function [7]. This was the first experimental reconstruction of a  $P$  function showing negativities, cf. Fig. 2.1, which is a direct demonstration of nonclassicality based on its original definition. For many quantum states such a reconstruction is impossible, e.g. for squeezed states or phase-randomized squeezed states. In such cases the nonclassical effects can be demonstrated by using characteristic functions or quantum statistical moments [6].

### Entanglement

Entanglement is the main resource of the rapidly growing field of Quantum Information Technology. This nonlocal and nonclassical property can be detected in various ways. One possibility is the violation of Bell-inequalities. Quantum states, which admit the local-hidden-variables model, cannot violate these inequalities. Such inequalities are based on measuring two observables of a two mode system. Using classical square identities, new Bell-type inequalities for up to eight observables have been derived [14]. They can be applied to multi-mode systems by using alge-



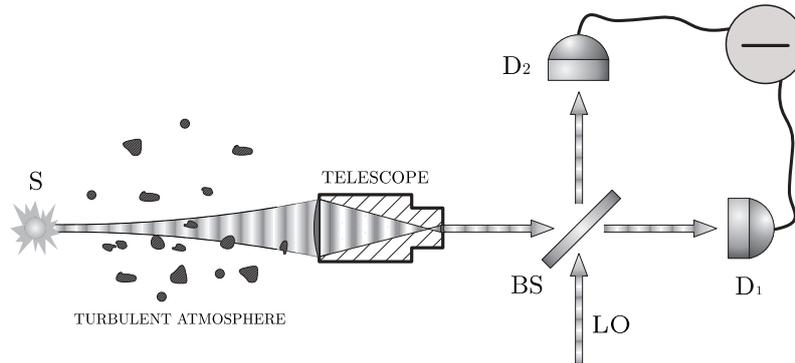
**Fig. 2.1:** Experimentally determined  $P$  function of a SPATS showing negativities (after [7]).

bras corresponding to quaternions and octonions. Another way for the identification of entanglement is given by linear entanglement witnesses. Equivalently, the formulation of optimized, necessary and sufficient entanglement conditions in terms of arbitrary observables has been derived [15]. The optimization procedure of these inequalities leads to a set of coupled eigenvalue equations, called separability eigenvalue equations (SEE).

In analogy to the  $P$  function for coherent states the definition of specific quasi-probabilities,  $P_{\text{Ent}}$ , shows that entanglement can be represented as a quasi-mixture of separable quantum states. However, such quasi-distributions are ambiguous. Again, the optimization over a manifold of possible distributions delivers the SEE [16]. The optimized  $P_{\text{Ent}}$  reveals negativities, if and only if the quantum state is entangled. Moreover, it has been shown that entanglement can always be detected within a finite dimensional subsystem, even if the compound system can only be described completely by continuous variables [17].

## Cavity QED

Cavities are of fundamental research interest since they are widely used in experiments. We studied absorption and scattering losses in a high- $Q$  cavity, by introducing additional terms for damping and noise in the quantum Langevin equations and in the input-output relations [10]. A direct measurement of the parameters of a realistic leaky cavity with unwanted noise has been studied [12]. Bringing a two-level atom into a lossy cavity, the quantum trajectory method is also appropriate to describe unwanted losses, e.g. photon absorption and scattering by the cavity mirrors, and spontaneous emission of the atom [3]. The shape of spatiotem-



**Fig. 2.2:** Scheme for the transmission of quantum light through the atmosphere (after [11]).

poral radiation modes emitted by the cavity depends on the interaction, and it is controllable through the interaction time.

In the framework of quantum electrodynamics in dispersing and absorbing media, emitted radiation of a two-level atom in a high- $Q$  cavity has been studied [5][4]. We considered also the case when the emitted photon belongs to a wave packet spread inside and outside the cavity, and we obtained the resulting spatiotemporal shape of the outgoing wave packet and the efficiency to carry a one-photon Fock state. The correlations between this approach and the quantum noise theory (inner and outer cavity field represent different degrees of freedom) has been studied.

A cascade of two atom-cavity systems driven by Raman interaction has been considered in the context of entanglement [1]. We used such a system to study the entanglement evolution between the atoms. Moreover, this setup can be used for storing entanglement by switching off the coupling. The emitted photon of two coupled cavities carries the entanglement information between both intracavity fields [2]. Thus, entanglement can be observed by the mode structure of a single photon. This method can be used to reveal the dynamics and the transfer of entanglement between the cavity modes.

### Propagation of Quantum Light through Media

We have studied the propagation of quantum light through semiconductor media. For this purpose we have combined methods of field quantization in macroscopic media with the microscopic theory of semiconductors. We have analyzed by these methods the propagation of squeezed input radiation through a semiconductor [19]. In this approach we were able to develop a unified treatment of the propagation of nonclassical light, both for conditions of absorption and gain in the semiconductor. We have further refined the theory by including results of microscopic semiconductor theory to study the propagation of squeezed light under more realistic

conditions [18].

Another situation of increasing interest is the propagation of nonclassical light through the turbulent atmosphere. A detailed understanding of the effects of turbulence on the quantum properties of the transmitted light is of great importance in the context of quantum communication, see Fig. 2.2. We have developed the basic concepts for the description of the effects of turbulence on the quantum effects of light during its propagation [11]. Besides developing general theoretical methods for dealing with the turbulence effects in the quantum domain, we could show that the quantum effects of weak light fields are more robust than those of bright fields.

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### 2.1.3 Semiconductor Optics

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#### General Outline of the Research

The main topics of our research are the study of *fundamental quantum processes in semiconductors* and *their interaction with light* on time scales from several hundreds of microseconds down to some femtoseconds ( $10^{-15}$ s), especially with respect to future applications in computer and communication technology.

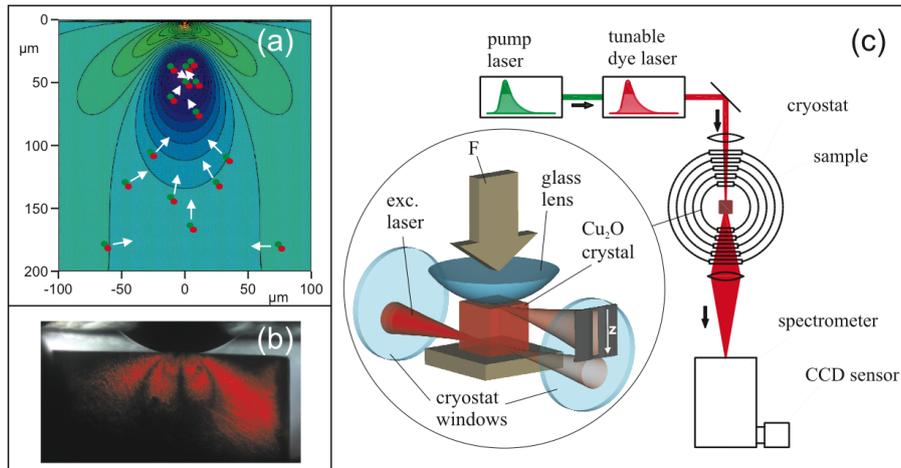
The main focus of our research has been the study of Bose-Einstein condensation of excitons in the collaborative research activity SFB 652 of the Deutsche Forschungsgemeinschaft ‘Strong correlations and collective effects in radiation fields: Coulomb systems, clusters and particles’.

A second topic has been the study of quantum optical properties of semiconductor nanostructures which has been financially supported by the Deutsche Forschungsgemeinschaft in the research group ‘Quantum optics of low dimensional semiconductors’ up to July 2009. Part of these research is continued in the SFB 652.

Initiated by the Interdisciplinary Faculty of the University we recently started together with the clinic of ophthalmology an interdisciplinary research project on spatially resolved light scattering from eye structures.

#### Bose-Einstein Condensation of Excitons

In semiconductors a new state of matter could be generated by exciting electron-hole pairs with intense laser pulses. This state is similar to that of common matter in many aspects: Bound states, very similar to the hydrogen atom, can build up which are called excitons. These could further form molecules (biexcitons) or even larger aggregates under adequate circumstances. Due to their tiny mass - the exciton mass is more than three orders of magnitude smaller than that of the hydrogen atom - excitons show up pronounced quantum properties already at temperatures of a few Kelvin which is quite different to common matter where temperatures of a few micro Kelvin are necessary. In the focus of this project are the thermodynamical properties of dense exciton systems. Especially, the existence of a theoretically proposed Bose-Einstein condensate and its interaction with the light field is of particular interest.



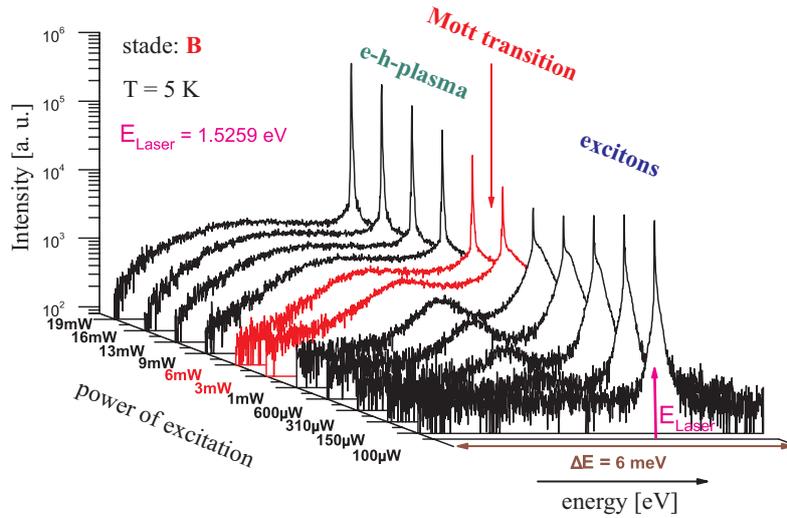
**Fig. 2.3:** Setup of the optical experiment to investigate the possibility of an excitonic Bose-Einstein condensate at ultralow temperatures. Part (a) shows the creation of the excitonic trap by Hertzian stress, part (b) shows the sample with applied stress at  $T=50$  mK between crossed polarizers to reveal the strain distribution by the induced double refraction. Part (c) shows the experimental setup with pulsed dye laser and spectroscopic equipment to resolve the luminescence both spatially and spectrally.

All previous studies, however, did not reach sufficient low temperatures of the exciton system. Here we could make a big advance by installation of a new magneto cryostat system which is unique by allowing direct optical access to the sample space at temperatures below 50 mK and magnetic fields up to 7 T (see Fig. 2.3).

In this project we are investigating two different types of systems:

a) Strong inhomogeneous electric fields shall be applied to high quality semiconductor quantum well samples which generate a parabolic-like potential in the quantum well plane such that the exciton motion becomes directed onto the potential minimum where the dense exciton matter shall arise. Furthermore, the excitons become aligned along the growth direction in the potential center due to band shifts along the electric field. Therefore, the wave function overlap between electron and hole will be reduced, so that the radiative decay of the excitons will be suppressed. This leads to a longer life time in which quantum correlations can build up. The excitons in these systems can be analyzed with the method of phase-sensitive reflection spectroscopy which we have developed for states in zero electric field [13, 11, 6].

b) High quality cuprous oxide samples [2] with homogeneous exciton linewidth in the nano electron volt range [2]. By applying stress to the sample surface via a spherical glass lens (see Fig. 1) we are able to create a potential trap for the excitons of a depths of a few meV, which is sufficient to collect optically excited excitons. For this purpose, we have build up a tunable pulsed dye laser system with small line



**Fig. 2.4:** Spectrally resolved intensity of resonance fluorescence from a size-confined electron-hole system in a quantum well. The spectra show the pronounced saturation of the excitonic resonance fluorescence and the transition to an electron-hole plasma at higher power. The sideband at moderate power is due to emission from a biexciton state. The size of the emitting spot is about  $1 \mu\text{m}$  in diameter. From [3].

width so that one can excite the excitons directly inside the trap. First experiments have already shown that we are able to create inside the trap an excitonic gas with high density at temperatures around 0.5 K in quasi-thermal equilibrium.

### Quantum Optics of Semiconductor Nanostructures

This research project aims to explore the quantum properties of the light emitted from semiconductors under resonant excitation. This re-radiation is commonly referred to as resonance fluorescence (RF). In semiconductor systems, quasiparticle excitations, like excitons, are fermions at the composite level. Since Coulombic many-body effects are usually strong in semiconductors, one may expect significant fermion contributions also in excitonic RF [14]. As a first step, we have investigated the RF from disorder localized excitons in high quality quantum wells and have been able to observe single excitonic RF for the first time. This opens up to study the dependence of the spectrum of RF on the intensity of excitation, where we expect to see strong changes due to the coupling to the light which will be significantly different whether excitons behave like bosons or more like fermions. While in the latter case, one expects the dressing of the exciton states to show up as kind of a Mollow triplet, in the bosonic case no splitting will be observed. This is indeed the case for our systems of weakly localized excitons as can be seen nicely in the excitation power dependence displayed in Fig. 2.4. With increasing power, the exciton

RF becomes saturated and shows a broadening and a slight spectral shift to higher energies. At a certain power level, however, the excitonic features vanish and the typical light scattering spectrum of an electron-hole plasma shows up with a broad contribution due to scattering by plasmons. We thus have been able to observe the Mott transition in the electron-hole system directly [3]. The quantum statistical properties of this RF is expected to show sub-Poissonian statistics and the possibility of squeezing below the quantum noise level [14]. Here experiments are under way.

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### 2.1.4 Theoretical Solid-State Optics

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#### **Photon Green's Function for Bounded Media: Splitting Property and Nonequilibrium Radiation Laws**

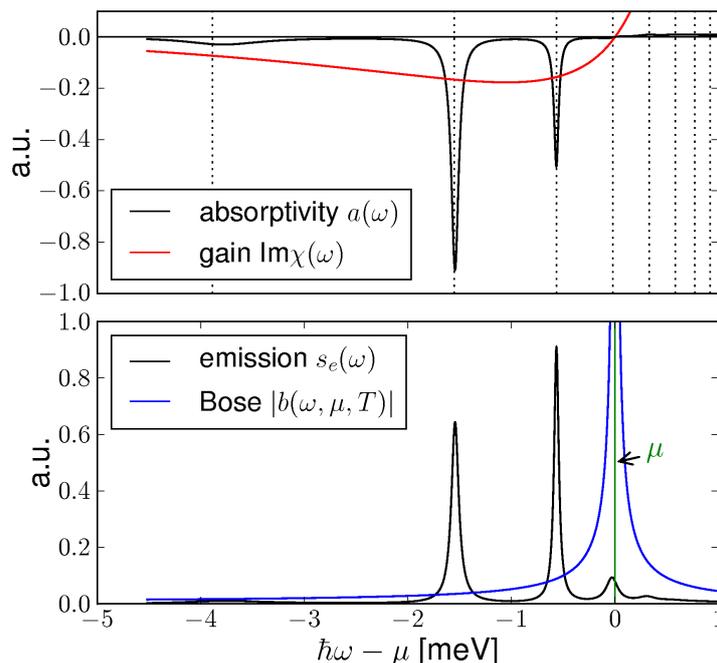
A radiation field coupled to a many-particle system in nonequilibrium can be described in a quantum-mechanically exact way using the photon Green's function on the two-time Keldysh contour. However, spatial inhomogeneity of the system, as induced, e.g., by the presence of medium boundaries, makes its exact treatment complicated. For the experimentally relevant slab geometry at stationary excitation we were the first being able to exactly take into account the spatial inhomogeneity. With the help of a careful re-definition of Poynting's theorem we proved that common approximations to this problem indeed fulfill the energy conservation condition, which was doubted for decades [6]. Starting from the photon Green's function we derived a radiation law generalizing Planck's and Kirchhoff's laws [5, 1]:  $s = s_e - s_a = (b - n)a$ . The (quantum statistical) emission  $s_e$  appears to be proportional to the (classically determinable) absorptivity  $a$ . Proportionality factors of emission and absorption  $s_a$  are distributions of internal ( $b$ ) and external ( $n$ ) excitations. In quasiequilibrium,  $b$  turns into a Bose function (KMS condition), the total equilibrium is the limiting case of Planck's law.

Including results from the theory of quantum condensation (see above), explicit predictions for optical signatures of a condensate in the medium could be made [5]: while there is no signature in the absorption spectrum, in the emission spectrum a  $\delta$ -shaped peak at  $\hbar\omega = \mu$  occurs, i.e., at the crossover from absorbing to amplifying behavior where no normal emission takes place.

Based on the above findings, we discussed and demonstrated the relations between absorption, emission, lasing, and spatial inhomogeneity in semiconductors at different excitation states and identified different mechanisms of emission [7], see Fig. 2.5 for absorptivity and emission spectrum of a highly excited ZnSe layer. Furthermore, some core relations could be generalized to arbitrary geometries and nonstationary excitation conditions while still fully considering exactly the spatial inhomogeneity problem [2].

#### **Propagation of Nonclassical Light Through Semiconductors**

Footing on the above results for the PGF description of radiation field coupled to a many-particle system, we have investigated the propagation of nonclassical light



**Fig. 2.5:** Absorptivity, gain, and emission spectrum of a highly excited ZnSe layer.

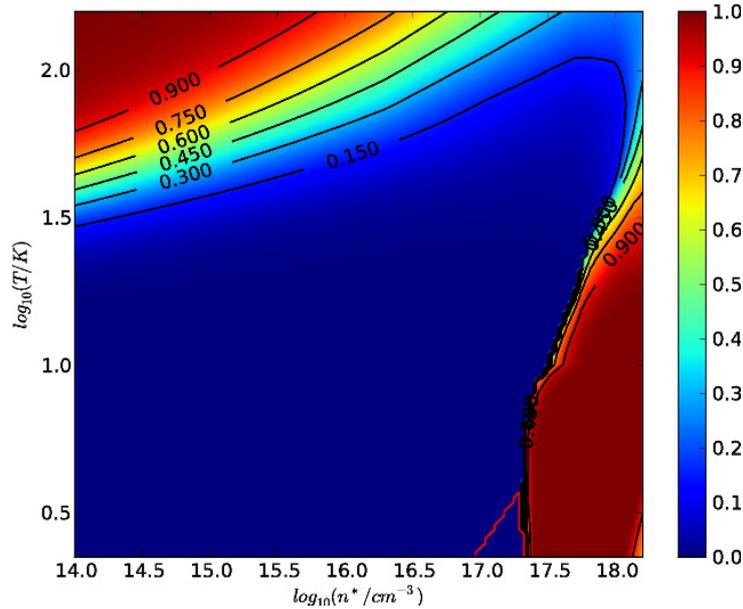
through semiconductors in cooperation with the group of W. Vogel (see Report of the Quantum Optics Group, [12, 13]).

### Ionization Equilibrium, Mott Effect, and Bose-Einstein Condensation in Excited Semiconductors

Excitons, bound electron-hole ( $e-h$ ) pair excitations in semiconductors, have been a favorite for the experimental realization of Bose-Einstein condensation (BEC) for decades. Their existence, however, is restricted by the Mott transition, i.e., the breakup of the bound states with increasing density. For very high densities, a crossover to a BCS-type condensate of weakly interacting  $e-h$  pairs is expected.

This area has been the subject of several publications of our group. In the framework of real-time Green's functions, we have developed a unified theory of quantum condensation in  $e-h$  plasmas relying on the feature of time long-range order (TLRO) occurring in the two-particle ( $e-h$ ) Green's function [3, 10]. Besides deriving a system of generalized Gorkov equations, we have analyzed the quasi-equilibrium case and obtained by solution of the gap equation a common phase boundary of the quantum condensate. This phase boundary comprises both limiting cases (BEC and BCS condensate) with a smooth crossover between them.

The analysis of the region of existence of an excitonic BEC requires a careful analysis of the ionization equilibrium of the partially ionized  $e-h$  plasma and the



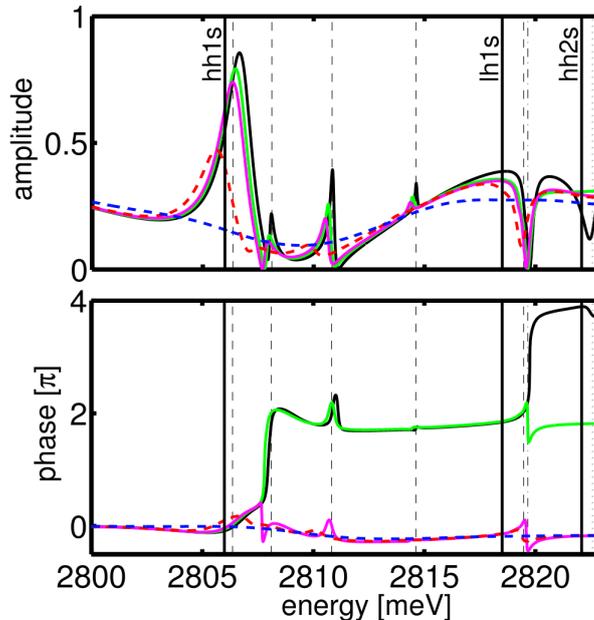
**Fig. 2.6:** Isolines of the degree of ionization in the density–temperature plane for ZnSe. The red triangle at the bottom borders the region where BEC of excitons is possible.

Mott effect [8, 11]. For this, we derived the carrier density in extended quasiparticle approximation which then can be split into free quasiparticle, scattering, and bound state contributions. Introducing a chemical picture by defining the bound  $e-h$  states (excitons,  $X$ ) as a new basic particle species leads to a general mass action law and, in the nondegenerate case, to the Saha equation. Many-particle effects occur, in particular, at two places: the carrier self-energies in the quasiparticle densities and the exciton energy. The self-energies have been calculated self-consistently in dynamically screened random phase approximation (RPA). The exciton ground-state energy has been obtained by solution of the semiconductor Bloch equations. A measure for the state of the  $e-h$  plasma is given by the degree of ionization defined by  $\alpha = n_e^*/n_e$ , where  $n_e^*$  ( $n_e$ ) is the free (total) electron density. Isolines of  $\alpha$  for zinc selenide (ZnSe) are shown in Fig. 2.6 in dependence on density and temperature. The most remarkable feature is the Mott transition appearing as a jump from  $\alpha = 0$  to  $\alpha = 1$  with a nearly temperature independent Mott density at low  $T$ . A window for the occurrence of BEC of excitons is opened at low temperatures just below the Mott density (red triangle).

### Phase Behavior of the Reflected Light at Semiconductor Layers

In the vicinity of the band edge the strong coupling of light with exciton resonances leads to a splitting of the light dispersion, known as polariton effect. In heterostructures the spatial dispersion leads in addition to the well-known Fabry-Perot modes to

an additional series of interferences of polariton waves above the exciton resonances. This is demonstrated in the figure below (black curves), where the amplitude, the phase of the reflected light from a ZnSe-ZnSSe heterostructure and the positions of the light- and heavy-hole excitons (lh, hh) are presented. The single polariton modes are marked by thin vertical lines.



**Fig. 2.7:** Amplitude (upper) and phase (lower) of light reflected at a shallow-confined ZnSSe heterostructure.

We have investigated the behavior of this modes both in the emission and in phase and amplitude of the reflected light in cooperation with the Semiconductor Optics Group of H. Stolz. Inspecting the experimental results for the reflection we could reconstruct the transmission and absorption in the sample theoretically. This enabled us to use the measured emission for the reconstruction of the spectral distribution of polaritons [6]. We found that the polariton distribution is strongly located in the polariton modes being far away from thermal equilibrium [9].

In [4] we have demonstrated that the appearance of pronounced polariton interferences in the phase-resolved reflection of shallow-confined ZnSSe heterostructures opens the possibility of a detailed study of the Mott transition of excitons due to excited carriers. In particular, the phase shows abrupt jumps by  $\pi$  at the polariton modes, which vanish with increasing excitation of carriers (see Fig. 2.7, the carrier density is ranging from  $n = 5 \cdot 10^{15} \text{ cm}^{-3}$  (green) to  $n = 2 \cdot 10^{17} \text{ cm}^{-3}$  (blue),  $n = 0$  (black)). We explain these carrier induced changes by many-body effects between excited carriers as the dynamical screening of the Coulomb interaction and quantum kinetic effects in the scattering.

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## 2.1.5 Clusters and Nanostructures

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Dipl.-Phys. Christian Peltz	Dipl.-Phys. Stefan Polei
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cand. phys. Christian Schumann	
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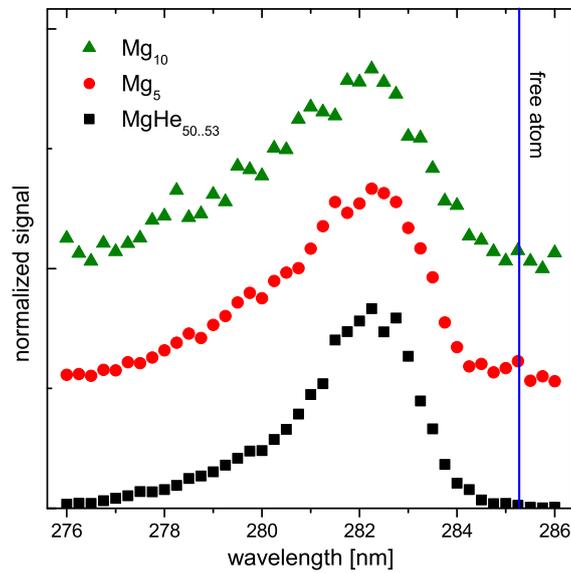
### General Outline of the Field of Research

Finite size, large surface fraction, limited capacity for heat and charge, and discrete electron states: these are characteristics of metal clusters and nanoparticles, addressed in the field of cluster physics. Our research is aimed at the remarkable consequences, many of which are accessible by spectroscopic means. Free clusters in a beam [3, 5, 8, 6, 7, 11, 10, 12, 14, 18, 23, 22, 26, 27, 28] allow for the investigation of the pure cluster properties where the coupling to the environment may be neglected. When deposited on a surface the cluster-substrate interaction becomes crucial and is a topic of intense research [20, 13, 17, 21, 24, 1, 25, 15, 2, 16, 29, 9]. A large part of the research has been conducted within the Sonderforschungsbereich SFB 652, the BMBF project FSP 301, and the DFG Priority Programme SPP 1153.

### Spectroscopy on Metal Clusters Embedded in Helium Droplets

Ultracold helium nanodroplets provide an interesting environment for studies on the interaction of clusters with a weakly interacting and superfluid matrix. A powerful method is applied to grow and prepare the clusters in the droplets, that is sequential pick-up of atoms by the nanodroplets. This technique provides a flexible tool to nearly independently adjust the size of either the droplets and the embedded species. By exploring the limits, cadmium clusters of up to 2000 atoms have been produced with this method [28]. For spectroscopy studies, resonant two photon ionization is applied to mass-select the embedded neutral metal clusters. In combination with photoelectron spectroscopy, e.g., the intermediate state dynamics of  $\text{Ag}_3$  was analyzed and the contribution of the helium environment was extracted [23]. In

contrast to  $\text{Ag}_N$ , magnesium clusters show a completely different behavior. These atoms instead form a weakly interacting foam where the Mg-He interaction gives rise to a tiny potential well at large interatomic distances. The spectroscopic analysis of the optical spectrum close to the bare sp transition reveals that a quite regular structure forms inside the droplets. Evidence for a cluster foam consisting of up to 14 Mg atoms have been proven [22], see Fig. 2.8. In femtosecond pump-probe studies the formation of metal ion helium snowballs ( $\text{M}^+\text{He}_N$ ) have been analyzed. This observable provides information about the local environment and only shows up when single metal atoms are present. Using this fingerprint, the caging effect in the light induced fragmentation of silver clusters have been monitored in real time and cluster reformation was observed on a timescale of several tens of picoseconds [6].



**Fig. 2.8:** The regular appearance of the optical spectra from magnesium atoms embedded in helium nanodroplets as measured for different cluster sizes gives evidence for the formation of a weakly bound complex.

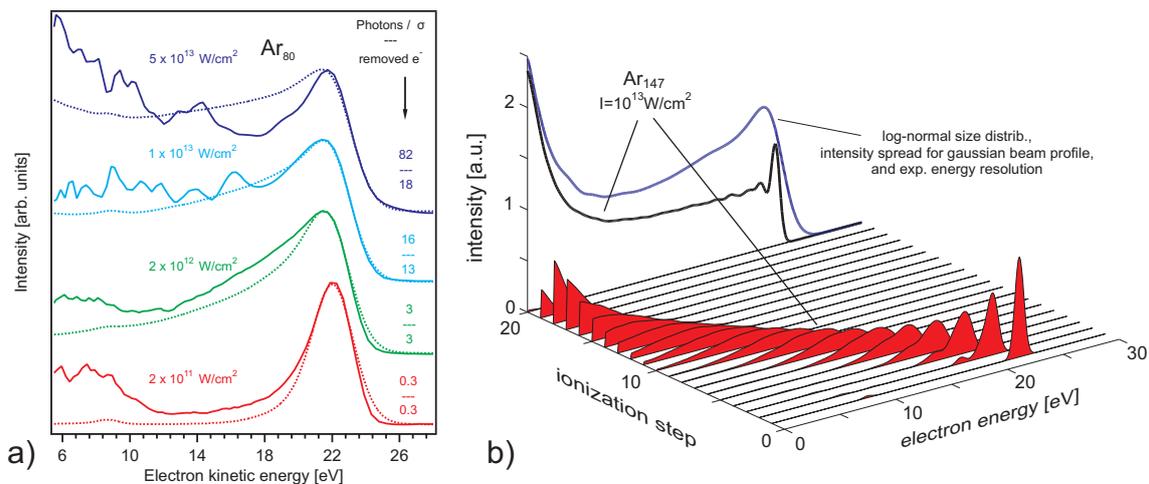
### Strong Field Excitations of Molecules and Clusters in the Optical Regime

In the interaction of intense light pulses with small particles, strong field induced phenomena could be analyzed [7]. For small molecular systems with only few active electronic degrees of freedom this allows to investigate correlated quantum few-electron processes like nonsequential double ionization [27]. Clusters, on the other hand, might serve as model systems to investigate multielectron dynamics relevant for other areas of intense laser matter research, e.g. laser driven particle and radiation sources. The many-body aspects of the finite-sized object introduce a special behavior of the cluster response, as is reflected by the emission of energetic MeV ions, fast keV electrons and short wavelength radiation up to the X-ray regime. In

contrast to atomic gas targets, the temporal pulse structure plays a significant role: stretched and double pulses are much more effective in the generation of these energetic species than ultrashort single pulses [18, 11]. Especially, the electron emission shows a surprising emission characteristics [10]. Due to the resonant interaction of the oscillating laser field with the collective mode of cluster electrons an efficient acceleration of electrons can be achieved. Our Vlasov simulations have revealed the nature of this interaction where the plasmon motion plays the dominant role, leading to attosecond electron bursts. Interesting issues are the mechanisms and the laser intensity thresholds for the generation of highly charged ions [12]. By carefully analyzing the focus conditions using the z-scan technique, first appearance intensity thresholds for multi-electron ionization of clusters have been determined [8]. Only recently we started to use adapted light fields to control the strong field laser-cluster interaction. The first experiments are quite promising, since they show that it is possible to adjust the charge state distribution nearly at will. A topical issue is the effect of a surrounding rare gas matrix to the dynamics of an embedded cluster, e.g., when using the Helium droplet pickup for the cluster growth. It could be shown that the presence of the matrix material induces complex feedback effects to the dynamics including an enhancement of ion charge states due to additional collective resonances in the shell material or delayed cluster expansion due to caging, sensitively depending on the shape of the exciting laser field [4].

### **Clusters in Intense Short-Wavelength Pulses from Free Electron Lasers**

The rapid advances in free electron laser (FEL) technology have opened up new avenues to drive, control, and analyze the structure and dynamics of matter. Several novel approaches such as single-shot coherent diffractive imaging or ultrafast time-resolved holography of nanostructures, small particles, or biological samples are presently in reach or have been demonstrated. A crucial fundamental question being closely related to all existing and upcoming applications of intense FEL light is how the interaction mechanisms of intense laser fields with matter develop in the spectral range from the extreme ultraviolet (XUV) up to the x-ray domain. Atomic clusters are an ideal testing ground for corresponding fundamental studies as great experience in their experimental and theoretical analysis is available [5]. A pioneering experiment [3] on argon clusters in intense XUV laser pulses (32 nm, 30 fs,  $10^{11}$ - $10^{14}$  W/cm<sup>2</sup>) has revealed that the ionization and heating processes strongly differ from those in the near-infrared or vacuum ultraviolet domain. In the latter cases clusters are rapidly turned into a nanoplasma and collisional and collective heating effects dominate the energy capture. Instead, the photoemission spectra under XUV excitation contain strong signatures of a multistep ionization process, without indications for notable collisional plasma heating. While the atomic photoline is dominant at low laser intensity (see Fig. 2.9a,  $E_{kin} = 22$  eV), a shoulder towards lower electron energies develops with increasing laser intensity that eventually turns into a plateau structure.



**Fig. 2.9:** Photoelectron spectra for  $\text{Ar}_N$  under intense XUV 30 fs laser pulses at  $\lambda = 32$  nm (intensities as indicated). The measured spectra for  $\text{Ar}_{80}$  (solid, left panel) show a pronounced non-thermal structure. Starting from the atomic photoline at 22 eV a plateau develops with increasing pulse intensity that can be reasonably explained by Monte-Carlo simulation results (dotted) [3]. The right panel displays the evolution of the underlying mechanism, e.g., sequential multistep ionization, as function of ionization step for  $\text{Ar}_{147}$ .

The main features of the spectra can be well explained with a multistep ionization process of sequential atomic photoemission in the developing cluster potential. The contributions of each ionization step to the final electron spectrum as calculated by corresponding Monte-Carlo simulations [3] are indicated in Fig. 2.9b. The development of the spectral contributions also indicates the onset of frustration of direct photoemission, which leads to a delayed nanoplasma generation at sufficiently high laser fluences. Even if a nanoplasma is produced, collisional heating is negligible and the excess energy of inner photoionization governs the electron dynamics [19]. This scenario underlines that strong-field laser matter interactions at short wavelength are connected to unique response mechanisms, the understanding of which will certainly lead to new fundamental insights and novel schemes for the analysis of ultrafast phenomena. In another experiment we use the VUV wavelength and the high photon flux delivered by FLASH to study the electronic properties of mass-selected clusters in the linear response regime. For lead, the shallow core level photoelectron spectra reveal a nonmetal to metal transition at clusters sizes around  $N=19$  [26]. In future studies the experiment will be equipped with a hemispherical analyzer which contains a delay line detector allowing for angular resolved measurements with improved resolution.

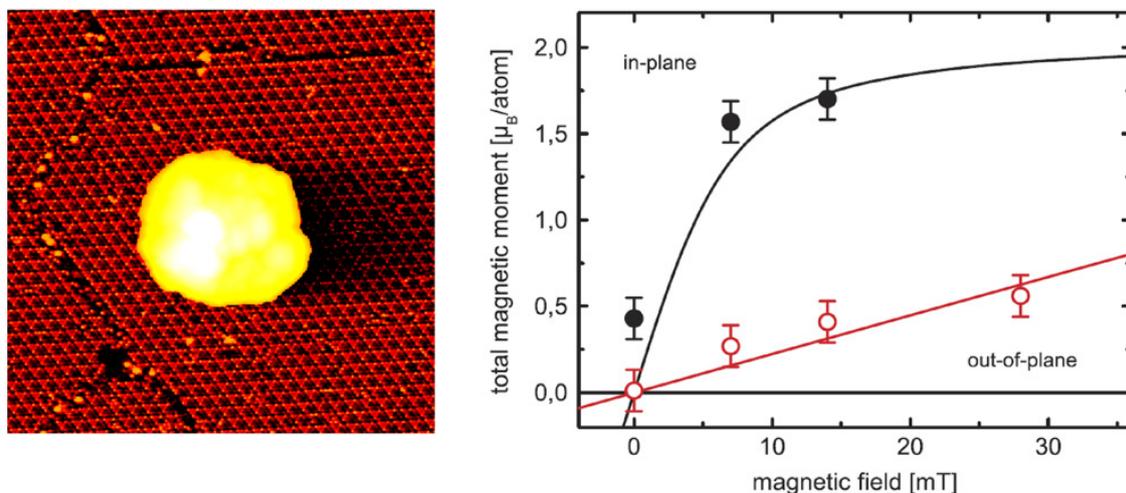
## Clusters at Surfaces

The properties of nanoclusters typically change substantially compared to the gas phase when brought into contact with surfaces. In view of potential applications a holistic understanding of the cluster-surface system is inevitable. The importance of this issue has been underlined by the Priority Programme SPP 1153 “Clusters at Surfaces: Electronic Structure and Magnetism”. This Priority Programme has been organized by our group and has been funded by the DFG over a 6 years period in order to foster concerted activities of the surface and cluster science communities (see [20] for a Topical Issue). One important event has been the “International Conference on Clusters at Surfaces” ICCS 2008, which attracted many scientists from numerous countries. It was held from May 25-29, 2008, in Warnemünde. Below we will sketch a few own activities concerning clusters at surfaces.

Structure and magnetism of deposited clusters: Clusters formed in the gas phase and deposited on crystal surfaces have been studied by various techniques. High resolution transmission electron microscopy images of individual Fe, Co, and FeCo alloy nanoparticles provide evidence for a crystalline structure [17]. Facets of large Co clusters deposited on Ge(110) could be resolved in scanning tunneling microscopy images after taking into account the shape of the tip [25]. From magnetization loops of Fe clusters an uniaxial magnetic anisotropy with the magnetic hard axis being perpendicular to the surface is found [15]. In case of Co particles the results hint at an temperature-dependent spin-reorientation transition [1]. An evaluation of the XMCD spectra of Co particles on W(110) revealed bulklike magnetic spin moments but strongly enhanced magnetic orbital moments with a strong size-dependence [16]. Spectroscopic data on the magnetism of individual Co nanoparticles could be obtained using photoemission electron microscopy (PEEM) [24]. As a result of these explorative studies it became possible to acquire funding of a new PEEM system which will be installed in Rostock in 2011.

Metal clusters as efficient nanocatalysts: Due to their distinct properties and the large surface-to-volume ratio nanoparticles are capable of efficient catalysis. The catalytic activity and dynamical shape changes in size-selected nanoclusters at work are studied under realistic reaction conditions by using a combination of simultaneous temperature-programmed reaction with in situ grazing-incidence small angle x-ray scattering. A rapid change of the shape of the catalyst has been found during the selective partial oxidation of propene [29].

Atomic Au chains on Silicon: Strongly anisotropic Au-induced reconstructions on silicon can be viewed as the ultimate nanowires and are used to investigate the physics of electrons in one dimension. Although the quasi one-dimensional system Si(111)5x2-Au has been discovered more than 40 years ago the atomic structure has remained unknown. Combining scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy the coverage-dependent phase diagram on Si(557) has been established and the Au content of Si(111)5x2-Au could be revised [2]. Comparison of spectroscopic STM images to density functional calcu-



**Fig. 2.10:** Left: Scanning tunneling microscope image of a single Ag cluster deposited on atomically resolved Si(111). Right: Measured magnetization (symbols) of Fe clusters on W(110) and the corresponding model fits (lines).

lations revealed a structural model which is in accordance with all existing experimental data [9].

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## 2.1.6 Dynamics of Molecular Systems

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### General Outline of the Field of Research

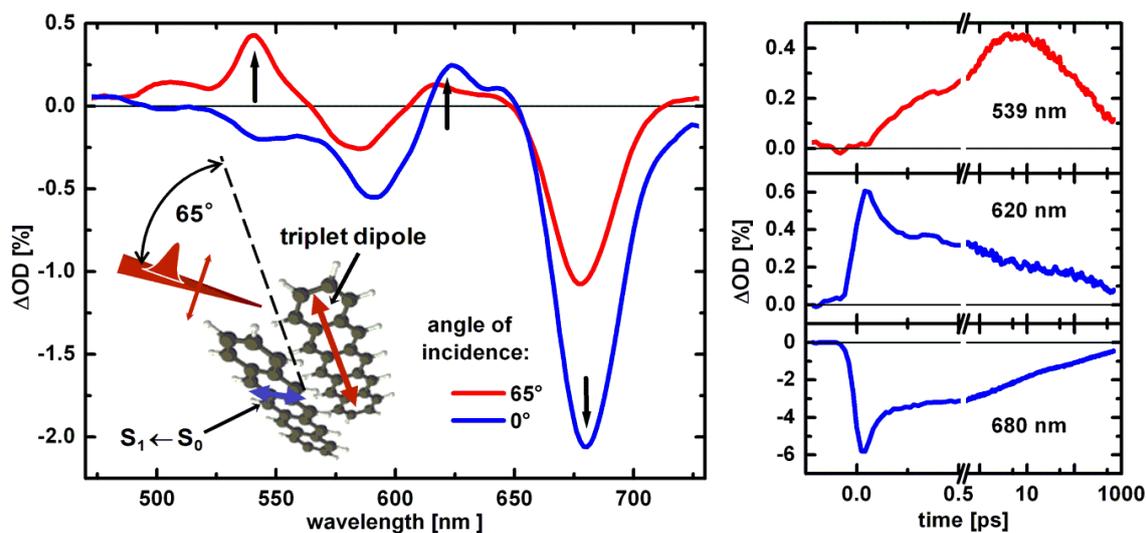
The group “Dynamics of Molecular Systems” started at the Institute of Physics in October 2007. The research focuses on photoinduced processes in molecules, supramolecular systems and organic materials. It follows two lines. One deals with intramolecular processes like charge transfer, the change of electronic states, the coupling to nuclear motions, and mechanisms of chemical reactions. The other line addresses organic materials and interfaces. In these systems we investigate the dynamics of electronic excitations, charge separation, and energy and charge transport. The results are highly relevant for functional materials, organic electronic applications and solar cells. Our main experimental technique is ultrafast spectroscopy with a resolution down to 10 fs [4, 14, 13], which allows to observe the processes in real time. The following topics summarize the current main activities.

### Dynamics in Microcrystalline Films and Supramolecular Structures

Fast processes in highly ordered organic systems are relevant for application of these systems in organic electronics. We investigate in collaboration with Bert Nickel (Ludwig-Maximilians-Universität München) the electronic dynamics in pentacene films which are used as active layers in organic transistors. Fig. 2.11 shows transient spectra and time traces after optical excitation of such a film [3, 7].

A 70 fs fast decay of the primarily excited Frenkel excitons is found [6]. Previously it was speculated that the fast process reflects fission into triplets. To observe triplet specific signatures we changed the angle of incidence from normal to 65°. In this geometry the probe field has a large projection on the strong triplet-triplet transition dipole. The corresponding absorption band appears at 539 nm. However, it is relatively weak and rises delayed compared to the ultrafast primary process. This shows that triplet formation is only a minor relaxation channel and not responsible for the first step. From the spectral signatures we concluded that an excimer like species is formed [3, 7]. The subsequent dynamics is governed by diffusion controlled annihilation and trapping processes. From its analysis we can deduce the mobility of the electronic excitations and the concentration of traps [6].

Aggregates are promising supramolecular structures for directed energy and charge transport. In first experiments on perylene bisimide H-aggregates we see that the original fluorescence is quenched within 200 fs due to structural rearrangements [2]. These changes of the local geometry result in an immobilization of electronic



**Fig. 2.11:** Left: Transient spectra of a pentacene film 8 ps after excitation at 669 nm for different angles of incidence. Right: Time scans at different probe wavelengths. Red lines denote measurements with an angle of incidence of  $65^\circ$  and blue lines with normal incidence.

excitations. Further studies will be extended to J-aggregates in which this effect is suppressed and where a high mobility of the excitons is expected.

### Transport in Disordered Organic Materials

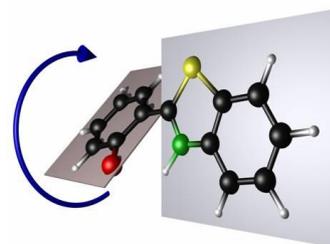
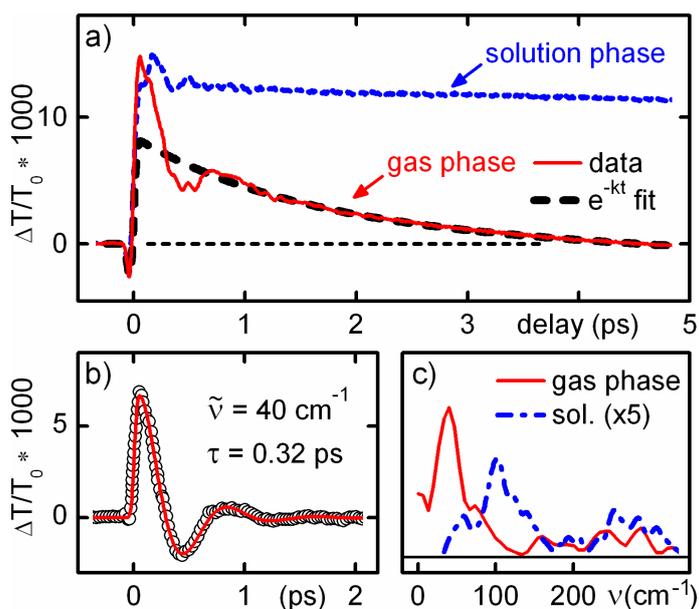
Organic materials with a low degree of order like many polymers show a very limited performance with respect to energy transfer and transport. We design transport pathways using dye molecules as active sites in polymer matrices. At high dye concentrations Förster energy transfer becomes quite fast and a high mobility for electronic excitations is achieved. Even so the structural disorder is still large, the energetic disorder is reduced since the dye molecules have well defined electronically excited states which are little affected by the environment [5]. The mobility is characterized by measuring the transfer time to acceptor sites which have a somewhat lower lying excited state. The acceptors collect all the excitons generated by the absorption of light and the composite material can be regarded as a simple light harvesting system.

### Vibronic Wave packets in Photoreactions

The mechanisms of photoreactions can be analyzed by observing in real time the fundamental steps which can be extremely fast. We find that in many cases ultrafast reactions proceed as ballistic wave packet motions which cause a subsequent ringing of the molecular skeleton in those vibrational modes which contribute significantly

to the reaction path. The analysis of the coherent vibrational excitations allows to reconstruct the reaction coordinate which provides direct insight into the mechanism [4].

In collaboration with Eberhard Riedle (Ludwig-Maximilians-Universität München) and his coworkers we investigate excited state intramolecular proton transfer [14]. Pronounced signal oscillations are observed due to ringing of the molecule in coordinates which affect strongly the distance between the hydrogen donor and the acceptor. This is a strong indication that after optical excitation the molecular skeleton contracts till the distance is short enough for the electrons to rearrange and to bind the hydrogen atom to the acceptor [17, 12]. After the transfer internal conversion (IC) occurs. Interestingly we find that the dynamics of the proton transfer is little affected by the environment whereas the subsequent IC evolves in gas phase dramatically different compared to solution (see Fig.2.12). In the latter case a rather slow decay of the excited state population is observed whereas in gas phase the signal exhibits an oscillatory contribution at a low frequency of  $40\text{ cm}^{-1}$  and a fast decay time of a few picoseconds [16].



**Fig. 2.12:** Transmission change after photoinduced proton transfer. The oscillatory signature results from a wave packet motion along a cis-trans isomerization coordinate.

These findings are interpreted as follows. There is a weak driving force along a cis-trans isomerization coordinate which results in a wave packet motion for the isolated molecule. The corresponding twisting of the molecular backbone leads to a strong increase of the ground state energy. When the two molecular moieties are about perpendicular to each other the electronically excited and the ground state form a conical intersection and an efficient IC is possible [1]. In solution friction due to the interaction with the solvent molecules occurs and inhibits the propagation of a wave packet along the isomerization coordinate. The excited state potential seems to be rather flat for this coordinate and the evolution proceeds as a diffusive

motion.

### Charge Transfer Processes and their Control by the Environment

Together with partners from Munich, Würzburg, and Warsaw we investigate charge transfer processes which play a key role in photovoltaic energy generation and biomolecular photo dynamics. In the case of Lactones we see that the solvent controls in a very subtle way the stationary equilibrium as well as the dynamics [11, 10]. Here two charge transfer states are involved which have different dipole moments. The time resolved absorption measurements show that after excitation of the lower lying state the solvation shell starts to rearrange to decrease the energy of the system. However, during this process the higher lying other charge transfer state is also strongly reduced in energy and since its dipole moment is larger its energy becomes lower than the optically excited state. As soon as both states are degenerate effective population transfer to the second charge transfer state sets in. We were able to model the process by applying Marcus theory with a time dependent energy gap in combination with the specific response times of the solvents [11]. The solvation dynamics can also depend on the structure of the solute and in particular on its symmetry. We studied the solvation after photoexcitation of a charge transfer state in a highly symmetric triple carbazole substituted triarylborane and compared it to a single carbazole substituted triarylborane [8, 9]. In polar solvents an accelerated solvation process is observed for the compound with three fold symmetry. The difference is particularly large for solvents with a slow response. The availability of three active sites with the same energy opens up the possibility of intramolecular excitation or charge transfer in addition to the intermolecular response of the solvent shell. Thereby, the static dipole moment of the excited state is essentially mobilized and can hop between the branches of the symmetric molecules [9]. This leads to an accelerated energy relaxation in comparison to the model compound with only one active site.

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## 2.2 Physics of Nanomaterials

### 2.2.1 Physics of New Materials

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Kerstin Witte      Stefan Flor      Barbel Przybill  
Ulrike Schroder

The main scientific activities of our group focus on the synchrotron radiation, field assisted processing (spark plasma sintering and microwave sintering), phase stability and transformation, nanostructured materials, quasicrystal materials, and porous materials. Novel functional materials (nano, quasi, and porous) with tailored physical properties are prepared by non equilibrium and hybrid technologies also using field assisted sintering. A large spectrum of analysis methods focus on synchrotron radiation spectroscopy, atomic and magnetic force spectroscopy and nano-indentation allows us to analyze the phase formation and stability of the prepared functional materials and explore their mechanical, magnetic, electronic or dynamic properties for their potential engineering, biomedical and energy applications.

- I. Field Assisted Processing
- II. Physics of Nanostructured Materials
- III. Physics of Quasicrystal Materials
- IV. Physics of Porous Materials

#### I. Field Assisted Processing

##### Spark Plasma Sintering

A Spark Plasma Sintering unit has been installed with a rapid gas cooling device in a worldwide unique configuration in the group of physics of new materials, at Institute of Physics in University of Rostock (Figure 2.13). The SPS process is based on the electrical spark discharge phenomenon: a high energetic, low voltage spark pulse current momentarily generates high localized temperatures, from several to ten thousand degrees between the particles resulting in optimum thermal and electrolytic diffusion. During SPS treatment, powders can be processed for diverse novel bulk material applications, for example nanophase materials, fine ceramics, functional gradated materials, hard alloys, biomaterials and porous materials etc.



**Fig. 2.13:** Hybrid FAST/SPS system HP D 250 (FCT Systeme GmbH)

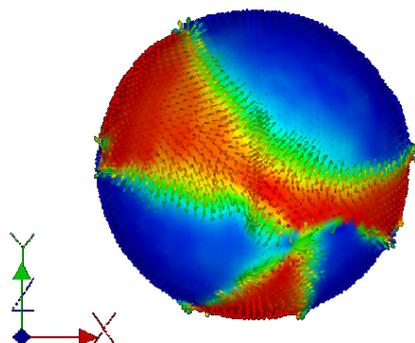
### **Microwave Sintering**

Microwave processing not only provides economical advantages towards conventional heat sources but also offers new physical aspects in the processing of materials. It offers new ways to improve properties of existing materials and possibilities to develop completely new materials. This makes microwave processing one of the most interesting and exiting tools for materials science these days. Microwave sintering has been developed and set up in our group.

## **II. Physics of Nanostructured Materials**

### **Pulsed electric field induced phase transformation to diamond from nanocarbon and graphite**

This research is supported by DFG BU 547/10-1. Diamond is a material with superlative physical qualities. In particular, diamond has the highest hardness and thermal conductivity of any bulk material. In this project, the pulsed electric field induced diamond conversion is studied through the selection of the appropriate carbon modifications, the incorporation of suitable catalysts and the optimization of the technological processes. Recent results show that diamond can be converted from carbon nanotubes and C60 without catalysts being involved by the SPS. The NiFe catalysts can achieve an effective enhancement of diamond transition from MWCNTs in the SPS. A model was proposed to describe the diamond growth and revealed as a layer-by-layer growth mechanism.



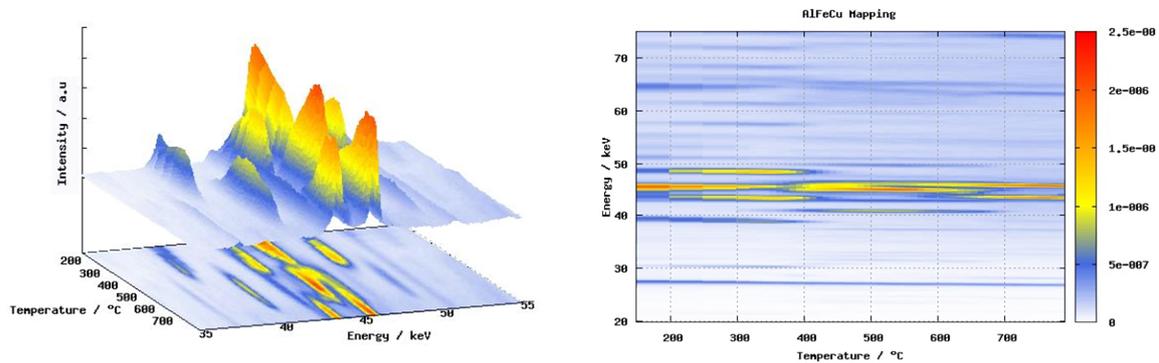
**Fig. 2.14:** The domain structure of a 200nm maghemite particle.

### **Magnetic Nanoparticles**

Investigation and simulation of magnetic materials: Numerical micromagnetism is a suitable method to treat magnetization dynamics on the nanometer scale. This is a theory that allows resolving magnetization inhomogeneities which goes back to Landau and Lifshitz 1935, where the configuration of the magnetic moment within a domain wall was described using a continuum approach. In order to be able to deal with general magnetization distributions advanced numerical tools are required. For complex structures like thin film heads, recording media, patterned magnetic elements, nanocrystalline permanent magnets or magnetic nanoparticles the finite element method is very suitable.

Magnetic coupling and anisotropy - Perpendicular recording: In magnetic recording the areal density is almost doubled every year. In old commercial hard disks the bit is stored parallel to the surface - longitudinal recording. Unfortunately, there is a physical limit which does not allow reducing the size of a bit. The spring 2005 world record in areal density is 230 GBits/in<sup>2</sup> which was realized with perpendicular recording. In our group we work intensively not only on the preparation of new layer systems with PVD (physical vapor deposition), but also on characterization of the magnetic materials with MFM (magnetic force microscopy), GXRR (grazing x-ray reflectometry) and MOKE (magneto optical Kerr - effect). Through combining the characterization methods and micromagnetic simulations we gain knowledge about the materials. The simulations give us the unique possibility to trace the changes in the coupling and anisotropy between the layer systems.

Magnetic nanoparticles for bio-medical applications: Nanostructured magnetic systems are playing a great role in material science nowadays because of the large range of possible applications. Magnetic nanoparticles commonly used in medicine are in the size range from several to hundreds of nanometers. To understand the system complexity and to improve its application we need to understand the relaxation phenomena. The Néel - relaxation is a phenomena occurring in all magnetic materials. The orientation of the magnetization of the material follows the changes in orientation of the external magnetic field by domain movement. Brown - relaxation occurs



**Fig. 2.15:** In situ high-temperature diffraction patterns of the Al-Cu-Fe alloy showing the formation of a single icosahedral phase at 750°C

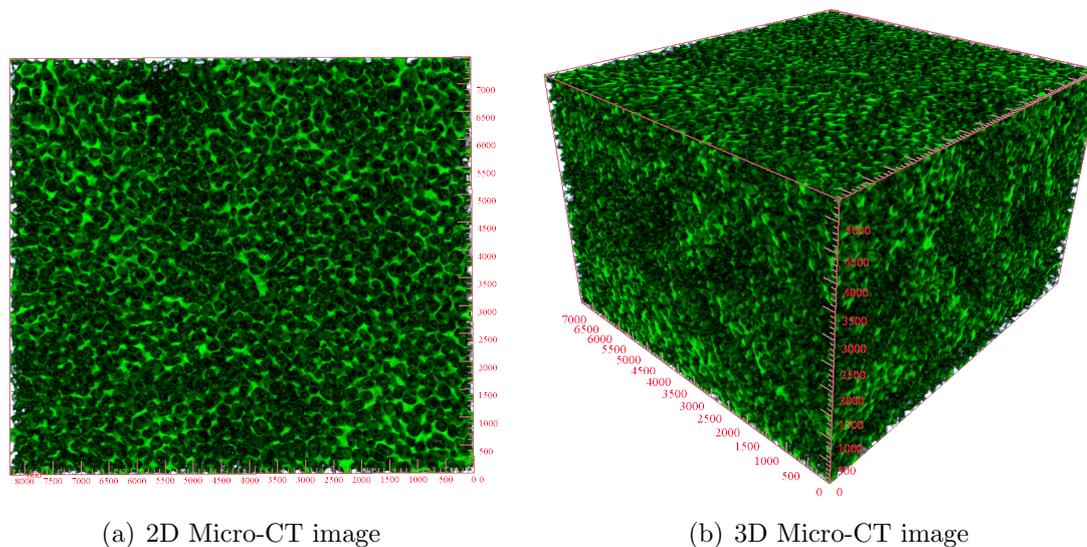
only in magnetic nanoparticle ensembles which are free to move. The nanoparticles adjust their magnetization to the changes of the external field orientation by physical rotation. The only possibility to predict the behavior of a single particle is through micromagnetic simulations as an example the multi domain state of a nanoparticle in Figure 2.14 shows.

### Synthesis and Consolidation of High Temperature Ceramic Systems With Well-Defined Nano- and Microstructure

This research focused on the use of in-situ synchrotron radiation methods to investigate phase transitions and structural stability of oxide ceramics with low positive and negative thermal expansion.  $\text{Al}_2\text{TiO}_5$ ,  $\text{ZrW}_2\text{O}_8$  and  $\text{Al}_2(\text{WO}_4)_3$  nanopowder materials are prepared and consolidated by sintering process at elevated temperatures, yielding bulk specimens. By implementing the sintering process using the new, innovative SPS technology, the control of grain growth while heating can be realized, conserving nanostructures. High heating rates, short dwell and applied pressure stand out due to this sintering technique. The bulk materials are characterized by transmission X-ray diffraction with synchrotron radiation, high-resolution electron microscopy and micro-computer tomography. Additionally dilatometry and nano/micro-indentation supplement the analysis.

### Nanostructured and Ultrafine Titanium-Based Alloys

The research is supported by DFG GRK 1505/1 (Welisa). Nanostructured titanium-based biomaterials with tailored porosity are important for cell-adhesion, viability, differentiation and growth. Nanocrystalline cp Ti, Ti-6Al-4V, Ti-Al-V-Cr and Ti-Mn-V-Cr-Al alloy powders were prepared by high-energy wet-milling and sintered to either full-density (cp Ti, Ti-Al-V) or uniform porous (Ti-Al-V-Cr, Ti-Mn-V-Cr-Al) bulk specimens by SPS. Cellular interactions with the porous titanium alloy

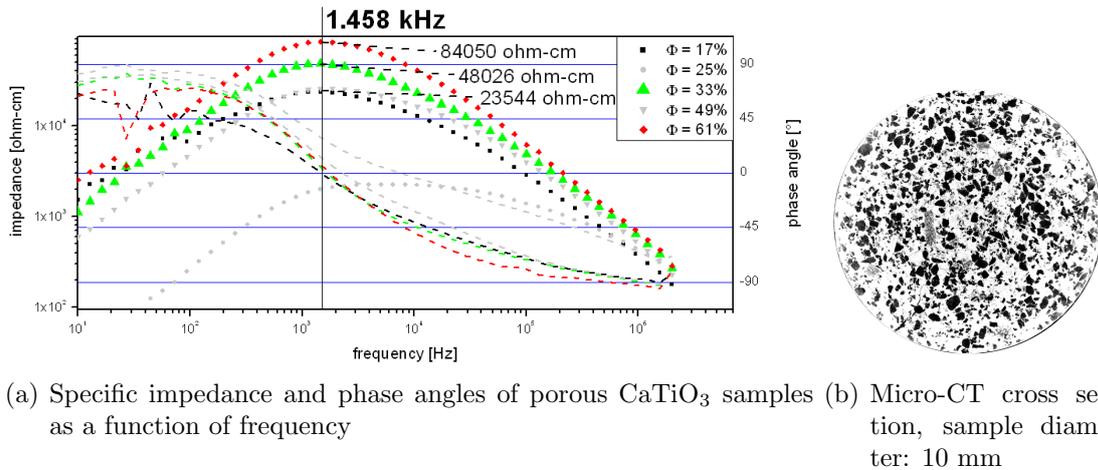


**Fig. 2.16:** Structure of porous Ti foams produced by Spark Plasma Sintering

surfaces were investigated with osteoblast-like human MG-63 cells. Additionally, titanium-manganese (TiMn) alloys with various manganese contents were prepared by using mechanical alloying and SPS techniques. The microstructures, mechanical properties including hardness, elastic modulus and ductility, cytotoxicity and cell proliferation properties of the TiMn alloys were investigated. Concentrations of Mn below 8 wt.% in titanium reveal negligible effects on the metabolic activity and the cell proliferation of human osteoblasts. The Ti2Mn, Ti5Mn and Ti8Mn alloys with supervisor mechanical properties and acceptable cytocompatibility have a potential for use as bone substitutes and dental implants.

### III. Physics of Quasicrystal Materials

The work on quasicrystalline Al-based alloys took place in the framework of the European Marie Curie EST Project Advanced Training in Hybrid Technologies for Nanostructured Composites (MEST-CT-2005-020986), 2005-2009. Quasicrystal-forming aluminium alloys have a strong potential for several technological applications due to their unique combination of low friction coefficients, high-temperature stability, low thermal conductivity. The formation of QC's during non-isothermal annealing of the Al-Cu-Fe nanopowders was studied by high temperature synchrotron radiation diffraction and differential scanning calorimetry. The in-situ X-ray diffraction experiments were performed under different pressure conditions at the MAX 80 installed at the F2.1 beamline of HASYLAB/DESY (Figure 2.2.1). Additionally, quasicrystal/UHMWPE composites were prepared. Our results show that quasicrystal/UHMWPE composites with a highly uniform dispersion of AlCuFe quasicrystal



**Fig. 2.17:** Dielectric properties (a) and cross section (b) of a cylindrical  $\text{CaTiO}_3$  sample

particles in the polyethylene matrix can readily be achieved by wet mixing. The chemical homogeneity and microstructure were investigated by SEM/EDX. The resulting composite powders were further shaped into bulk solid bodies by pressing or extrusion. Microwave heating was used in order to selectively heat the quasicrystalline particles inside the ‘microwave-transparent’ UHMWPE matrix. The observed partial melting of the polymer originated from the particle-matrix-interface may be further used to tailor the properties of the composite material. The effects of the composition on the microstructure and mechanical properties were analyzed.

#### IV. Physics of Porous Materials

##### Porous Metallic Foams

The research is also supported by DFG GRK 1505/1 (Welisa). Porous titanium (Ti) and its alloy were widely used in the biomedical field due to their outstanding mechanical properties, low density, chemical resistance and biocompatibility. Macroporous pure titanium (Ti) foams with porosity of 30-70% and pore size of 125-800  $\mu\text{m}$  were fabricated by using the SPS. The resulting Ti foams consist of pure  $\beta$ -Ti phase with interconnected macropores in square cross sections. Figure 2.16 shows 2D and 3D micro-CT images of porous Ti foams produced by SPS. The plateau stress and Young’s modulus agree with the Gibson-Ashby models, and coarsely follow of linear decline with the increase of the pore sizes, and exponential decay with the increase of the porosity. The macroporous Ti foams with plateau stress 27.2-94.2 MPa and Young’s modulus 6.2-36.1 GPa may have a potential to be used as bone implants.

### Dielectric Properties of Porous Calcium-Titanium Based Ceramics ( $\text{CaTiO}_3$ )

The research on calcium titanate - based ceramics for bone repair is supported by DFG (Welisa) ("Analysis and simulation of electrical interactions of implants with bio-system"), an interdisciplinary research training group (GRK 1505/1) which focuses on technical implant systems. Calcium titanate is known to improve the bonding between titanium and hydroxyapatite, to have better mechanical properties and a 4.5 times higher osteoblast adhesion rate than hydroxylapatite. Nanocrystalline calcium titanate powder is produced by the wet-chemical sol-gel-synthesis and applicable as porous scaffolds formed by conventional sintering and pore-forming agents, as high-densed implants realized by SPS. Figure 2.17 shows the specific impedance and phase angles of porous  $\text{CaTiO}_3$  samples as a function of frequency. First studies of sintered pellets show a direct relationship between their porosity and specific impedance being in the range of human bone material which is expected to improve the acceptance by the surrounding tissue.

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## 2.2.2 Polymer Physics

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### General Outline of the Field of Research

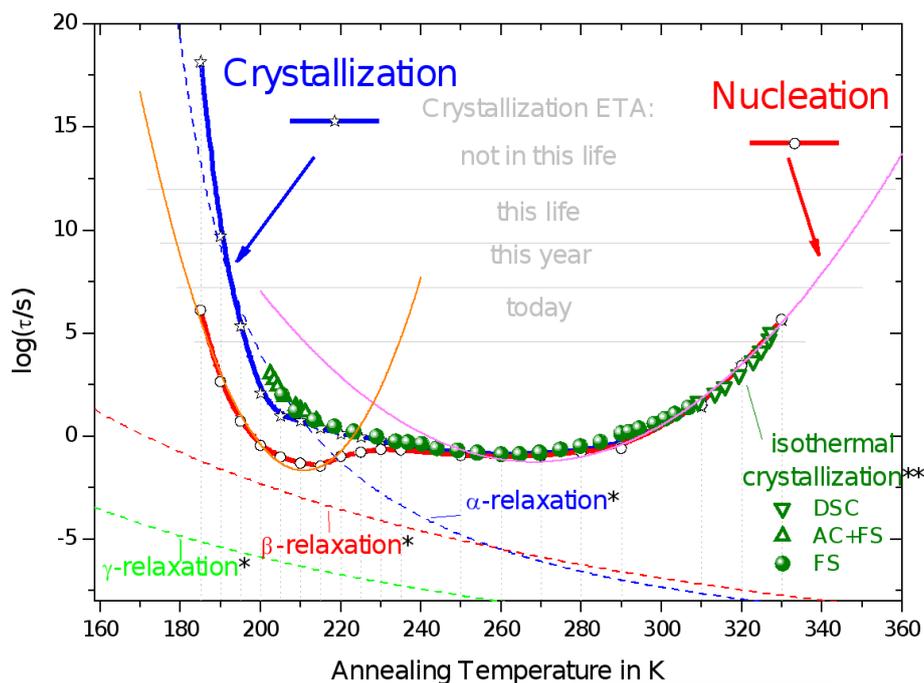
For engineering materials, solidification during processing is a very important step. It is proceeded either by crystallization or by a glass transition. Both routes show a characteristic energetic signature, which can be followed by calorimetry. Solidification kinetically depends on many parameters – material properties as well as processing conditions. Calorimeters covering a dynamic range from  $10^{-4}$  K/s up to  $10^6$  K/s in cooling and heating are available in the Polymer Physics Group and were used to study solidification of different materials.

### Crystal Nucleation and Growth in Poly( $\epsilon$ -caprolactone)

Crystallization is commonly considered as nucleation, followed by a growth process. Nevertheless, a complete description of polymer crystallization is far from being achieved. Several theories are in contradiction with experiments. Often, a decisive conclusion regarding the validity of a theory is not possible because of a lack of appropriate experiments. A new experimental technique for temperature control of a sample and determination of its heat capacity during temperature treatment at high cooling and heating rates was, therefore, developed. Both crystal nucleation and growth characteristic times were determined simultaneously in the range of temperatures where crystallization occurs – from below glass transition up to the equilibrium melting temperature (Fig. 2.18).

The setup developed has opened new possibilities to shed light on the processes of polymer crystal nucleation and growth. The investigation of nucleation as a part of the crystallization process was of special interest.

The crystallization was studied starting from below glass transition up to the melting temperature, for times from  $10^{-2}$  to  $10^5$  s. The homogeneous nucleation was studied simultaneously with crystallization in the same range of temperatures. The study provides information about crystal nucleation and overall crystallization in the polymer which was not available before.



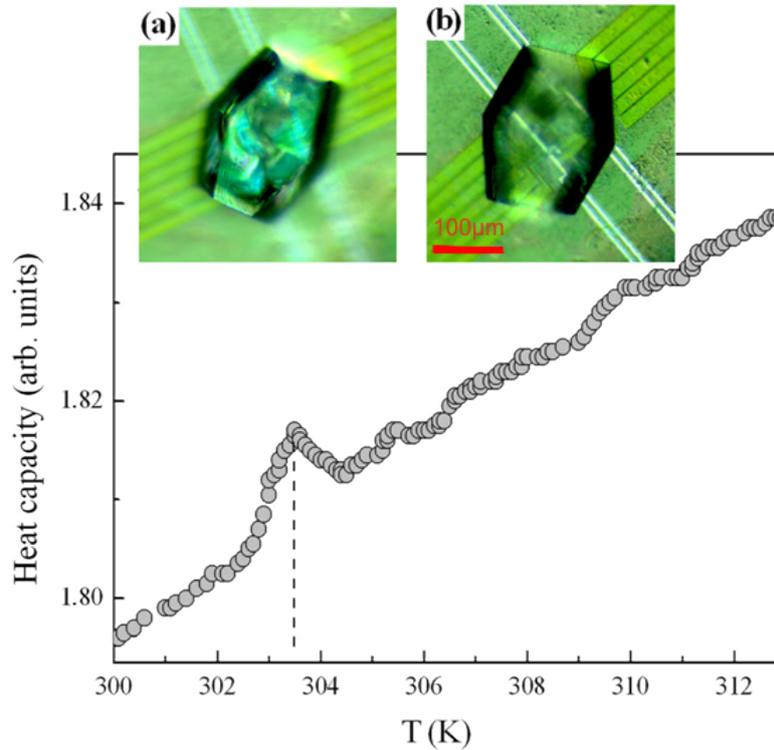
**Fig. 2.18:** Activation diagram for nucleation and crystallization processes at temperatures from below glass transition up to melting temperature and 20 orders of magnitude time range. They are compared to dielectric relaxation data (dashed curves).

### Nano Sized AC Chip Calorimetry

With a differential AC-calorimeter based on a chip sensor, which is also used for fast scanning calorimetry, we achieve a sensitivity in the pico Joule per Kelvin range, which allows us to measure samples below one nanogram. The calorimeter also allows heat capacity measurements in the frequency range 1 Hz to 10 kHz for films below 10 nm thickness. In a controlled humidity environment, investigations of small biological systems and thin films under different conditions are possible. Fig. 2.19 shows the phase transition in a tetragonal hen egg-white lysozyme single crystal. The system is also adapted for use under ultra high vacuum for investigations of extraordinary stable glasses deposited in situ in the vacuum chamber directly onto the calorimeter chips.

### Crystallization of Polymer-Based Nanocomposites

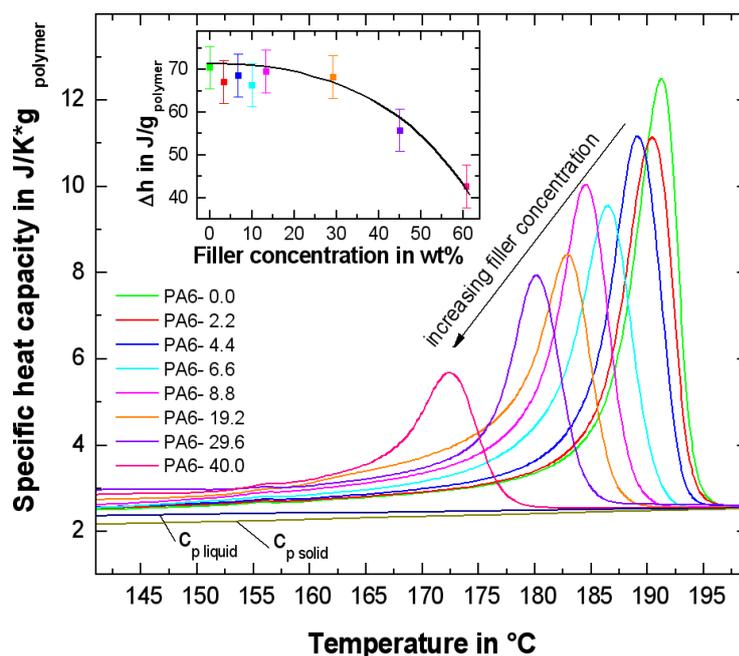
The solidification of polymers is determined by local processes on a length scale of a few nanometers. The addition of only a small amount of nano-sized inorganic particles often results in a dramatic change of the solidification behavior and/or the structure on different length scales as well as the macroscopic properties of semicrys-



**Fig. 2.19:** AC-calorimetric response of the phase transition in a tetragonal hen egg-white lysozyme single crystal. As inset the pictures of the crystal before (a) and after (b) the measurement are shown.

talline polymers. The effectiveness of nanofillers, in comparison to traditionally used microfillers, is due to its large surface. Crystallization behavior and final properties of polymer based nanocomposites depend therefore on the interaction between the filler particle and the matrix polymer at the interface. Nano-sized materials like clay often act as nucleating agents. Depending on the number of these, heterogeneous nuclei crystallization kinetics and final product properties can vary. For increasing processing efficiency and structure-property tailoring, this effect is widely used during industrial polymer processing. But sometimes the opposite effect occurs. The addition of a nanofiller results in lower crystallization kinetics. In Fig. 2.20, an example of crystallization from cooling for a polyamide6/clay nanocomposite is shown. By increasing filler concentration at identical experimental parameters, crystallization appears at lower temperatures (slower) and crystallization enthalpy (final crystallinity) becomes smaller.

A detailed calorimetric analysis of the crystallization and melting processes, as well as glass transition, of these PA6/clay nanocomposites leads to the result showing strong interaction between polymamide6 and the clay particles. Finally, this interaction is responsible for a significant decrease in mobility of an amorphous material



**Fig. 2.20:** Specific heat capacity of PA6 and its nanocomposites during non-isothermal crystallization from cooling at 10 K/min from the melt at 250 °C, measured from DSC scan experiments, and normalized to the polymer mass fraction. The inset shows crystallization enthalpies, normalized to the polymer mass fraction, as a function of filler concentration.

at the surface of the nanofiller, and, therefore, for the decrease of crystallization kinetics.

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### 2.2.3 Electron Scattering – Insulator Physics

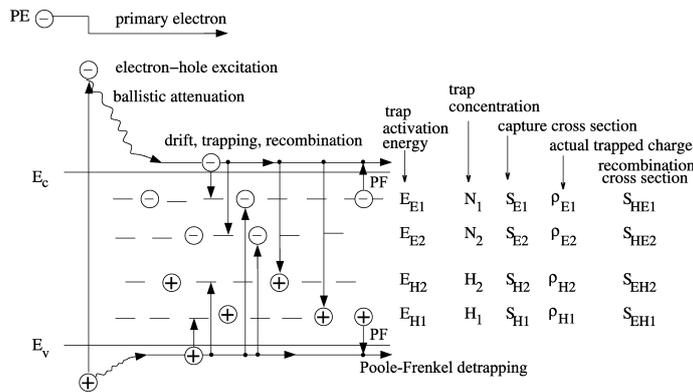
Head: Prof. Dr. Hans-Joachim Fitting

#### General Outline of the Field of Research

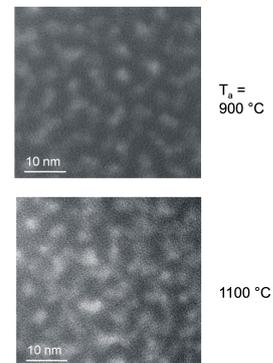
The research group is dealing with electron scattering, spectroscopy, and microscopy mainly in wide-gap dielectrics and insulators. Therefore, the electron energies cover the wide range from meV to MeV. Consequently, elastic and inelastic interactions of electrons with atoms, with core and valence band electrons as well as collective interactions with plasmons and phonons are taken into account.

All these scattering mechanisms have been transformed to Monte-Carlo (MC) simulations associated to our experiments of electron emission, spectroscopy, and microscopy in thin layers and structured solids as well as of hot and ballistic electron transport in semiconductors and dielectric layers. Here basic materials of micro- and optoelectronics are under investigation: e.g. compound semiconductors like BN, AlN, GaN or ZnS and high attention is paid to silicon-based systems ( $\text{SiO}_2\text{-Si}$ ) especially modified, e.g. by ion implantations.

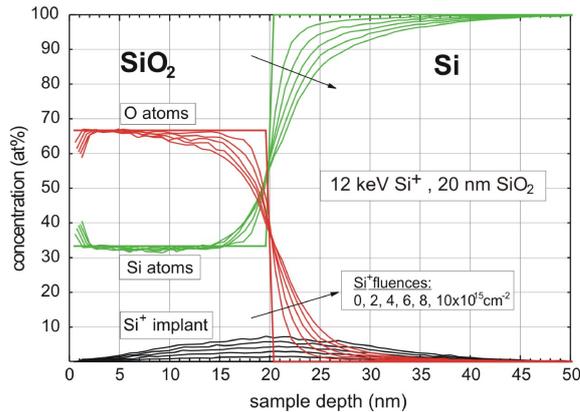
Already in 1980 we have started to calculate the energy balance of hot electrons in  $\text{SiO}_2$  by means of respective Monte Carlo simulations and 1990 we first have investigated the vacuum emission (VE) and spectroscopy of ballistic electrons emitted from planar ZnS electroluminescence (EL) devices.



**Fig. 2.21:** Scheme of the flight-drift model FDM including the ballistic flight of electrons and holes with their attenuation followed by diffusion and drift, trapping or recombination as well as Poole-Frenkel release from traps, altogether resulting in a selfconsistent charge transport.



**Fig. 2.22:** Energy-filtered transmission electron micrograph (EFTEM) of Si clusters in a  $\text{SiO}_2\text{:Si}$  matrix after thermal annealing at  $T_a$ , using the characteristic Si plasmon loss (17 eV).



**Fig. 2.23:** TRIDYN simulation of the ion beam mixing process showing the  $\text{Si}^+$ , Si and O atom concentration profiles across the former  $\text{SiO}_2/\text{Si}$  interface.

The experimental work is performed mainly in a digital scanning electron microscope (SEM) equipped with energy-dispersive X-ray analysis (EDX), cathodoluminescence (CL), electron beam induced conductivity (EBIC) and field-controlled vacuum emission (VE) of hot and ballistic electrons. Furthermore, we use Fourier transform infrared spectroscopy (FTIR) for investigation of local defects in amorphous networks of dielectrics. During the last years, in cooperation with French groups in Lyon and St. Etienne, special attention was paid to electron beam charge injection into high-insulating ceramics and the related selfconsistent charge transport and charging processes in these materials, see Fig. 2.21. Respective charging measurements have been performed by SEM and EDX techniques. Moreover, CL spectroscopy in SEM technique is a powerful method enabling high sensitivity and high spatial resolution detection of defect and luminescent centers, especially in small volumes and thin nano-layers. E.g., in modified  $\text{SiO}_2$  layers we have either enhanced or replaced the first and second constituent silicon and/or oxygen isoelectronically by elements of the IV and VI group. Especially additional  $\text{Si}^+$  or  $\text{Ge}^+$  ion implantation with thermal post-treatment lead to nanocluster formation in the silica ( $\text{a-SiO}_2$ ) host matrix, see Fig. 2.22. For the first time we developed and applied “ion beam mixing” across the interface of a  $\text{SiO}_2$ -Si layer system and have obtained a  $\text{SiO}_x$  buffer layer with decreasing stoichiometric factor from  $x = 2$  gradually down to  $x = 0$  over about 15 nm, see Fig. 2.23.

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## 2.2.4 Physics of Nanomaterials

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### Nanostructure Processing of Advanced Biomaterials

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 material.

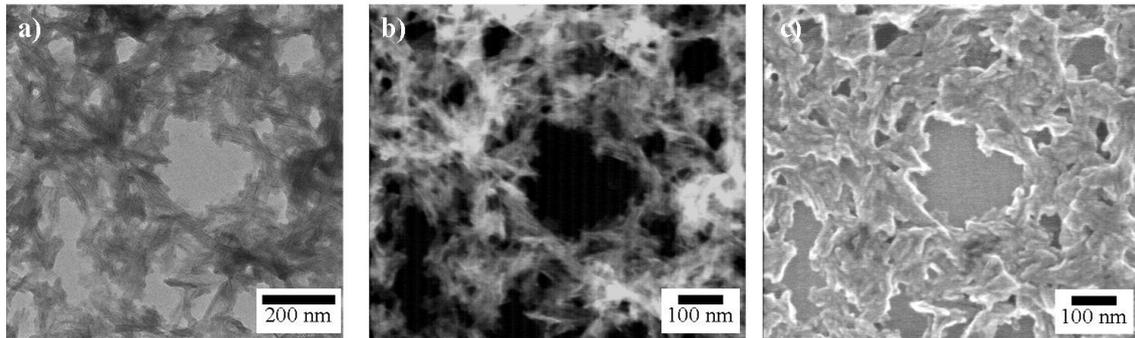
The improvement of the acceptance of a synthetic material in living tissue is of great importance. Therefore we developed a synthetic nanostructured biomaterial with special properties. The interaction between the synthetic material and autologous proteins is achieved by using a synthetic matrix of defined 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.

The interdisciplinary 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.

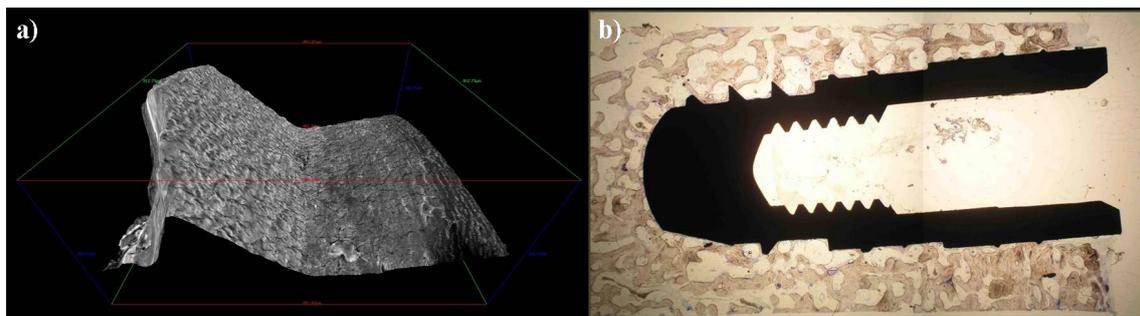
Three examples are given to demonstrate the fields of our interest [1, 2, 3, 4, 5, 6, 7, 8, 9].

### Development of a Nanostructured Biomaterial Coating

The goal of this part was to improve the osseointegration of implants by offering an osseoinductive and permanent hydrophilic surface. Therefore we transcribed the properties of the synthetic bone grafting material NanoBone<sup>®</sup> as a coating material. This coating material is characterized by nano crystalline, synthetic hydroxyapatite that is embedded in a highly porous matrix of silica gel which is derived by using the sol gel technique. Hydrolysis of TEOS (tetraethylorthosilicate) under acid condition form a particular sol which condensates together with synthetic bone-like hydroxyapatite during a drying process into a three-dimensional network. The crossover from sol to gel network occurs on the implant surface. The SiO<sub>2</sub>-matrix completely encloses the HA-plates which results in a porosity in the nanometer scale, Fig.(2.24a) a transmission electron micrograph of the coating material. Figure (2.24b) is a dark field image in the STEM mode (scanning transmission electron microscopy) of the same region showing the HA-plates because of the higher scattering contrast. The



**Fig. 2.24:** a) TEM-picture of the coating. b) Dark field image, this mode is sensible for the hydroxyapatite crystals caused by the scattering contrast. c) SE-picture in STEM mode of the coating gives a topographic overview of the HA-crystals embedded in a silica matrix.



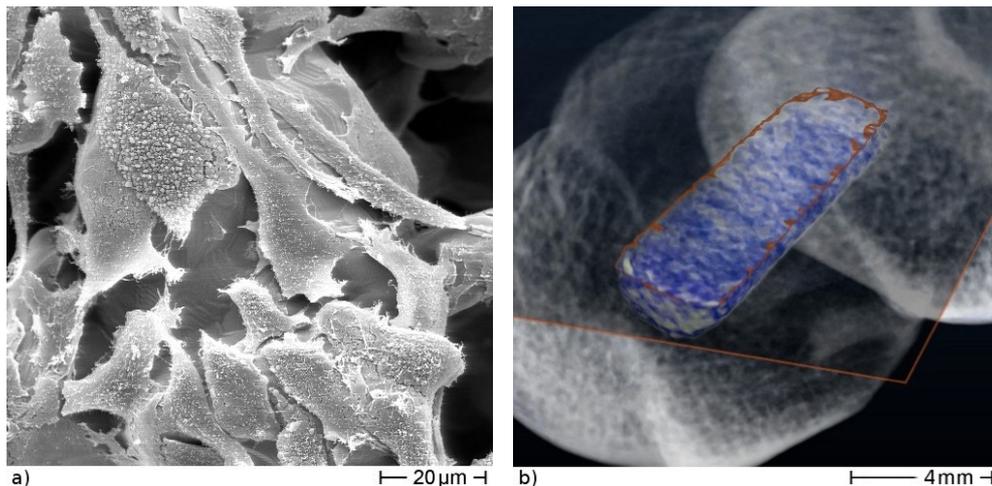
**Fig. 2.25:** a) Screw thread of a dental implant coated with a homogeneous layer in a 3D SEM. b) Histologic cross section of the implant inserted in the bone of a minipig.

topography of the coating and the embedding of the HA-crystals are shown in Figure (2.24c), a SE image made in STEM mode.

First animal studies reveal an improvement of the behavior of osseointegration, (Fig.2.25). Coated and uncoated implants were inserted in the frontal bone of minipigs. The BIC (bone implant contact) of commercially (uncoated) dental implants (e.g. ix2<sup>®</sup>, M.&K.) degenerates during the early stages of implantation (2 weeks: 69%, 4 weeks: 61%, 6 weeks: 46%). The BIC of a coated implant is improved on the same timescale (2 weeks: 73%, 4 weeks: 71%, 6 weeks: 78%). Fig.(2.25a), 3D SEM, shows the geometry of the screw thread and the implant surface covered with the coat. The insertion of the implant into the bone and the histologic cross section is displayed in Fig.(2.25b).

### Sponge-Like Structural Design With Interconnected Porosity Instead of Conventional Screw Thread Dental Implants

The titanium sponge is produced by grouting titanium powder with a placeholder. In the next step the green body can mechanically designed for the requested application. Finally, the placeholder is removed before the starting sinter process creates sponge-like material from the powder. The particle size of the placeholder and the mixing ratio between powder and placeholder define the porosity.

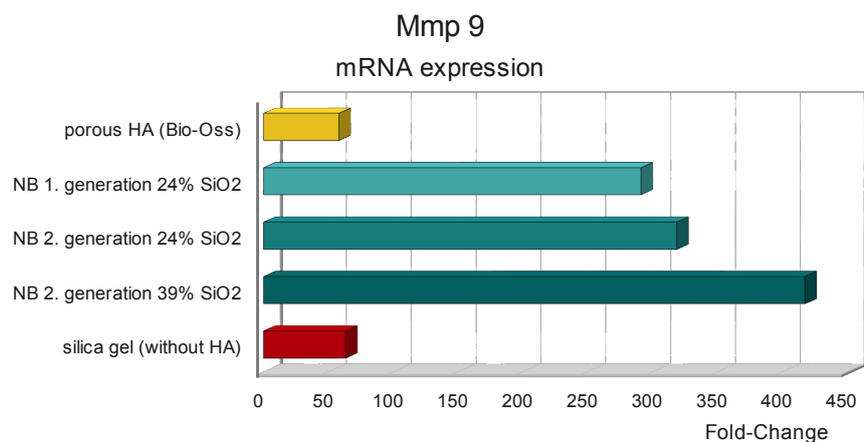


**Fig. 2.26:** a) Scanning electron micrograph of the titanium sponge after a cytotoxic test. The surface is completely coated with cells. This result demonstrates good biocompatible attributes of the new material. b)  $\mu$ -computer-tomography of the implanted titanium sponge in a knee joint of a rabbit after four weeks.

The properties of the titanium sponge are analyzed by stress measurement. The surface is tested by energy dispersive X-ray spectroscopy, scanning and transmission electron microscopy. The interaction between bone remodelling and implant is checked by cytotoxic tests (Fig.2.26a). After osseointegration the result will be analysed by  $\mu$ -computer-tomography (Fig.2.26b) and by optical microscopy on histomorphometric cross section of the implant inserted in the bone (like Fig.2.25b)

### Correlation Between Biomaterial Structure and Gene Expression

For a better understanding of ectop bone formation mechanisms, differentiation of mesenchymal stem cells to bone forming cells was analyzed via differential gene expression. Hence, the aim of one project was the determination of specific biomaterial-initialized genes, which have been expressed in a rat model during bone formation. Five different biomaterials (NanoBone<sup>®</sup>(NB) 1. and 2. generation 24% SiO<sub>2</sub>, NB 2. generation 39% SiO<sub>2</sub>, Bio-Oss<sup>®</sup>, Silicagel) have been tested subcutaneously in the adipose neck tissue in comparison to defects in the tibia of rats. After 12 days,



**Fig. 2.27:** Fold-change of samples with biomaterial implanted subcutaneous after 12 days against adipose tissue. Matrix metalloproteinases (MMPs) play a role in osteoclastic bone resorption.

grafts were removed and differentially expressed genes were determined by microarray technology. The sample labelling, hybridization and staining have been carried out according to the Protocol for Affimetrix<sup>®</sup> GeneChip<sup>®</sup> Rat Gene 1.0 ST Array System.

Data from all chips has been analysed and many bone specific genes have been identified. The expression profiles were similar in all used biomaterials. Osteoblastic (e.g. Osteoactivin, Fibromodulin) as well as osteoclastic genes (e.g. Cathepsin K, Chemokines, Matrixmetallopepdidases) and genes encoding extracellular matrix components (e.g. Collagenases, Fibonectin, Laminin) could be detected. Furthermore, specific genes for Osteoclasts showed expression pattern dependent on biomaterials. In addition, in adipose neck tissue high expression levels of bone specific genes have been verified.

In bone grafts the highest gene expression has been shown using biomaterials with defined SiO<sub>2</sub>-percentage. In addition, correlations to the influence of SiO<sub>2</sub> concentration on the tissue and therewith on the formation of new bone were shown.

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## 2.3 Physics of Particles and Fields

### 2.3.1 Quantum Theory and Many-Particle Systems

**Head:** Prof. Dr. Gerd Röpke (until 09/2009)  
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Dipl.-Phys. Susanne Killiches	
Marina Hertzfeldt	

#### **Non-Local Dynamic Correlations in Dense Plasmas**

We investigated the wave-vector dependence of dynamical correlations in dense plasmas using different methods. In particular, a new interpolation scheme that accounts for dynamic collisions and electron correlations (local field corrections) has been established. Consequences for plasmon dispersion and Thomson scattering has been studied.

A self-consistent approach to the single-particle spectral function in dense plasmas has been developed [77]. Extensive calculations for classical one-component plasmas have been carried out. The application of the non-local dynamic structure factor is also of interest for nuclear reactions in dense plasmas.

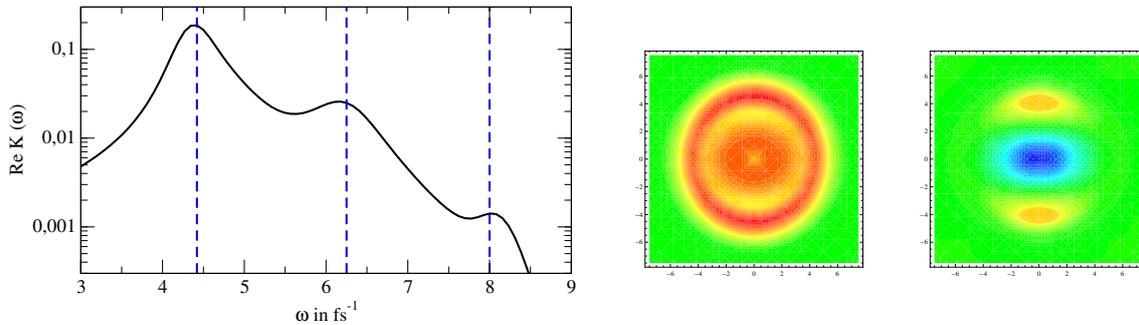
#### **Dynamical Structure Factor and Optical Properties of Dense Plasmas**

A fundamental quantity to describe the interaction of light and matter is the dynamical structure factor. Within linear response theory, transport coefficients are related to different equilibrium correlation functions that have been calculated numerically or analytically using quantum statistical approaches. The resulting dynamical collision frequency was applied to bremsstrahlung, Thomson scattering, absorption and reflection of light by strongly correlated Coulomb systems.

In contrast to infinite matter, finite systems such as nanostructures show new and interesting properties. Clusters of solid state densities can form nanoplasmas after laser irradiation with intensities of  $10^{13} - 10^{16} \text{ Wcm}^{-2}$ . The time evolution of the

electron ion system is simulated by semi-classical molecular dynamics (MD) simulations using a pseudo-potential adapted to sodium [43]. Time dependent plasma properties like temperature and density are introduced when local thermal equilibrium is established.

Dynamical correlations for finite systems via restricted MD simulations (fixed ion configuration) are investigated [42]. We study the bi-local frequency dependent structure factor for clusters at various temperatures, densities, particle numbers and ionization degree. A resonance structure has been found, see Fig. 2.28 (left). Different collective excitations have been identified and characterized by the spatial distribution of the current auto-correlation function, see Fig. 2.28 (middle, right). To compare with bulk properties, size effects of dynamical properties are investigated. In particular, we identified the size effects for the Mie mode and the bulk plasmon excitation. Furthermore, we found that the damping rates are increasing with the cluster size.

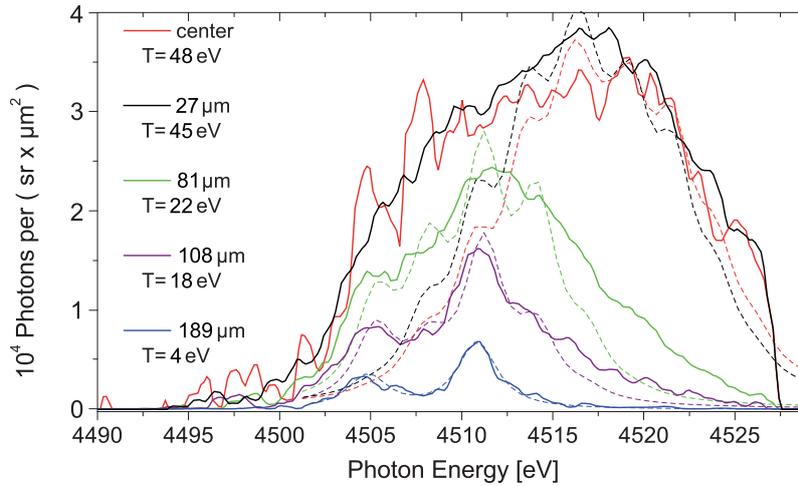


**Fig. 2.28:** Laplace transform of the current auto correlation function of electrons in excited clusters (left). Spatial distribution of currents in the first mode of excited cluster (middle). Spatial distribution of currents in the third mode of excited cluster (right).

### Spectral Line Profiles in Dense Plasmas

Due to the interaction with surrounding particles, spectral lines in dense plasmas are strongly modified compared to their isolated, atomic counterparts. The quantum statistical approach has been further elaborated and applied to laser ignited dense Lithium plasmas.

Of high interest for the diagnostics of dense plasmas is x-ray spectroscopy.  $K_\alpha$  spectra of mid- $Z$  atoms such as Si, Cl, and Ti, produced by strong laser irradiation, have been analyzed. A blue-shift due to ionization/excitation satellites and a red-shift due to screening by free electrons in the plasma compete to form the  $K_\alpha$  line profile. Analyzing recent experimental spectra, the temperature and density profile of the laser-excited plasma has been inferred [61, 62].



**Fig. 2.29:** Comparison of radially resolved theoretical (dashed) and experimental (solid) Ti  $K_{\alpha}$  spectra.

### Clusters and Quantum Condensates in Nuclear Matter

The equation of state (EoS) of nuclear matter at finite temperature and density with various proton fractions has been worked out [52], in particular the region of medium excitation energy given by the temperature range  $T \leq 30$  MeV and the baryon density range  $\rho_B \leq 10^{14.2}$  g/cm<sup>3</sup>. Standard approaches such as Dirac Brueckner Hartree-Fock (DBHF) or Relativistic Mean Field (RMF) are not applicable in that region. In addition to the mean-field effects, the formation of few-body correlations, in particular light bound clusters up to the  $\alpha$ -particle ( $1 \leq A \leq 4$ ) have to be taken into account. The calculation is based on a many-particle approach, the medium modification of the light clusters is described by self-energy and Pauli blocking effects.

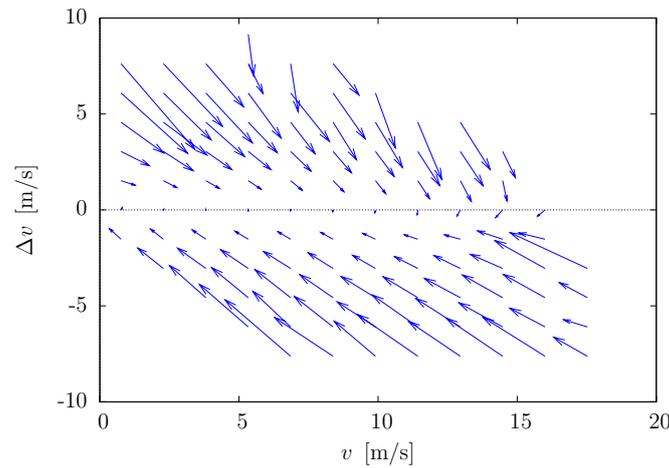
Applications are heavy-ion collisions [52] and supernova explosions in astrophysics [67]. In particular, the influence of cluster formation on the symmetry energy has been investigated [70].

An interesting phenomenon is the Bose-Einstein condensation of alpha clusters. New results have been elaborated for nuclear matter [64]. Intense investigations have been performed with respect to the cluster structure of low-density excited states of <sup>12</sup>C (Hoyle state) and <sup>16</sup>O, see also [13].

### Kinetic Theory and Decoherence in Quantum Systems

Kinetic equations and linear response approach are extended to relativistic systems. For photons in relativistic dense plasmas, a kinetic equation has been derived that distinguishes between real and virtual photons and gives a systematic approach to Cerenkov radiation and bremsstrahlung within a many-particle QED [37]. Generalized quantum master equations have been derived for open systems, in particular

for Rydberg atoms in a plasma. Decoherence in the time evolution of the open quantum system leads to localization and the transition from quantum to classical behavior. Quasiclassical approaches give an adequate description of transition rates for highly excited atoms coupled to a radiation field and interacting with a plasma [21].



**Fig. 2.30:** Speed and speed difference change within one second (NGSIM data).

### Traffic Flow Theory

The car following behavior is described with an optimal velocity model. This on forces based model leads to a new view on traffic flow, which puts the energy in the focus of discussion. The model can be compared with data from the NGSIM-program (*Next Generation Simulation*). Fig. 2.30 shows the speed and speed difference change within one second in the data. The clear dependence of the velocity change on the velocity difference to the car in front can not be reproduced by the model yet.

### Time-Dependent Density Functional Theory

The expertise of Prof. Röpke's successor Prof. Bauer lies in the theory and numerical simulation of intense laser-matter interaction. Prof. Bauer took up his employment in September 2009. The work published within the last four months of the period covered by this Research Report was devoted to the foundations of a Kohn-Sham description of time-dependent density functional theory [49, 50].

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## 2.3.2 Statistical Physics

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### Warm Dense Matter and Ab Initio Molecular Dynamics Simulations

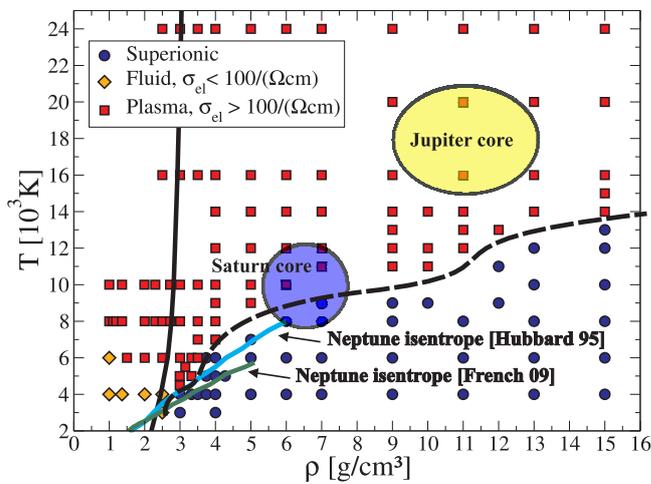
The thermophysical properties of light elements (e.g. H, He, H-He mixtures; C, O, N and their hydrides) at high pressures are of great importance for interior models of stars, brown dwarfs, and giant planets as well as for inertial confinement fusion experiments. A precise knowledge of the equation of state (EOS) as well as of the electrical conductivity is needed for a large domain of densities and temperatures, especially for high densities as typical for condensed matter and for temperatures of several eV, i.e. for *warm dense matter (WDM)*.

The EOS of H [7], He [2], H-He mixtures [25, 39], water [17], and Li [3] was derived from *ab initio* molecular dynamics simulations (AIMD) which combine a classical treatment (molecular dynamics) for the ions with a full quantum description for the electrons (within density functional theory). Besides the EOS, the electrical conductivity, the diffusion coefficients, and the pair correlation functions can be extracted. These quantities are evaluated in order to describe the high pressure phase diagram in more detail, especially the transition from non-metallic to metallic behavior. Chemical models predict that this electronic transition is accompanied by a thermodynamic phase instability [6, 38, 37] which would affect models of planetary interiors and the evolution of giant planets strongly.

As an example we present the high-pressure phase diagram of water which is one of the prevalent materials in nature and has a variety of structural transitions. Water is known to be a major constituent of Neptune and Uranus as well as of Jupiter and Saturn. Interior models for these planets require accurate EOS data in order to meet the observational constraints; see Refs. [25, 26, 21, 27] for details. Thermodynamic conditions as occurring deep in the interior of giant planets have not been realized experimentally yet so that AIMD simulations are a valuable tool in this context. We have performed AIMD simulations for water up to ultra-high-pressures of 100 Mbar and several thousand Kelvin. Of special interest is the identification and location of the phase transition between superionic water and dense water plasma. The exotic superionic phase is characterized by highly mobile protons diffusing through a solid bcc oxygen lattice [17].

We have determined the phase diagram from 3000 K to 24000 K and for densities

up to  $15 \text{ g/cm}^3$ , see figure 2.31. Our main result is that superionic water and strongly dissociated fluid water are the only occurring phases above 4000 K. Dissociation is inferred from the systematic difference between the diffusion coefficients of both ion species. We find that water at present Jupiter core conditions is in a fluid dense plasma phase, regardless of the planetary model. Hence, the initial Jupiter core may have been larger than today due to erosion of its water component. However, the Saturn core conditions are very close to the superionic phase boundary. Thus, superionic water may exist in Saturn's core which offers an explanation why it is larger than that of Jupiter.

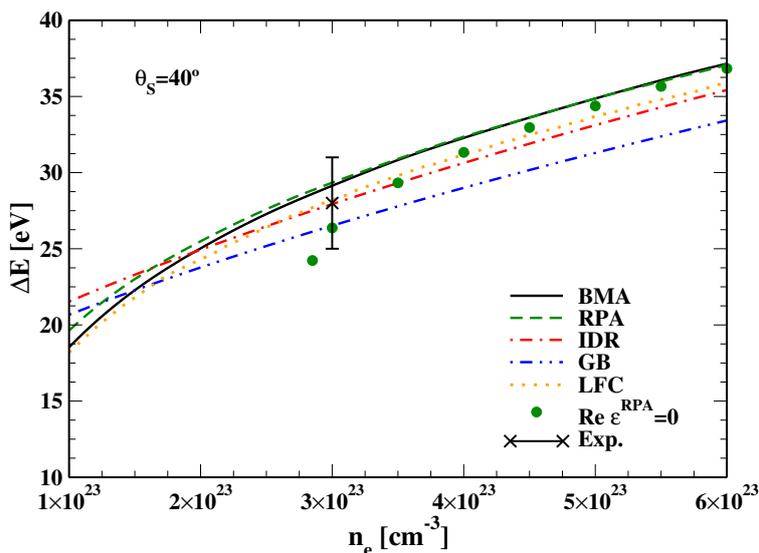


**Fig. 2.31:** Phase diagram of warm and ultra-dense water for temperatures above 3000 K [17]. Each colored point represents a simulation in equilibrium. The plasma-to-superionic phase boundary (black dashed line), the principal Hugoniot curve (black solid line), and two Neptune isentropes are also shown. The ovals embrace the range of conditions in the cores of Jupiter and Saturn.

## Interaction of Plasmas With Electromagnetic Fields

X-ray Thomson scattering has demonstrated its capacity as a reliable and versatile tool for the diagnostics of dense plasmas [29, 1, 30, 12, 5, 31, 4]. X-rays emitted from laser produced plasmas can probe the WDM region with temperatures of several eV and densities close to solid density up to compressed matter well above solid density and electron temperatures between 0.1 eV and several 10 eV. Collective X-ray Thomson scattering experiments yield information on the density and temperature of dense plasmas via the plasmon peaks. Their frequency position is directly related to the free electron density, see figure 2.32, and the temperature is derived from the detailed balance relation. The range of applicability of the standard Gross-Bohm (GB) dispersion relation and of an improved dispersion relation (IDR) in comparison to calculations based on the dielectric function in random phase approximation (RPA) was investigated [28]. This approach has been generalized by including collisions within the Born-Mermin approximation (BMA) [1, 10, 9]. It has been shown that the consideration of collisions is important in the WDM region and in the transition region from collective to non-collective scattering.

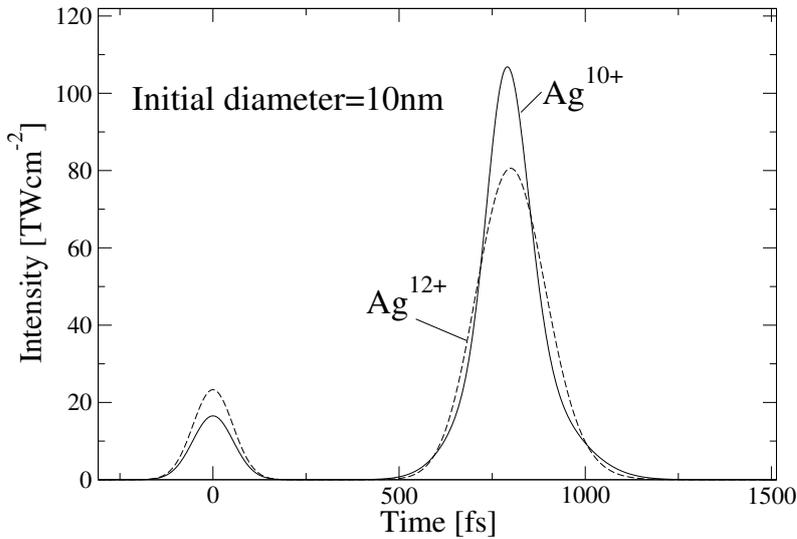
The development of an appropriate theory for X-ray Thomson scattering experiments as performed at the Free electron LASer Hamburg (FLASH), the Linac Coherent Light Source (LCLS) in Stanford, and at the future European XFEL in Hamburg is an important challenge to plasma diagnostics and treated in a close collaboration with partners at the FSU Jena, DESY Hamburg, U Oxford, and the LLNL in Livermore. In this collaboration various experiments with intense ultra-short laser pulses at short wavelength were performed with different target materials [16, 35, 8]. Especially, a novel collective Thomson scattering experiment on liquid hydrogen droplets was realized at FLASH. In this context the influence of plasma inhomogeneities in hydrogen targets on the Thomson scattering spectrum was investigated by comparing density and temperature averaged scattering signals to calculations assuming homogeneous targets. We have found discrepancies larger than 10% between the mean electron density and the effective density as well as between the mean temperature and the effective temperature [10].



**Fig. 2.32:** Comparison of the maximum position  $\Delta E$  of  $S_{ee}(k, \omega)$  calculated in different approximations as a function of the electron density  $n_e$  for a beryllium plasma with  $Z_{\text{eff}} = 2.5$ ,  $T_e = 12$  eV, and the laser wavelength  $\lambda_0 = 0.42$  nm and scattering angle  $\theta_S = 40^\circ$ . The green points are the zeros of  $\text{Re } \epsilon(k, \omega)$  and the experimental point is taken from [29].

### Interaction of Clusters With Laser Fields

Recent studies have demonstrated the potential of dual-pulse excitations to explore and control the laser-cluster interaction process. The response of sodium clusters to dual-pulse laser fields of moderate intensity has been studied by a systematic comparison of semiclassical Vlasov and Vlasov-Uehling-Uhlenbeck simulations [13]. Electron-electron collisions were found to significantly enhance the non-resonant absorption whereas the maximum ionization at optimal pulse delays – mainly determined by resonant plasmon excitations – are practically unaffected.



**Fig. 2.33:** Optimization of laser pulse shapes for a maximum yield of silver  $\text{Ag}^{10+}$  ions (solid) and  $\text{Ag}^{12+}$  ions (dashed) in clusters of initial diameter of 10nm. The pulse energy corresponds to a single Gaussian pulse with peak intensity  $160 \text{ TWcm}^{-2}$  with a duration of 130 fs (FWHM) and  $\lambda=810 \text{ nm}$ .

A further optimization of the ion yield is possible by pulse shaping. For an understanding of the dynamics, a theoretical description using a genetic algorithm and basing on the nanoplasma model was used which allows to describe different physical processes like ionization, heating and expansion that occur during the laser-matter interaction on a hydrodynamic level. The original model of Ditmire et al. was modified in some important points [33, 23] like inclusion of the lowering of ionization energies. For the collision absorption, we used improved expressions based on quantum statistical theory [11]. The genetic algorithm was used to optimize the yield of specific ion species [20, 24]. For the intensity envelope of the pulse,  $I(t)$ , we used a superposition of 5 Gaussians with three free parameters each and kept the fluence constant. Similar to experimental results, there comes out a double peak structure with a first pulse of lower intensity followed by the main-pulse with higher intensity, see figure 2.33. This second pulse in the vicinity of the Mie resonance leads to a resonant energy input into the plasma leading to an enhanced impact ionization.

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### 2.3.3 Physics of Elementary Particles

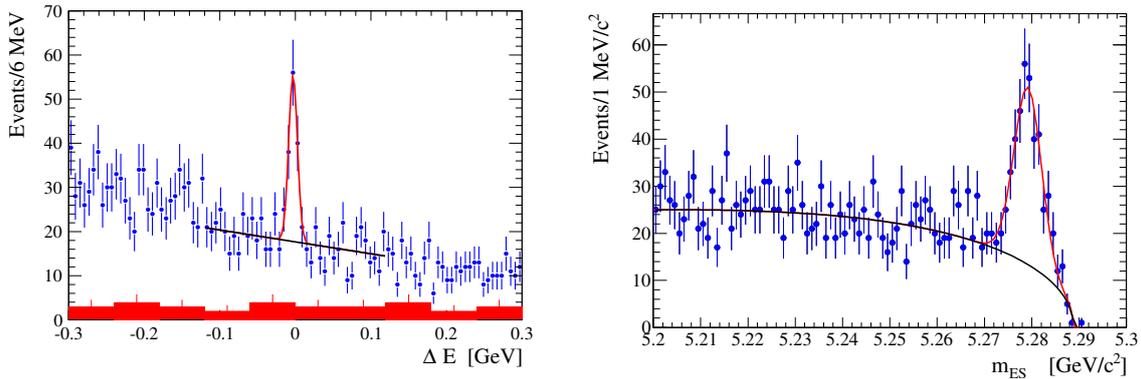
**Head:** Prof. Dr. Henning Schröder

<b>Staff:</b>	Priv.-Doz. Dr. Michael Beyer	Priv.-Doz. Dr. Roland Waldi	
	Dr. Alexander Kaukher	Dr. Stefan Strauß	
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	Dipl.-Phys. Martin Hierholzer	Dipl.-Phys. Torsten Leddig	
	Dipl.-Phys. Oliver Schäfer	Dipl.-Phys. Erik Schmidt	
	Yanjun Cong	Sebastian Dittrich	Christian Voß

#### Experiment BABAR

Since summer 2000 the group participates in the BABAR-experiment at the SLAC Accelerator Laboratory in California (USA), supported by the BMBF. This experiment studies multi-particle final states produced in the electron-positron-annihilation at a center of mass energy of 10.58 GeV. At this energy, the  $\Upsilon(4S)$ -resonance is produced, which decays exclusively into a pair of  $B$ -mesons, massive particles heavier than a helium nucleus. The main aim of the experiment is the investigation of a time dependent CP-asymmetry (particle-anti-particle asymmetry) in the decay of neutral  $B$ -mesons. The main achievement of BABAR was the first observation of this CP asymmetry in 2001. In the last three years, subsequent studies have revealed also direct CP violation, and improved the precision of the parameters of the Cabibbo-Kobayashi-Maskawa matrix which are responsible for this effect. These results established the predictions made by Kobayashi and Maskawa in 1972. Consequently, these theorists were awarded the Nobel prize in 2008. Among the most interesting recent results is the comparison of various decay channels with CP violation that may be differently affected by physics beyond the Standard Model. Although some hints have been found, we can not establish a significant discrepancy with this successful theory.

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 500 million  $B\bar{B}$  pairs collected are used to study much more details than CP asymmetries. The recent 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 found new decay channels (Fig. 2.34), and investigated the features of new and established baryonic final states. Many of those decays exhibit an enhancement of the decay rate at the threshold of the baryon-anti-baryon mass, which still puzzles the theorists working in this area. We will continue our investigations, and will contribute to the understanding of this unexpected feature by comparing modes with different



**Fig. 2.34:** Two clear signals for the  $B$  meson decays to final states with baryons:  $\bar{B}^0 \rightarrow \Lambda_c^+ \bar{p} K^- \pi^+$  (left, showing the distribution of the energy difference to a  $B$  meson) and  $\bar{B}^0 \rightarrow \Lambda_c^+ \bar{p} \pi^0$  (right, showing the mass distribution seen in the experiment).

underlying decay patterns.

### Experiment OPERA

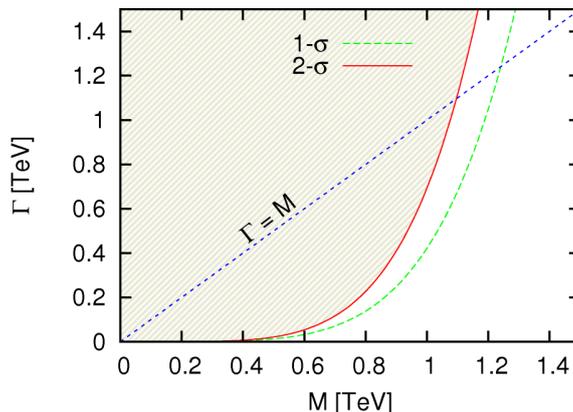
OPERA is an experiment to investigate tau-neutrino appearance from a muon-neutrino beam due to neutrino oscillations. The German groups in the OPERA-experiment (University of Hamburg, University of Münster, University of Rostock) were constructing the muon spectrometer of the OPERA detector, which has been installed in 2006 in the Gran Sasso laboratory in Italy. The Rostock group is responsible for the TDC-read-out electronics of the muon spectrometer. The CERN neutrino beam is operational, and data taking has started in 2007. Within about ten years of data taking, only a few events of tau neutrino appearance are expected from the Standard Model.

### Monte Carlo Studies for ILC

The next generation of particle accelerators will operate at 1000 GeV scattering energy and above (Terascale). The most urgent questions of interest are: i) What is the origin of the masses of elementary fermions and of the electroweak symmetry breaking? ii) What is the structure of space at small scales and are there hidden dimensions? iii) What is the nature of dark matter and dark energy?

The Large Hadron Collider (LHC) at the European Research Laboratory CERN has started operation in September 2008, and is providing proton proton collisions since March 2010. Another collider for electrons and positrons is under exploratory studies and could be realized as an International Linear Collider (ILC). Our group participates in the detector development and the physics program for this machine.

High precision analysis of physics questions such as the electroweak symmetry breaking requires a close collaboration of experimentalists and theorists. This is



**Fig. 2.35:** The confidence regions in parameter space (mass, width) of a new scalar resonance that could be exchanged in  $W$ - $Z$ -scattering. The green and red lines limit the parameter range where this particle could be observed with 1- $\sigma$ - and 2- $\sigma$ -significance.

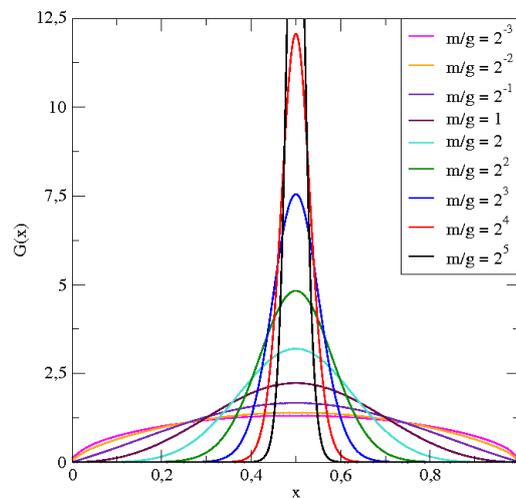
realized by simulating theoretical models and the complex experimental set-up in depth, starting from an effective Lagrangian quantum field theory that includes alternatives to the Standard Model approach for mass generation. Using this theory, a Monte Carlo event generator simulates intermediate three vector boson states produced in  $e^+e^-$  collisions, their decay, the hadronisation of six quark final states and gluons, and the detector response. New physics is expected to manifest itself in the interaction of the vector bosons. The most prominent example is a neutral spin-0-resonance replacing the Standard Model Higgs boson. The simulated events are reconstructed to determine the sensitivity of an ILC experiment to new physics encoded in the effective Lagrangian, and the regions in the parameter space of the non-standard Higgs boson where the real experiment could make a discovery or exclude the existence of such a particle (Fig. 2.35).

### Detector Research and Development

An important component of the detector at ILC is the readout electronics for the time projection chamber (TPC) that is a crucial component for charged track reconstruction and identification of particles. A TDC-based read-out for the TPC has been developed in our group, and has been used for further studies of the TPC performance. We have also built a prototype chamber for small-scale tests. This work is at the forefront of electronics development, and is supported through a European network EUDET.

## Theory

We investigate strongly-coupled gauge field theories at finite temperature within the discrete light-front quantization approach. Light-front quantization of low-dimensional models, such as the massive Schwinger model (Fig. 2.36) and quantum chromodynamics in 1+1 dimensions ( $\text{QCD}_{1+1}$ ) serve as theoretical test bed before one addresses questions in four-dimensional QCD. This framework is in particular suitable for the investigation of nuclear matter under extreme conditions as occurring, e.g., in heavy ion collisions that will be performed at CERN (Geneva) and GSI (Darmstadt).



**Fig. 2.36:** The momentum structure function of the Schwinger boson in the massive Schwinger model. Coupling strengths  $m/g$  varying from very weak to very strong have been investigated.

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### 2.3.4 Molecular Quantum Dynamics

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The Molecular Quantum Dynamics group at the University of Rostock has been established in January 2008. The focus of our research is on computer simulations of the dynamics, spectroscopy, and laser control of molecular systems from gas phase clusters, solvated or solid-state embedded chromophores, aggregates to biomolecules. Here, dynamics comprises chemical reactive and nonreactive processes of the nuclear degrees of freedom (adiabatic dynamics in the electronic ground state) as well as coupled (non-adiabatic) electron-nuclear dynamics as it occurs in Photophysics and Photochemistry. Spectroscopic methods range from nuclear magnetic resonance to stationary as well as ultrafast infrared and optical spectroscopy. Furthermore, we are active in the area of laser control, where pulse design is used not only to drive molecular dynamics, but also enable spectroscopic characterization of non-equilibrium states [2, 3, 9, 10, 11, 12, 14, 13, 15, 1, 4, 7, 6, 5, 8].

The study of Molecular Quantum Dynamics requires to solve the time-dependent Schrödinger equation. For the case of many coupled degrees of freedom approximate numerical schemes have to be invoked; among the most successful ones ranges the Multiconfiguration Time-dependent Hartree (MCTDH) method which has been pioneered by Meyer and coworkers in Heidelberg. Here the quantum mechanical state vector is written as a linear combination of time-dependent basis vectors which facilitates a compact representation of the moving wave packet. During the last years MCTDH has been our working horse and our efforts have been particularly focused on the development of efficient and flexible ways to determine molecular Hamilton operators for MCTDH wave packet propagation [2, 14, 13, 15, 1, 5].

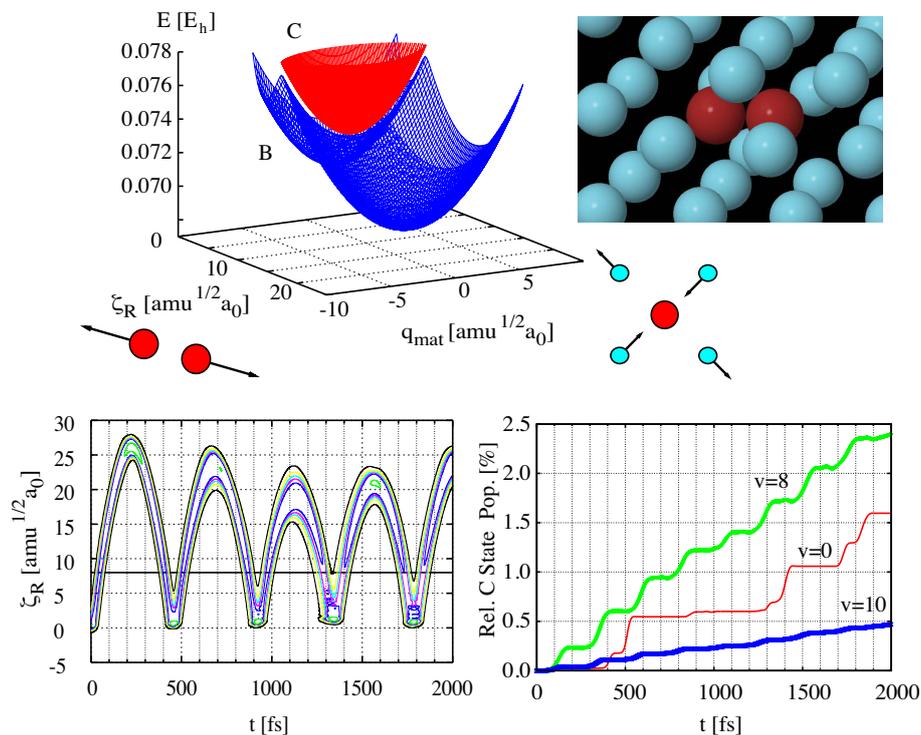
In condensed phase situations approximations to the dynamics have to be invoked and we utilize either the Master Equation approach [9, 10, 11] or quantum-classical hybrid techniques [12]. In the latter, trajectory-based formulations of spectroscopic linear and nonlinear response functions are combined with quantum mechanics/molecular mechanics (QM/MM) approaches to the determination of the interaction potentials. A variant, the semiempirical diatomics-in-molecules (DIM) method is particularly useful for the consideration of small chromophores embedded in low-temperature matrices [2, 1]. These hybrid methods replace purely quantum mechanical electronic structure approaches which are used for model systems in gas phase [3, 14, 15, 4, 6].

Hydrogen bonds are a prominent example for systems showing effects of multi-dimensional quantum dynamics. On the one hand side, the proton as the lightest nucleus is bound, e.g., to delocalization, tunneling, and zero point energy effects. On the other hand, its motion is strongly coupled to that of the surrounding atoms

and in particular their charges. Using a full-dimensional (9D) ab initio description we have studied the microsolvated  $\text{OH}^-$  ion,  $\text{H}_3\text{O}_2^-$ , which is prototypical for strong hydrogen bonds [14]. The particular question which has been addressed concerned the relative stability of different isotopomers. It was found that the hydrogen bond in  $\text{HOHOH}^-$  is slightly more stable than the deuterium bond in  $\text{HODOH}^-$ , a fact which is of relevance in the context of isotope fractionation. A second system, the protonated ammonia clusters,  $\text{NH}_4^+(\text{NH}_3)_{1-4}$ , has been studied as a model for ammonia wires being able to shuttle protons, e.g., in transmembrane ammonia channels. The dimer,  $\text{N}_2\text{H}_7^+$  turned out to be the most interesting system from the perspective of quantum effects and spectroscopy. Here, despite a rather high reaction barrier ( $> k_B T$ ) the proton is delocalized due to zero point motion. As a consequence the molecular structure becomes symmetric, whereas it would be asymmetric in the classical limit. Further, whereas typical NH-stretching absorptions are located above  $3000\text{ cm}^{-1}$ , the deformation of the potential energy surface due to hydrogen bonding gives rise to an absorption around  $400\text{ cm}^{-1}$ . This theoretical prediction has been confirmed by measurements at the free electron laser (FELIX) in Nieuwegein [15].

A second focus has been on the double hydrogen bonds in DNA base pairs. While the geometric properties of DNA hydrogen bonds are well-studied, their fluctuation dynamics on a femto- to picosecond time scale became accessible with the emerging ultrafast spectroscopy in the infrared domain only. To state the problem: The interesting NH-stretching vibrations absorb in the range above  $3000\text{ cm}^{-1}$ . However, stability of the DNA requires the presence of water which dominates this spectral range with its OH-stretching absorption band. From the perspective of linear IR spectroscopy, the NH-stretching absorption is completely hidden underneath the water band. However, in collaboration with the experiments we could show that two-color nonlinear pump-probe spectroscopy can unravel the characteristics of the NH absorption of the hydrogen bonds [3, 6]. Specifically, excitation in the fingerprint region around  $1600\text{ cm}^{-1}$  by a first pump pulse leads to a transient response in the  $3000\text{ cm}^{-1}$  that can be measured by a second probe pulse. Ab initio calculations of anharmonic couplings for the two hydrogen bonds enabled us to unravel the coupling pattern which is responsible for the correlated quantum dynamics of DNA base pairs. While for these calculations gas phase models had to be designed, individual base pairs can also be studied in non-aqueous solution. Here we focused on an adenine-uracil pair to clarify the origin of the line broadening of the NH-stretching vibration. Studying energy gap fluctuations on the basis of QM/MM (Gromacs/Car-Parrinello) trajectory simulations, relevant collective motions coupling to this stretching vibration could be identified [12].

Dihalogen molecules embedded in low-temperature rare gas matrices are an ideal test ground for quantum dynamics in the condensed phase. Upon photoexcitation it is the possibility for non-adiabatic electronic transition triggered by nuclear motions which adds to the challenge of a quantum description. Using the DIM method we have designed four- and five-dimensional [2, 1] model Hamiltonians suitable for studying the coupled dynamics on the electronic  $B$  and  $C$  states after excitation



**Fig. 2.37:** Non-adiabatic quantum dynamics and laser control of  $\text{Br}_2$  in solid Ar (upper right). Upper left: Conical intersection between the electronic  $B$  and  $C$  states along the bond distance and the asymmetric cage deformation coordinates. Lower left: Reduced density of the wave packet dynamics on the  $B$  state. Lower right: Relative  $C$  state population due to  $B$  to  $C$  pre-dissociation in dependence on the vibrational pre-excitation in the electronic ground state [2, 1].

from the ground  $X$  state (cf. Fig. 2.37). Of particular interest has been the pre-dissociation from the initially excited electronic  $B$  to the  $C$  state which is mediated by a conical intersection. First, nuclear motions responsible for triggering this transition could be identified (matrix cage deformation). Second, it was found that the efficiency of pre-dissociation depends on the initial vibrational excitation of the Br-Br bond in the electronic ground state. In principle this would give a handle on controlling the pre-dissociation. In practice one faces the challenge that this homodimer cannot be vibrationally excited directly, i.e. by means of IR radiation. Using Optimal Control Theory we could demonstrate that vibrational pre-excitation of the electronic ground state can be achieved by a pump-dump like scheme, where the pump pulse launches a wave packet on the  $C$  state which is dumped back to the electronic ground state after a certain delay time, thus achieving vibrational pre-excitation [1].

Finally, we have considered the topic of single molecule electron transfer on the

basis of a Generalized Master Equation in collaboration with V. May from the Humboldt University Berlin [9, 10, 11]. In single molecule electron transfer the coupling between electronic and nuclear degrees of freedom of the molecule leads to the appearance of additional vibrationally mediated transport channels. However, under certain conditions it had been shown previously that transfer is blocked due to poor vibrational wave function overlap (Franck-Condon blockade). We could demonstrate that this Franck-Condon blockade can be overcome and a switching of the transport can be achieved by means of optical excitation of the molecule.

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## 2.4 Institute of Atmospheric Physics Kühlungsborn

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<b>Address:</b>	Schlossstr. 6, 18225 Ostseebad Kühlungsborn Germany
<b>Director:</b>	Prof. Dr. Franz-Josef Lübken
<b>Telephone:</b>	+49 (0)38293 68-0
<b>Fax:</b>	+49 (0)38293 68-50
<b>Web:</b>	<a href="http://www.iap-kborn.de">http://www.iap-kborn.de</a>
<b>Source for more information:</b>	Institute report (every two years)
<b>Other locations:</b>	Außenstelle Juliusruh, Drewoldke 13 18556 Juliusruh, Germany

### 2.4.1 Main Areas 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, in particular at Arctic 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 ( $\sim 10\text{--}120$  km).

The main building of IAP being located in Kühlungsborn provides modern offices, laboratories, high speed computer facilities, and administrative and technical infrastructure. 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 is located at  $69^{\circ}17'N$  and  $16^{\circ}01'E$  ( $2^{\circ}$  poleward of the Arctic circle) and hosts instruments from several international institutes. The IAP also operates a mobile lidar (= light radar) in a container which was stationed at various locations and is currently prepared for a campaign in 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 2 and 54 MHz. Furthermore, instruments are installed on sounding rockets to measure dust, and 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. Since 2009 a new microwave spectrometer is installed at Kühlungsborn to measure water vapor profiles up to  $\sim 85$  km. The experimental investigations are accompanied by model calculations and theoretical studies. The scientists at IAP cooperate with

several international research institutes and universities both on experimental and theoretical aspects of atmospheric physics.

### **Supplemental Information**

Typically 70 individuals were employed at the IAP, amongst them 22 scientists and 20–25 students. In the period 2007–2009 the following staff members of the IAP gave courses and seminars at the Rostock University in the field of physics of the atmosphere: Prof. Dr. F.-J. Lübken, Prof. Dr. E. Becker, Prof. Dr. M. Rapp, Dr. habil. U. Achatz (now professor at the Frankfurt University), and Dr. habil. D. Peters. They also provided opportunities for students to work at the IAP for their bachelor, master, diploma and Ph. D. thesis.

In the following we provide some examples of typical research results in the three departments of the IAP. More details can be found in 149 science papers published by IAP scientists in the period 2007–2009. A list is provided in the appendix of this report.

## 2.4.2 Optical Sounding of the Atmosphere

**Head:** Prof. Dr. Franz-Josef Lübken

**Staff:** Prof. Dr. Götz von Cossart

Dr. Gerd Baumgarten

Dr. Uwe Berger

Dr. Jens Fiedler

Dr. Ronald Eixmann

Dr. Michael Gerding

Dr. Josef Höffner

Dr. Gerd Sonnemann

8 PhD students

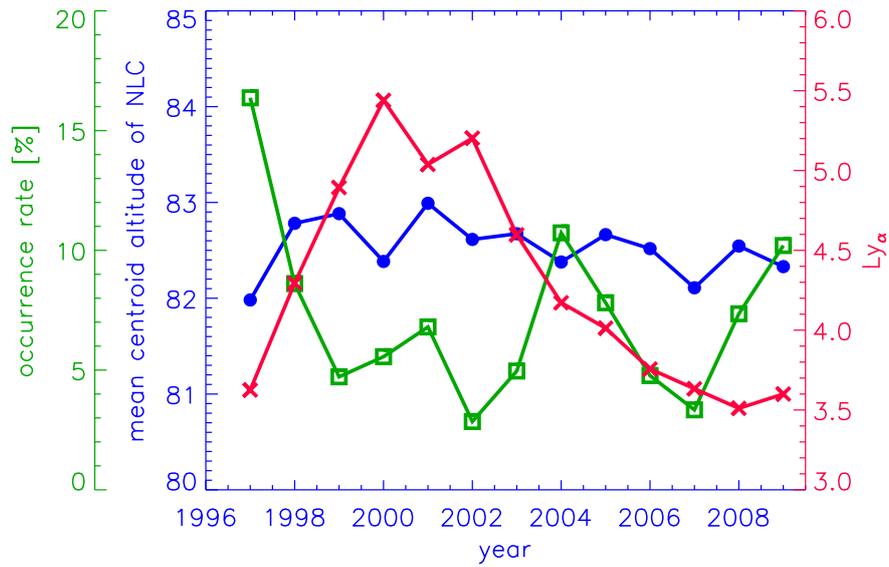
3 Dipl./MSc/BSc students

Main areas of research 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 (mesopause = pronounced temperature minimum near 90–100 km altitude), (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 mounted on balloons. A global scale model called LIMA (Leibniz Institute Model of the Atmosphere) is used to interpret ice cloud measurements and their connection to background conditions.

In the following, we present an example of results from our Rayleigh/Mie/Raman lidar at ALOMAR. This lidar measures temperatures in the 30–90 km altitude region as well as noctilucent clouds. NLC were first observed at mid latitudes by naked eye in the summer season more than 110 years ago. Today we know that NLC consist of water ice particles which can only exist in the very cold summer mesopause region at mid and high latitudes where temperatures occasionally drop below  $-140^{\circ}\text{C}$ . Since several years NLC are detectable by lidars even within the polar circle, i. e., during full daylight.

Science experts worldwide speculate that NLC might be sensitive indicators for long term changes in the upper atmosphere related to anthropogenic activities. But NLC are also subject to natural variations caused by, for example, solar activity. NLC are attractive for trend studies because they are very sensitive to temperatures and water vapor concentrations. In the last 13 years IAP scientists have collected a total of  $\sim 1700$  hours of NLC observations at ALOMAR which is the largest data-set worldwide. In Fig. 2.38 we show mean altitudes and occurrence rates for strong NLC, more precisely with backscatter coefficients larger than  $\beta = 13 \cdot 10^{-10} / (\text{m} \cdot \text{sr})$ . As can be seen the NLC altitudes are basically constant from year to year and are in fact very similar compared to historical observations (not shown here). This limits any speculation about long term trends of temperatures and/or water vapor at NLC heights. Fig. 2.38 also shows that occurrence rates are not simply anti-correlated with solar activity but show a more complex behavior. This is contrary to conventional expectations. We need to understand natural variability of NLC better before we can exploit the role of NLC for climate change detection.

Except from observations by lidars we also study the creation of ice clouds and their morphology by the LIMA model dealing with microphysical processes of ice particles in an atmospheric background with spatial and temporal variability. With



**Fig. 2.38:** Seasonal mean centroid altitudes (blue) and occurrence rates (green) of noctilucent clouds observed by the IAP lidar at ALOMAR. The solar Lyman- $\alpha$  radiation is shown (red) as an indicator of solar activity.

LIMA we have been able to reproduce long term variations of ice clouds as observed by satellite instruments and also to elucidate the influence of solar activity on NLC.

### 2.4.3 Radar and Rocket Borne Soundings of the Atmosphere

**Head:** Prof. Dr. Markus Rapp

**Staff:** Dr. Jürgen Bremer    Dr. Norbert Engler    Dr. Peter Hoffmann  
Dr. Ralph Latteck    Dr. Werner Singer    Dr. Gunter Stober  
Dr. Boris Strelnikov    Dr. Irina Strelnikova    Dr. Marius Zecha  
Dieter Keuer    Jens Mielich  
5 PhD students  
4 MSc students

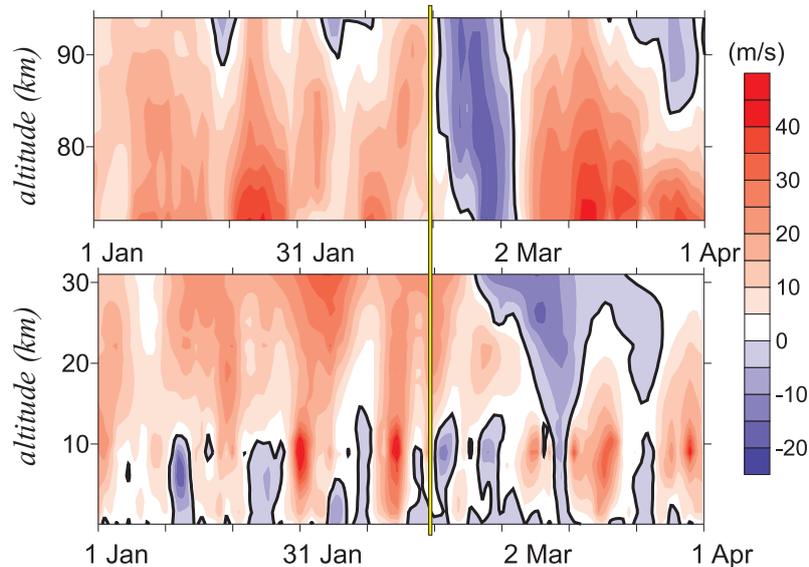
Main areas of research are the dynamical structure of the mesosphere and lower thermosphere (MLT, 60–120 km altitude) and of the troposphere and lower stratosphere (0–20 km altitude), the coupling of the MLT to the troposphere and vice versa, the composition of the MLT, and finally the detection and interpretation of its long term variability (forced by both natural and anthropogenic effects). All these areas are addressed using radar systems at various frequencies ( $\sim 100$  kHz to  $\sim 1$  GHz) as well as sounding rockets for in-situ observations. Radar observations are both made at mid-latitudes (Kühlungsborn and Juliusruh) and polar regions in Northern Norway. The latter is important since many atmospheric effects show their largest amplitudes at the poles like, e.g., the seasonal cycle leading for instance to the unique phenomenon of mesospheric ice clouds. In addition, the nearby location of the Andøya Rocket Range offers the operational opportunity to launch sounding rockets and hence allows us to combine state-of-the-art radar and lidar remote sensing with high resolution in-situ measurements.

As a particularly striking example for the topic of atmospheric coupling from the ground to altitudes of about 100 km, we present wind observations from a so-called stratospheric warming event in Fig. 2.39.

A stratospheric warming is characterized by strong planetary wave activity in the lower atmosphere which ultimately induces a reversal of the zonal wind (zonal = East to West) in the stratosphere which is accompanied by a strong warming. The latter may exceed several tens of degrees.

Fig. 2.39 reveals that the wave activity in the troposphere does not only induce a circulation change and heating in the stratosphere but also dramatic changes in the mesosphere. I.e., the IAP observations reveal that the wind reversal actually starts in the mesosphere after which the effect propagates down into the stratosphere, and in this case, even into the troposphere. Intriguingly, the mesospheric signal is observed several weeks before it finally reaches the ground hence also fostering speculations whether such mesospheric observations may successfully be implemented into weather forecast approaches. This issue is subject of current research at the IAP.

Investigations with sounding rockets are typically complementary to the ground based observations with radars in the sense that specific quantities can not at all be measured remotely like for example tiny nanoparticles of meteoric origin which are thought to be key players in the microphysics of the above mentioned mesospheric ice



**Fig. 2.39:** Characteristic changes of zonal winds (upper panel: mesosphere; lower panel: troposphere and lower stratosphere) above Andenes, Northern Norway, during a stratospheric warming event in winter 1998/99 (mesospheric data: Andenes MF radar; tropo- and stratospheric data: European Center for Medium range Weather Forecast, ECMWF). The vertical line indicates the onset of the wind reversal in the mesosphere.

clouds. Another benefit of in-situ measurements is the accessibility of quantities that can remotely not be measured with sufficient spatial resolution. A corresponding subject under consideration at the IAP is the characterization of the turbulent heat production following the breakdown of waves which are excited in the troposphere and propagate into the MLT. This heat production occurs on spatial scales of meters and less and is hence inaccessible for any state-of-the-art remote sensing technique. Our in-situ measurements reveal that corresponding heating rates are significant contributions to the heat budget of the MLT with values in excess of the direct radiative input.

### 2.4.4 Theory and Modeling

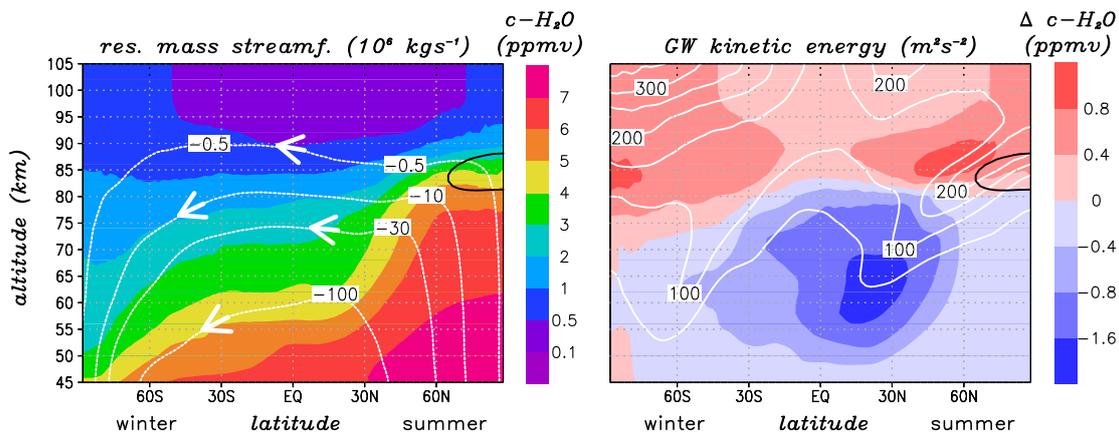
**Head:** Prof. Dr. Erich Becker

**Staff:** PD Dr. Dieter Peters  
Dr. Axel Gabriel                      Dr. Mykhaylo Grygalashvyly    Dr. Norbert Grieger  
Dr. Urs-Schaefer-Rolffs            Dr. Christoph Zülicke  
2 PhD students  
2 diploma thesis students

The main field of research is the 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 coupling of the atmospheric layers is controlled by radiative transfer, by the distribution of chemically and radiatively active minor constituents, and particularly by atmospheric waves. The latter are found on vastly different temporal and spatial scales. Atmospheric waves predominantly originate in the troposphere, they propagate upward and dissipate at higher altitudes, giving rise to so-called wave-mean flow interactions. By this mechanism the waves ‘drive’ a global mass circulation which leads to huge deviations from the radiatively determined state. In the upper mesosphere this circulation reaches from the summer to the winter pole.

In recent years much work has been devoted to understand the role of atmospheric waves for long-term changes in the middle atmosphere. The conventional picture of increased radiative cooling due to increased CO<sub>2</sub> can only partly explain the observations. We found that mesospheric cooling over Europe results in addition from a stronger and westward shifted planetary Rossby-wave pattern which in turn is related to trends in the ozone distribution. Furthermore, a purely dynamical mechanism was identified which strongly contributes to mesospheric cooling in summer. According to our model simulations, global tropospheric warming may result in an intensification of the energy cycle, which in turn induces stronger gravity-wave activity and, as a remote signal, a stronger pole-to-pole circulation in the mesosphere.

Gravity waves have typical horizontal and vertical scales of a few 100 km and 1–20 km, respectively. Using a suitable parameterization of turbulence within the global circulation model developed at IAP, gravity waves can now be simulated explicitly up to 100 km height. Combining the circulation model with a chemistry-transport model, also developed at IAP, we have found that gravity waves lead to a considerable mixing of minor constituents in the mesosphere, where the wave amplitudes are strongest. A similar effect has long been assumed to cause vertical mixing in the ocean. It is one of the results of the International Leibniz Graduate School ILWAO joined by IAP, IOW, and LSM that vertical mixing due to gravity waves could be established as an important process for understanding the physics of the middle atmosphere.



**Fig. 2.40:** Results from a high-resolution simulation showing the effect of gravity-wave mixing on water vapor during the summer solstice. Left: Mean water-vapor concentration (color) and mass streamfunction (white contours). Right: Change in water-vapor concentration resulting from wave mixing (colors) and mean kinetic energy of gravity waves (white contours, interval  $50 \text{ m}^2 \text{ s}^{-2}$ ). The mixing can be either along (summer) or against (winter) the mean transport by the mass streamfunction. For reference, the black lines indicate the cold summer mesopause by the 150 K temperature contour.

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

**Director of the institute:** Prof. Dr. Bodo v. Bodungen

**Head of the department:** Prof. W. Fennel

**Deputy:** Prof. H. Burchard

### **Introductory Remarks**

The Leibniz-Institute for Baltic Sea Research Warnemünde is a member of the Science Association Gottfried Wilhelm Leibniz and is jointly funded by the federal government and the state of Mecklenburg-Vorpommern. The institute has an interdisciplinary profile comprising the basic disciplines of marine sciences. The IOW is associated with the University of Rostock where the IOW department heads are Professors and contribute to the teaching of Biology, Chemistry and Physics. Similarly, the section ‘Marine Geology’ is associated with the University of Greifswald.

The research of the IOW is focused on marine systems in coastal and marginal seas using the Baltic Sea as an example. For more detailed information we refer to the annual reports of the IOW and invite the reader to visit our web site ([www.iowarnemuende.de](http://www.iowarnemuende.de)).

The department of physical oceanography is linked to the Institute of Physics of the Faculty of Mathematical and Natural Sciences of the University of Rostock. During the last three years, six members of our department, Prof. Fennel, Prof. Burchard PD Dr. Hagen, PD Dr. Lass, Dr. Umlauf and Dr. Neumann were teaching at the University of Rostock.

The oceanographic research encompass four elements: Observations with research vessels and moored instruments, theoretical studies and numerical modeling, satellite oceanography and work in of the Baltic Monitoring Programme. Further activities outside the Baltic are mainly focussed on the Benguela Current System off Namibia, South Africa and Angola. The department is also strongly involved in multidisciplinary modeling of marine ecosystems.

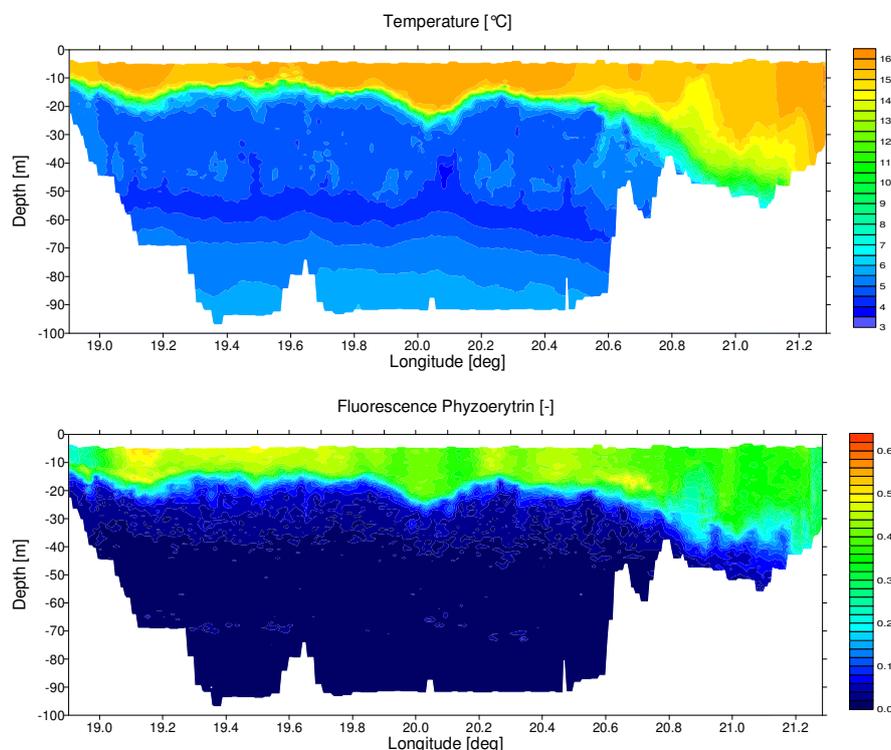
### **Upwelling in the Baltic and in the Benguela System**

V. Mohrholz, H. U. Lass, M. Schmidt, and W. Fennel

Upwelling processes are well known elements of the dynamics of coastal oceans, providing vertical transports of water and nutrients from deeper layers into the euphotic layers. On a global scale, the major upwelling systems, such as the Benguela, are among the most productive regions of the world ocean and play an important role

in the carbon cycle. In the Baltic sea upwelling is during the summer season the most effective process, that provides nutrients to the surface layer. The quantitative understanding of how upwelling related physical- biological interactions affect the system on small scale, mesoscale, and on regional scale, is of critical importance for a science based sustainable management of the marine environment.

In the Baltic Sea the vertical transport of nutrients into the surface layer by turbulent diffusion is impeded by the very stable three layer stratification during the summer season. However, upwelling of cold water, originating from the intermediate winter water layer, occurs frequently within narrow coastal belts. The location and the frequency of upwelling events depend on the coastal topography as well as the direction and duration of the alongshore wind.



**Fig. 2.41:** Transect observed with a towed instrument (ScanFish) from the east coast of Gotland (left) to the Latvian coast (right). The temperature (upper panel) showed that the upwelling at the east coast of Gotland caused an uplift of thermocline. The Ekman transport in the surface layer advected warm water towards the Latvian coast, where it caused accumulation and downwelling of surface water. The lower panel depicts the Phycoerytrin fluorescence as measure for cyanobacteria concentration. Highest fluorescence was found at the upwelling front of Gotland, where phosphate is supplied to the surface waters.

The role of upwelling for triggering cyanobacteria blooms in the central Baltic

sea was recently investigated in an interdisciplinary project at the IOW. Two field campaigns, conducted in summer 2007 and 2009 in the eastern Gotland basin, delivered the required multiparameter data set. The aim of the investigations was to elucidate the pathways of phosphate from the intermediate winter water into the surface mixed layer and how this phosphate flux fosters phytoplankton growth. In the period before these field campaigns the deep water of the Gotland Basin was exposed to enduring stagnant conditions with denitrification due to anoxic conditions resulting in nitrogen to phosphorus ratio much lower than the Redfield ratio. During summer the intermediate winter water was completely depleted of nitrate but contained a significant phosphate pool of about  $0.40 \mu\text{M}$ . The surface mixed layer was depleted of both nitrate and phosphate. Pulses of westerly wind with maximum wind speed of about  $15 \text{ m/s}$  forced upwelling at the east coast of Gotland and downwelling near the Latvian coast, Fig. 2.41. The corresponding eastward Ekman offshore transport moved surface water within about three days through the coastal boundary. Mesoscale eddies were observed off the south eastern coast of Gotland, which supported upwelling filaments near the southern tip of this island.

Within the coastal boundary layer, the upwelling transported phosphate from the intermediate winter water into the surface layer off Gotland where it was mixed with the phosphate depleted surface water. Generally, the upwelled phosphate was taken up by the plankton community of the surface mixed layer already within the coastal boundary layer and transformed completely into the particulate and dissolved organic phase. However, at sites where upwelling filaments develop, dissolved phosphate is transported over a distance of about three times the internal Rossby radius in offshore direction. The phosphate transport into the surface mixed layer of the eastern Gotland Basin by upwelling exceeded the corresponding transport by turbulent mixing through the seasonal thermocline by about one order of magnitude during typical summer-like wind conditions (Lass et al. 2010). In the Baltic, upwelling is episodic and the role of coastally trapped waves, such as Kelvin waves can be studied with a new generation of towed instruments and high resolution models. It is assumed that a substantial part of the vertical mixing is mediated by mesoscale processes including upwelling. The quantification of total vertical transports on event scales and during the annual cycles will be pursued in a new project 'Pathways and time scales of nutrient transports in the Baltic', funded by DFG. The study is based on simulation of scenarios with the numerical model of the Baltic Sea (see below).

The IOW continued the work in the Benguela upwelling region with two expeditions of the RV Merian and RV Meteor in 2008, (Fig. 2.42). The investigations were focused on the large scale dynamics of the system and on small scale process studies. A large scale CTD station grid was worked to extend the existing data set and to improve the seasonal coverage. Former observations in the northern Benguela suggest that the summer season 2008 was characterized by exceptional high surface temperatures and an increased frequency of coastal hydrogen sulphide outbreaks. In view of global change it will be important to clarify whether the uncommon

conditions were caused by a so-called inter-annual anomaly, the Benguela Niño, or whether it signals a long term change.

Small scale process studies at selected stations on the mud belt aimed at elucidating the role of turbulent mixing for vertical fluxes of nutrients and oxygen. Recent observations depicted a well mixed bottom layer of 10 to 30 m thickness on the shelf that could not be explained with the available current measurements. Using a bottom mounted ADCP in high resolution mode in combination with a Microstructure probe (MSS) for estimation of dissipation rates of turbulent kinetic energy (TKE), it could be shown that swell and internal waves play a dominant role in mixing in the bottom boundary layer. The near bottom current velocity caused by the swell and internal waves was in order of 10 to 20 cm/s. This value exceeds the observed mean current velocities near the bottom by the factor of 3 to 4. The consequences of this result for re-suspension of sediments will be one of the key issues in the ongoing research.

Since May 2009 the IOW is involved in the project ‘Geochemistry and Ecology of the Namibian Upwelling System’ (GENUS), funded by the BMBF until 2012. The project represents a national German contribution to IMBER and embraces several key issues identified by the IMBER Science and Implementation Strategy. The general aim is to clarify relationships between climate change, biogeochemical cycles, and ecosystem structure in the large marine ecosystem of the northern Benguela/SW Africa. An integral part of the project is building and enhancing capacity in marine sciences in Namibia. For detailed information refer to the project homepage (<http://genus.zmaw.de>).

The field measurements in the Baltic Sea and in the Benguela current system are supplemented by numerical investigations with coupled circulation and ecosystem models based on the MOM-4 code developed by GFDL extended by special code contributions of the IOW for regional model applications. The appropriate representation of coastal upwelling and the related physical processes requires enhanced horizontal model resolution that in turn could be achieved only by using super computer capabilities. Numerical simulations of the dynamics of the upwelling cell at the southern tip of Gotland in comparison with field and remote sensing data could demonstrate that numerical models resolving the baroclinic Rossby radius can produce realistic hindcasts of the upwelling dynamics. Hence, a numerically produced data set is currently used to quantify coastal upwelling in the Baltic Sea.

A numerical circulation model of the equatorial ocean and the eastern boundary current system off southern Africa coupled to a bio-geochemical model could be validated successfully against field data and is currently used to quantify transports through the Angola-Benguela frontal zone that separates a tropical ecosystem from the Benguela upwelling area.



**Fig. 2.42:** The German Research Vessel Maria S. Merian during the cruise in March 2008.

### **Ecosystem Model**

T. Neumann and W. Fennel

In the last three years the further development and application of the IOW ecosystem model focused on two main topics:

- analysis of the changes of the ecosystem of the Baltic Sea in response to future climate scenarios,
- bridging the gap between the lower and upper part of the marine food web.

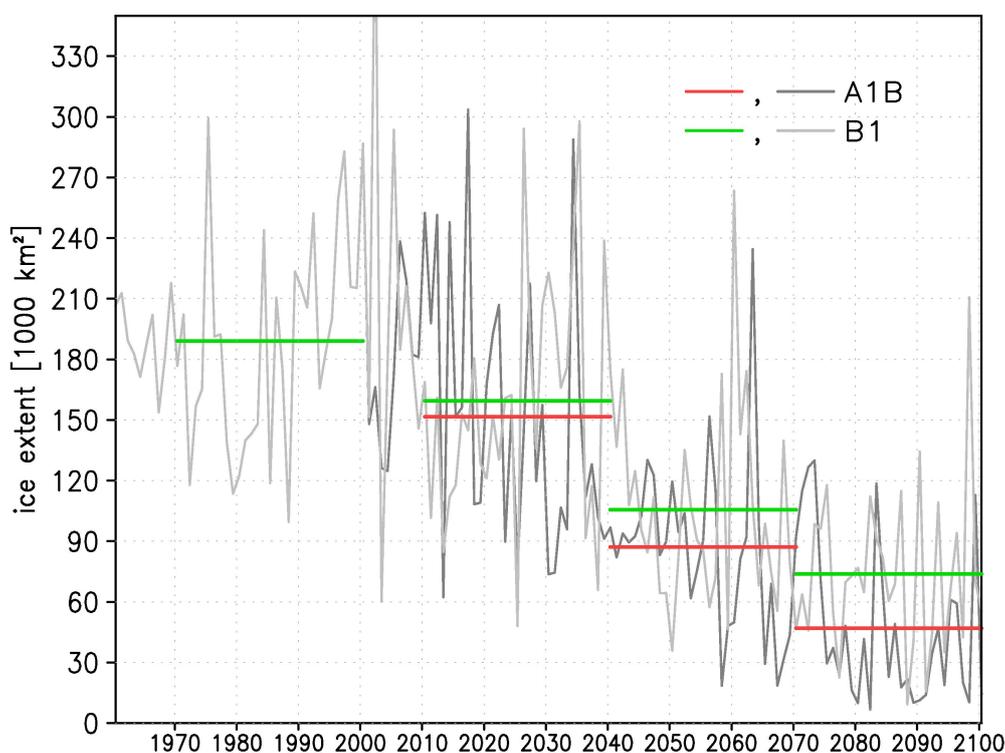
Within the last years super computer capabilities have largely increased, especially due to the setup of the second generation of the HLRN server (Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen). Together with some technical improvements of the IOW three-dimensional ecosystem model of the Baltic Sea, we are now able to simulate the Baltic Sea ecosystem for periods of more than 100 years.

The development of the Baltic Sea ecosystem in the response to changing climate is of particular concern. To answer this question, a high degree of uncertainties is involved. On the one hand, projections for a future climate cover a wide range of changes for the meteorological and hydrological variables. For example the global warming for the next 100 years is expected to be in the range of 2-4K. On the other hand, the Baltic Sea ecosystem is mostly controlled by its catchment area. Changes in land use, population patterns, the hydrological cycle etc. may have even a stronger impact on the Baltic Sea than the direct climate change.

At IOW we started to study the impact of climate change on the Baltic Sea ecosystem with the aid of IOW's model ERGOM (ecological regional ocean model).

One prerequisite was the availability of regional climate projections. These scenarios are derived from dynamical downscaling to nest regionally restricted climate model with high spatial resolution into a global climate model. Such data set are now available and the number of different scenarios runs increases.

The experiments at IOW focused on the direct impact of climate change with the assumption that nutrient loads from the catchment will not change. Results show especially decreasing sea-ice coverage and increasing water temperatures. There are some indications that salinity will decrease, however this is not a robust result because different models from different institutions give a wide spread of salinity changes. The model simulations do not indicate that biogeochemical cycles may change dramatically. For cyanobacteria a certain probability exists that the season will prolong, however this scenario did not consider changes in the catchment. As an example, Fig. 2.43 shows the decrease of sea-ice; a detailed description of the model experiments is in Neumann (2010).

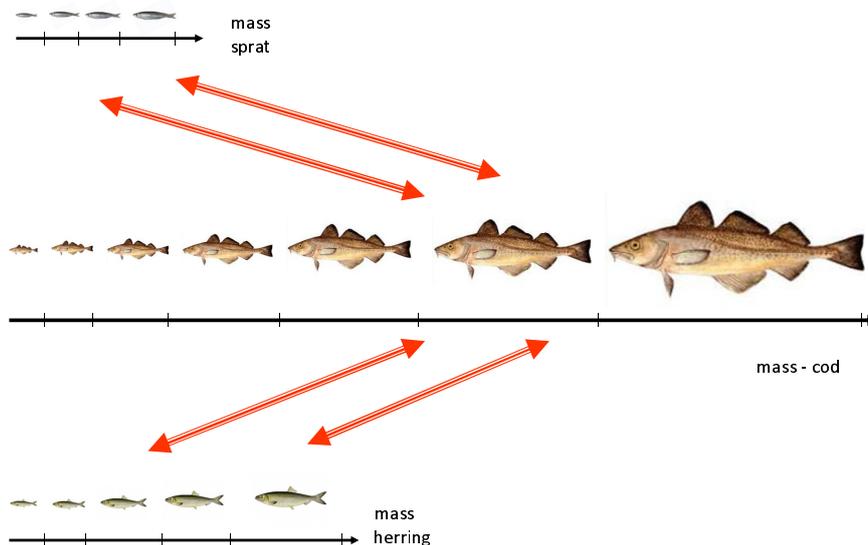


**Fig. 2.43:** Expected maximum sea-ice extent for the emission scenarios A1B (black and thick solid) and B1 (gray and thick dashed). Black and gray lines are the annual mean sea-ice extent, thick solid and dashed lines the 30-year means.

With regard to the food web modeling, we developed a mass-class dependent fish model in order to provide a consistent theoretical approach that bridges the gap between biogeochemical models and fish-production models. The linkage of

the different models requires coupling of a *NPZD*-model (*N*utrients *P*hytoplankton, *Z*ooplankton, and *D*etritus) with a fish production model to generate a *NPZDF*-model, (or *WFM*-*W*arnemünde *F*ood web *M*odel). Using the Baltic Sea as example system is an advisably point of departure, because the food web is relatively simple and the fish dynamics is here dominated by two prey species (sprat and herring) and one predator (cod). Nevertheless, the approach is formulated in a general manner and can also be applied to other systems with a few modifications in the parameter sets (Fennel, 2008).

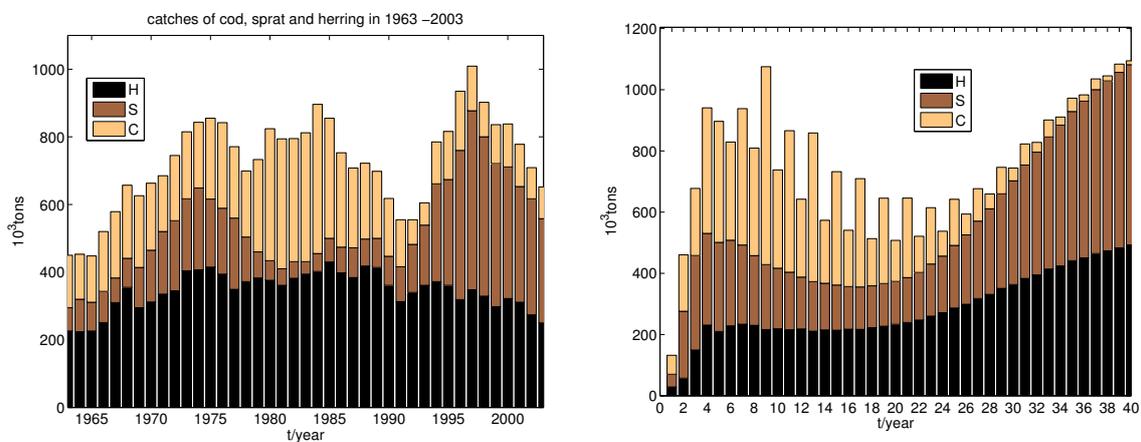
The fish model is size-structured by means of mass intervals, as sketched in Fig. 2.44. The state variables are concentration of biomass and number of individuals per unit of volume. The growth dynamics enhance the fish biomass, while the numbers of individuals is controlled by birth of recruits and mortality (natural, predation and fishing). The dynamics of the fish model is driven by size dependent predator-prey interactions, consumption of zooplankton, reproduction as well as natural and fishing mortality. The mass of the average individual is simply given by the ratio of biomass to numbers of individuals in each mass class. The relationship between the model components of the lower and upper part of the food web is established through feeding of prey fish on zooplankton and recycling of fish biomass to nutrients and detritus. The model conserves strictly mass. The challenge for the development of the fish model was to provide a consistent formulation of the complex interaction processes and fluxes of matter between the state variables. The work was done on the basis of a simple box model with a strongly simplified biogeochemical model component.



**Fig. 2.44:** Sketch of the size-structured prey-predator interaction

In order to demonstrate the model performance, several loading and fishing sce-

narios were tested. The result of a scenario simulation with simplified but realistic histories of the reproductive volume of cod, nutrient loads and fishing activities is shown in Fig. 2.45, and compared with observed fishery data (ICES). In spite of the strong simplifications of a box model, the observed order of magnitude and the structure of the species of catches can be reproduced, but the resulting phases do not match the observations (Fennel, 2010). This implies the need of further work with more realistic forcing and, in particular, the transition from a box model to a 3d-approach. Such a comprehensive *NPZDF*-model provides the possibility to analyze the effects of food web truncation. In particular, it is possible to quantify how choices of parameterizations in truncated *NPZD* models reflect the representation of unresolved processes (Fennel, 2009).



**Fig. 2.45:** Observed (left) and modeled (right) catches cod, sprat and herring from 1963-2003 for the Baltic Sea. Although the model is strongly simplified, it displays the right order of magnitudes, but the phases of the changes are poorly reproduced.

The model enables building the fish model into a three dimensional ecosystem model of the Baltic Sea or other systems. The next step is the implementation of a spatially explicit model where the development of fish in the phase space includes the three dimensional physical space.

## Thermodynamics of Seawater

R. Feistel

A precise knowledge of the thermodynamic properties of seawater and its composites with ice, water vapor and humid air is indispensable for the understanding and modeling of the changing terrestrial climate system, as well as the design of energy-efficient technical devices such as, e.g., desalination plants to meet the growing demand for potable water. To address the related problems and to revise the

partly obsolete standards of 1980, SCOR/IAPSO founded the Working Group 127 on Thermodynamic and Equation of State of Seawater, Fig. 2.46.



**Fig. 2.46:** First meeting of the SCOR/IAPSO WG127 in Warnemünde. From left to right: C.T.A. Chen (Taiwan), F.J. Millero (USA), B.A. King (UK), R. Feistel (IOW), D.G. Wright (Canada), T.J. McDougall (Australia), G.M. Marion (USA).

In close cooperation with the International Association for the Properties of Water and Steam (IAPWS) and various other partners such as the German universities of Rostock and Bochum, the TH Zittau and the PTB Braunschweig, a qualitatively advanced and very comprehensive new standard for oceanography was developed, and has eventually been endorsed as TEOS-10, the International Thermodynamic Equation of Seawater 2010, by UNESCO/IOC in summer 2009 in Paris. TEOS-10 is based on a new salinity measure, the Reference-Composition Salinity Scale, which replaces the SI-inconsistent oceanographic unit “psu” by a mass fraction in g/kg and assigns a chemical composition model to IAPSO Standard Seawater (Millero et al., 2008).

The work of WG127 is presented in a compact form in the monograph “IOC, SCOR and IAPSO: The international thermodynamic equation of seawater - 2010: Calculation and use of thermodynamic properties. Intergovernmental Oceanographic Commission, Manuals and Guides No. 56, UNESCO (English), 196 pp., Paris, 2010” and is available online from [www.TEOS-10.org](http://www.TEOS-10.org). Intended to be a fundamental reference document for oceanographers in the coming decades, it was critically reviewed by a number of external experts and by the members of WG127, and successfully defended on the 25<sup>th</sup> IOC Assembly in front of all UNESCO member states in Paris 2009.

As its Primary Standard, TEOS-10 combines very accurate empirical thermody-

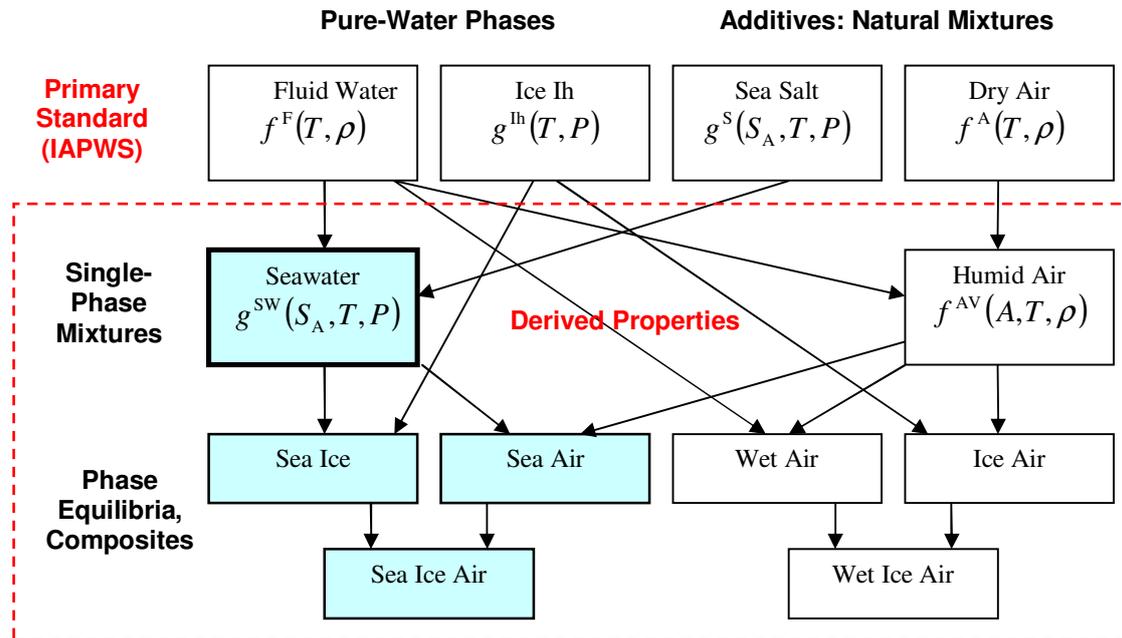
dynamic potentials that are formulated as official IAPWS documents for liquid water and water vapor, for ice, for seawater (Feistel, 2008) and for humid air (Feistel et al., 2010b). All the thermodynamic properties of those substances and their mutual phase equilibria can be computed from the Primary Standard by purely mathematical operations without additional empirical coefficients or equations, Fig. 2.47.

The Primary Standard of TEOS-10 consists of the IAPWS documents:

- Release on the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater, Berlin, Germany, 2008,
- Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. Doorwerth, The Netherlands, 2009,
- Supplementary Release on a Computationally Efficient Thermodynamic Formulation for Liquid Water for Oceanographic Use. Doorwerth, The Netherlands, 2009,
- Revised Release on the Equation of State 2006 for H<sub>2</sub>O Ice Ih. Doorwerth, The Netherlands, 2009, and
- Guideline on an Equation of State for Humid Air in Contact with Seawater and Ice, Consistent with the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater, to be adopted in Niagara Falls, Canada, July 2010.

Four of those five documents were mainly developed at the IOW and proposed to be endorsed by IAPWS as international standards. For this purpose, submitted IAPWS documents regularly undergo an extended and meticulous review and revision process over several months conducted by an Evaluation Committee of three international experts, established for this particular purpose, and must successfully be defended on an annual IAPWS meeting. IAPWS documents are available online at [www.iapws.org](http://www.iapws.org).

To assist the user, a comprehensive source-code library for “Sea-Ice-Air” (SIA library) for TEOS-10 was developed by WG127 with leading contributions from IOW, available from a Special Issue of Ocean Science ([www.ocean-sci-discuss.net/special-issue23.html](http://www.ocean-sci-discuss.net/special-issue23.html)). TEOS-10 is supported by various novel studies of properties of seawater and its interaction with ice and water vapor (Feistel and Marion, 2007; Feistel and Wagner, 2007; Tchijov et al., 2008; Feistel, 2008b, 2010; Sun et al., 2008; Feistel et al., 2008; Safarov et al., 2009). Further work is in progress regarding the metrological traceability of salinity measurements to ensure the comparability of measurement results on a century time scale, and to develop tools for the analysis and description of seawater composition anomalies, in particular with regard to the marine impact of rising CO<sub>2</sub> levels in the atmosphere (Feistel and Weinreben, 2008; Marion et al., 2009; Feistel et al., 2010a).



**Fig. 2.47:** Hierarchical structure of selected modules of TEOS-10. From the Primary Standard, the thermodynamic properties of the single phases and their equilibria can be derived mathematically.

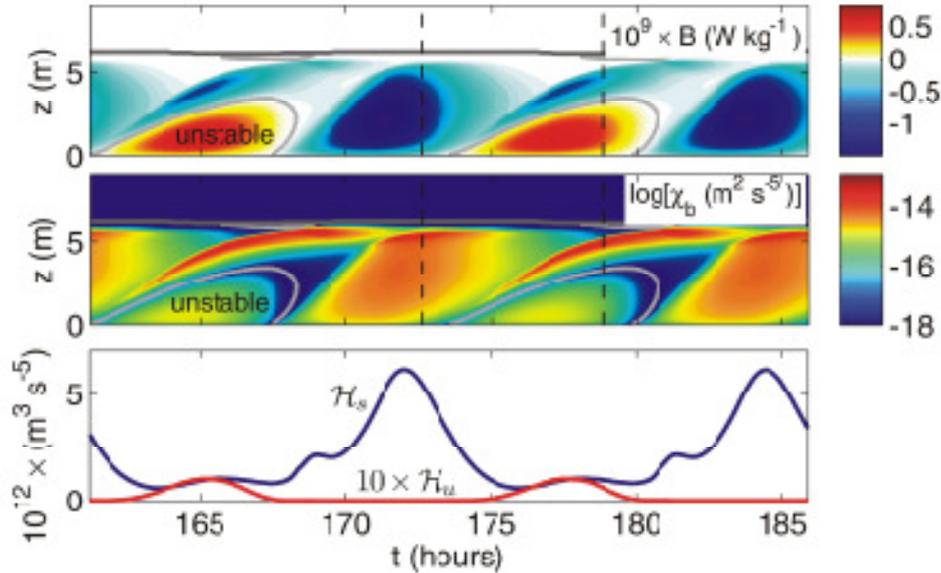
## Mixing and Residual Transport in Stratified Oscillating Bottom Boundary Layers

H. Burchard, L. Umlauf, and J. Becherer

Oscillating bottom boundary layers are an ubiquitous phenomenon in oceans and lakes. In the ocean they occur typically at semi-diurnal tidal frequency, while in tideless stratified marginal seas (like the Baltic Sea) and lakes internal waves at eigenfrequencies of the individual basins, driven by inflows or changes in wind forcing are cause of the oscillations. Stratification interacting with these oscillations in the bottom boundary introduces asymmetries which lead to a number of interesting phenomena relevant for the transport of solutes and particulate matter.

The Coastal Ocean Physical Process Studies (COPPS) group at IOW has concentrated parts of their scientific interest in investigating the impacts of these asymmetries in the Wadden Sea (Burchard et al. 2008), deep basins of the Baltic Sea and stratified lakes (Lorke et al. 2008).

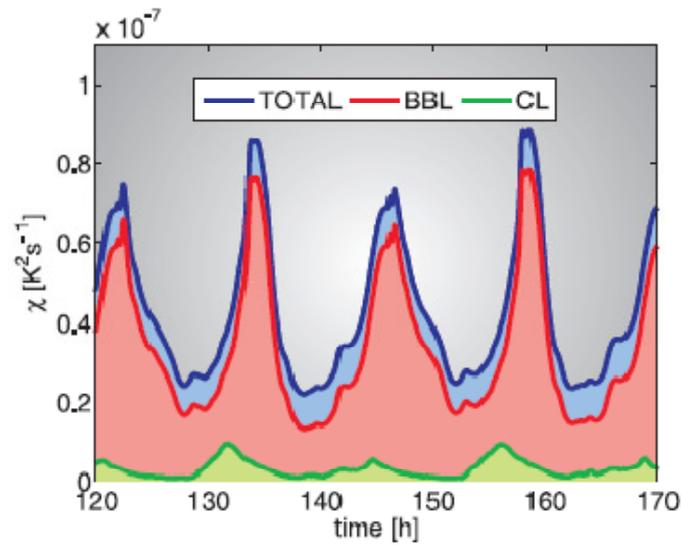
In a recent model study the problem of oscillating sloping bottom boundary layers in lakes and coastal sea basins has been idealized (no along-slope gradients except for background stratification) such that a 1D water column model can be applied (Umlauf and Burchard, 2010). In the upslope phase near-bottom shear (caused by



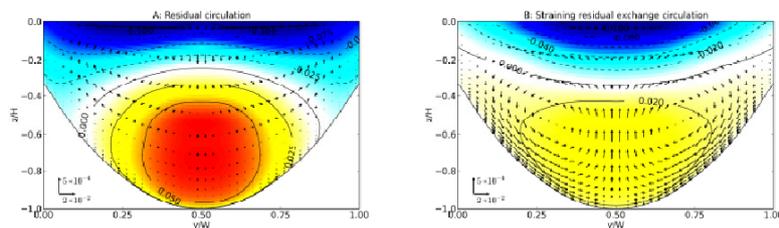
**Fig. 2.48:** Mixing in an oscillating and sloping bottom boundary layer during two periods. Upper panel: buoyancy flux  $B$ ; middle panel: dissipation of microstructure buoyancy variance,  $\chi_b$ , lower panel: vertical integral of  $\chi_b$  for stable ( $H_s$ ) and unstable ( $H_u$ ) stratification. Figure taken from Umlauf and Burchard (2010).

the no-slip bottom boundary condition for momentum) denser water moves over less dense water generating a destabilization of the water column and consequently strong turbulence production, high eddy diffusivity and upward (positive) buoyancy flux  $B$ . In the downslope phase, the opposite happens: less dense water is moved over denser water, suppressing turbulence. Fig. 2.48 shows 1D model results two periods for a bottom boundary layer of 5 m thickness, starting with the upslope phase. The unstable ( $B > 0$ ) region during upslope flow and the stable region ( $B < 0$ ) during downslope flow are clearly seen. In their modeling study Umlauf and Burchard (2010) found that mixing (defined as dissipation of microstructure buoyancy variance,  $\chi_b$ , see middle panel in Fig. 2.48) is much stronger during the downslope than during the upslope phase, although the eddy diffusivity (not shown) is much larger during the upslope phase. They could also show that the vertical integral of  $\chi_b$ ,  $H$ , is a good estimate for the irreversible upslope buoyancy flux. The great advantage of this theory is that  $\chi_b$  can be directly measured with a microstructure profiler, whereas observations of the buoyancy flux in an oscillating boundary layer would be very inaccurate. Becherer (2010) and Becherer et al. (2010) could show with a high resolution model for a small lake that almost all mixing occurs in the bottom boundary layer during stable stratification (Fig. 2.49).

Asymmetric oscillating bottom boundary layers interacting with buoyancy gradi-



**Fig. 2.49:** Composition of mixing (average temperature variance dissipation,  $\chi$ ) in a small lake during three oscillation periods: TOTAL: total mixing; BBL: bottom boundary layer mixing; CL: bottom boundary layer mixing during unstable stratification. Figure taken from Becherer (2010).



**Fig. 2.50:** Residual circulation (normalized by tidal velocity amplitude) in a cross-section through a tidal channel. Red: landward currents; blue seaward currents. Arrows show lateral circulation. A: Tidal residual; B: Tidal straining contribution to tidal residual. Figure taken from Burchard et al. (2010).

ents occur also in the Wadden Sea since Wadden Sea water is generally less dense than North Sea water (Burchard et al. 2008). This phenomenon is called tidal straining, which is known to be generating near-bottom landward residual flows. Burchard and Hetland (2010) could show that for tidally energetic flow tidal straining contributes to 2/3 of this residual current. In a recent model study, Burchard et al. (2010) demonstrated how this tidal straining circulation contributes to the residual currents for a cross-section through a tidal channel (Fig. 2.50). It will be a major task for the future to confirm these theoretical results with field observations in the Baltic Sea and in the Wadden Sea.

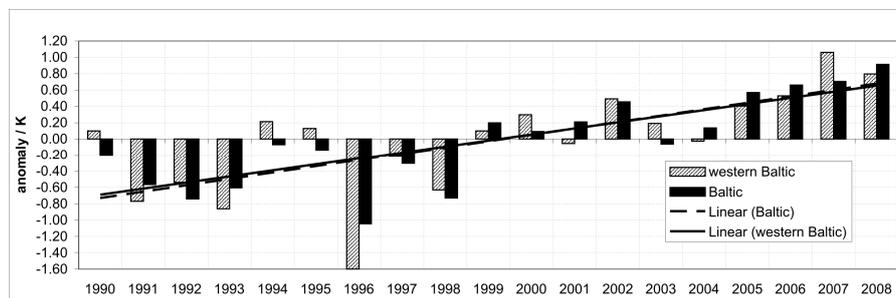
## Satellite Oceanography

H. Siegel

Remote sensing is a method providing coherent pictures of oceanographic processes which leave signatures at the sea surface. Both the synoptic character and the high repeating rate allow the mapping of variable structures in space and time. The application of satellite data in the IOW was focussed on sea surface temperature (SST) development of the Baltic Sea, the development of phytoplankton blooms, dynamical processes, and coastal discharge. SST maps are derived from data of the Advanced Very High Resolution Radiometer (AVHRR) of the NOAA weather satellites received from the BSH Hamburg. Ocean color data of MODIS and MERIS provided by NASA and ESA are used to derive optically active water constituents. In the frame of the ESA-ENVISAT mission IOW contributed to the MERIS- validation program.

SST data are evaluated to investigate seasonal and inter-annual variations in the temperature development of the Baltic Sea. The seasonal development in each year is described in the yearly hydro-chemical assessments of the state of the Baltic Sea prepared by IOW (Nausch et al. 2008, 2009) and in the HELCOM indicator fact sheets (Siegel and Gerth, 2008, 2009). The analysis of the SST was continued for the entire Baltic Sea and focussed on the dynamically high variable western Baltic Sea in front of the German coast (Siegel et al. 2010 submitted). The period 1990-2008 was characterized by a positive linear trend in the yearly mean SST with an increase of 1.41°C, (Fig. 2.51). In contrast to the global temperature development and that of the northern hemisphere the increase in the Baltic Sea continued until 2008. A decrease started in the Baltic 2009. The temperature increase in the Baltic Sea is approximately three to four times higher than for the northern hemisphere and for the globe but lower than the air temperature increase in the northern polar region. The trend is positive in all seasons and strongly depending on seasons and regions. The highest temperature increase occurred in July in the Bothnian Sea, Bothnian Bay, and Eastern Gotland Sea. The western Baltic Sea is strongly influenced by dynamical processes such as the water exchange between North and Baltic Seas and wind induced upwelling processes. Solar radiation and the shallow water depth lead to earlier warming in spring and earlier cooling in late autumn than in the Baltic Proper. Because of the structured alignment of the coast parts are excluded from the dynamical processes. The western Baltic has the highest yearly mean SST of the entire Baltic Sea and the different parts are highly correlated from Kiel Bight to the Bornholm Sea. The yearly mean air temperature of Warnemünde is in the same order of magnitude as the yearly mean SST in the western Baltic and highly correlated. The described processes and conditions reduced the trends of yearly mean SST in the central parts of the western Baltic to 0.9-1.2°C for the period 1990-2008. In areas which are excluded from the dynamical processes such as Greifswald Bay and Kiel Bight the trends are slightly higher with 1.44 and 1.42°C than that of the entire

Baltic.

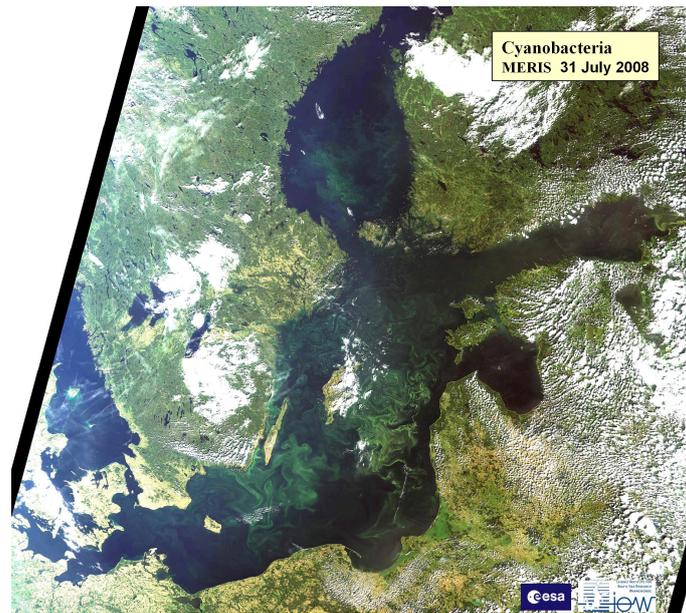


**Fig. 2.51:** Anomalies of yearly mean SST of the western and entire Baltic Sea including the linear trends

Seasonal variations in the satellite derived chlorophyll development of the Baltic are caused by a spring bloom of diatoms and dinoflagellates and after a stagnation period in June by a summer bloom of cyanobacteria. In 2007 satellite data on 12 March already showed relatively high chlorophyll concentrations in the western Baltic which developed in the following time further east and covered end of May the entire Gotland Sea. Although the summer 2007 was not very warm, but very cloudy and partly windy, there was a pronounced long lasting cyanobacteria development including the Bothnian Sea. The year 2008 was characterized by a mild winter and first indications of the spring bloom were observed on 10 February. During March and April the development continued while propagating eastward and reached the eastern Gotland Sea in May. End of June beginning of July first filaments of cyanobacteria were observed and covered already on 3 July areas from the Gotland Sea to the Arkona Sea (Fig. 2.52). Around 25 July the Baltic Sea was affected from the Kiel Bight to the Bothnian Sea which lasted until End of July. Beginning of August a number of low pressure systems passed the Baltic which stopped the bloom mid August.

In the second phase of the BMBF funded German-Indonesian Cooperation (SPICE) which started in September 2007 the interdisciplinary pollution studies were extended to the 5 major rivers of South-East-Sumatra (Indonesia). Remote sensing investigations combined with ground-truth measurements of optically active water constituents and water colour in different seasons of the years 2007-2009 were focused on the identification of different sources of water masses in the tributaries and estuaries and on the discharge into Malacca and Karimata Straits.

Within the joint research project SOPRAN (Surface Ocean Processes in the Anthropocene) financed by BMBF, the influence of Sahara dust on the radiation budget and the circulation in the tropical/subtropical Atlantic was investigated together with the IfM Hamburg. The IOW part was focussed on the spectral modification of the solar radiation and optical characteristics in the water column by Sahara dust as well as on the biological reaction of the ecosystem on the nutrient impact



**Fig. 2.52:** Example of a Cyanobacteria bloom on 31 July 2008 covering the entire Baltic Sea

based on ship-borne measurements and satellite data. Dust events occur sporadic and reduced in measured examples the incident irradiance by up to 40% with higher influence in the short-wavelength range.

In the BMBF funded Beibu-Project (Holocene environmental evolution and anthropogenic impact of Beibu Gulf, South China Sea) which started in June 2009 a subproject is dealing with detailed investigations on hydrography and biogeochemistry of the Beibu Gulf including remote sensing and modeling. The contribution of remote sensing is the investigation of the distribution of different water masses, the biological activity and suspended matter transport in relation to driving forces.

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## 2.6 Didactics of Physics

### 2.7 Physics Education

**Head:** Prof. Dr. Heidi Reinholz

**Staff:** Dr. Viola von Oeynhausen  
Dipl.-Paed. Falk Eberlein  
Dipl.-Paed. Christa Nier  
Prof. em. Hans-Erich Riedel  
Marion Pauer

The goals of our activities are multilayered. 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 want to reach out to the broader community as well as base our activities on empirical research with respect to teaching methods and media.

#### 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 media. Questions of motivation, diagnostics in teaching, interdisciplinary teaching are discussed as well as practically oriented seminars and activities have been introduced. In cooperation with schools and pre-school institutions, individual school projects on topics relevant for the considered age group and the curriculum have been developed and performed with student groups. Examples are *What do you know about water?* for primary school children and *Alternative energies* for secondary school students.

The experimental resources for the school related lab work have been renewed in order to stay on top with modern experimental equipment for teaching. First teaching experiences in school are seen as particularly helpful to students and teaching staff. They are organized in close collaboration with teachers in schools.

A new course on *Physics and technology* focuses on physical concepts relevant for technological applications in every day life contexts. This is combined with teaching soft skills by getting the students actively involved in development of teaching material and its presentations. A seminar on *IT-media in teaching* is now offered again, with focus on special applications for physics teaching (simulations, applets, computer interface for experimental data analysis), legal questions and interesting web resources for teaching.

The group is involved in (re)writing textbooks for schools according to changes

in the school curriculum of Mecklenburg-Vorpommern and other federal states [10]. A new formula collection for school students has been compiled recently [9].

### Outreach Activities

Since 2003, the Institute of Physics has organized the yearly **Lighthouse competition** [3] for the schools of Mecklenburg-Vorpommern which compete against each other for the lighthouse cup. After a prequiz about the main topic of the year (2007: water, 2008: light, 2009: energy), the best teams have to find good scientific explanations for experiments which are presented on stage. Afterwards, the labs of the institute are open to be visited and hands on activities are available to do. Last not least, a lecture with lots of impressive experiments repacked in a new story every year is been prepared and presented by a large number of physics students, including teachers students.



**Fig. 2.53:** Students of the Käthe-Kollwitz-Gymnasium Rostock, winner of the Lighthouse competition in 2009.

Science is fun. This is the reason, a group of scientists and students came together in 2005 to work on this project. Every year in August, Rostock welcomes 1.5 Mio visitors to the Hanse Sail, a meeting of large sailing boats. During this time, our event **Science@Sail** [1] is already a yearly runner for young and old. They have an opportunity to learn about science, interesting facts and fascinating experiments. Close to the sea you can smell the salt in the air - can I really trust my nose?

Under the water tap you can see a floating drop - but is it really true or are my eyes mistaken? The visitors of Science@Sail can probe their senses on more than 70 experiments and get the science behind them explained. In 2009, e.g., the focus was on astronomy.

**PhySch (*Physik und Schule*)** [2] is the newest of our projects on the interface between science and schools. University students who are trained to become science teachers are involved. They design experiments which complement the school curriculum in two possible ways. Either by an experiment which can not easily be done in schools, e.g. Franck-Hertz-experiment, or experiments which go beyond the school curriculum but contain various aspects already taught at school, e.g. intelligent glass (heat absorption/emission). Instructions for the school students are prepared at an appropriate level. The university students are also responsible to lead the school students through the projects which are offered at university venues or in the schools. Additionally, talks or presentations on specific topics relating to current research areas or as requested by schools [4, 5] are offered by scientists of the institute. Thanks to financial support by the Hochschulpakt, a half position was created in order to help with the link to the schools.

### Research

The group is involved in the activities of the ZLB (Centre for teacher education and education research by participating actively in only recently established working groups, like *Videography*, *Science and schools* as well as *Theory and practice*. In the latter we aim at a closer collaboration between university and schools in order to find ways to incorporate new research findings into every day teaching or investigating empirically teaching methods. Presentations at workshops and conferences are leading to new inspirations [7, 6, 8]. A PhD project on *Electricity in every day life* aims at revisiting the water model for introducing electricity.

Jointly we - scientists, teachers, parents, students - look for new ways to take science into the classroom and beyond. We started various projects on different interfaces between teachers and learners which interrelate and complement each other. By involving future science teachers in particular, we are creating highly qualified multipliers of science. What we want to achieve with all these activities is reach out to a broad public audience and get them interested and excited about science. For this, the specialists have to explain complex structures and how it all works in an easier way. It is a great challenge to communicate with generally understandable explanations and not using too detailed scientific terminology. At outreach activities, we like to present good examples and encourage more and more scientists to get involved in presentations and activities for the general audience.

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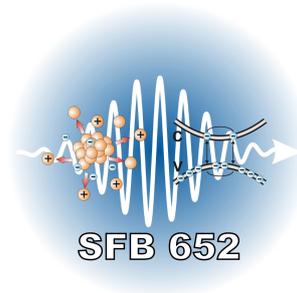
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# 3 Collaborative Research

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

**Executive Board:** Prof. Dr. Karl-Heinz Meiwes-Broer <sup>a</sup>  
Prof. Dr. Ronald Redmer <sup>b</sup>  
Prof. Dr. Gerd Röpke <sup>c</sup>  
Prof. Dr. Heinrich Stolz  
Prof. Dr. Stefan Lochbrunner <sup>d</sup>



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

<sup>a</sup>spokesman  
<sup>b</sup>vice-spokesman  
<sup>c</sup>until 30.06.2009  
<sup>d</sup>since 01.07.2009

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 first funding period of the Sfb652 ended on June 30, 2009. The DFG has granted a second funding period that started on July 1, 2009 and ranges to June 30, 2013.

### 3.1.1 Projects and Project Leaders

A1	Matter exposed to VUV- and X-ray radiation (1st and 2nd period)	Prof. Dr. Karl-Heinz Meiwes-Broer, Prof. Dr. Ronald Redmer, PD Dr. Josef Tiggesbäumker
A2	Thomson-scattering and correlations in warm dense matter (1st and 2nd period)	Prof. Dr. Ronald Redmer

A3	Correlated processes in laser-excited trapped cluster ions (1st and 2nd period)	Prof. Dr. Lutz Schweikhard*, Dr. Gerrit Marx*, Prof. Dr. Karl-Heinz Meiwes-Broer
A4	Many-body quantum electrodynamics and dielectric response (1st period)	Prof. Dr. Gerd Röpke, PD Dr. Heidi Reinholz
	Impact of dynamical correlations on optical properties in dense Coulomb systems and clusters (2nd period)	PD Dr. Heidi Reinholz
A5	Controlled strong-field excitation of clusters and particles by shaped laser pulses (1st and 2nd period)	PD Dr. Josef Tiggesbäumker, Prof. Dr. Karl-Heinz Meiwes-Broer
A6	Quantum kinetics of dense Coulomb systems in laser fields (1st and 2nd period)	Prof. Dr. Manfred Schlanges*, PD Dr. Thomas Bornath
A7	The phase of the light in optically excited semiconductor structures (1st period)	Dr. Günter Manzke, Prof. Dr. Heinrich Stolz
A8	Microscopic description of atomic clusters in intense laser fields (2nd period)	Dr. Thomas Fennel
A9	Simulation of quantum dynamics in strong laser fields using density functional theory (2nd period)	Prof. Dr. Dieter Bauer

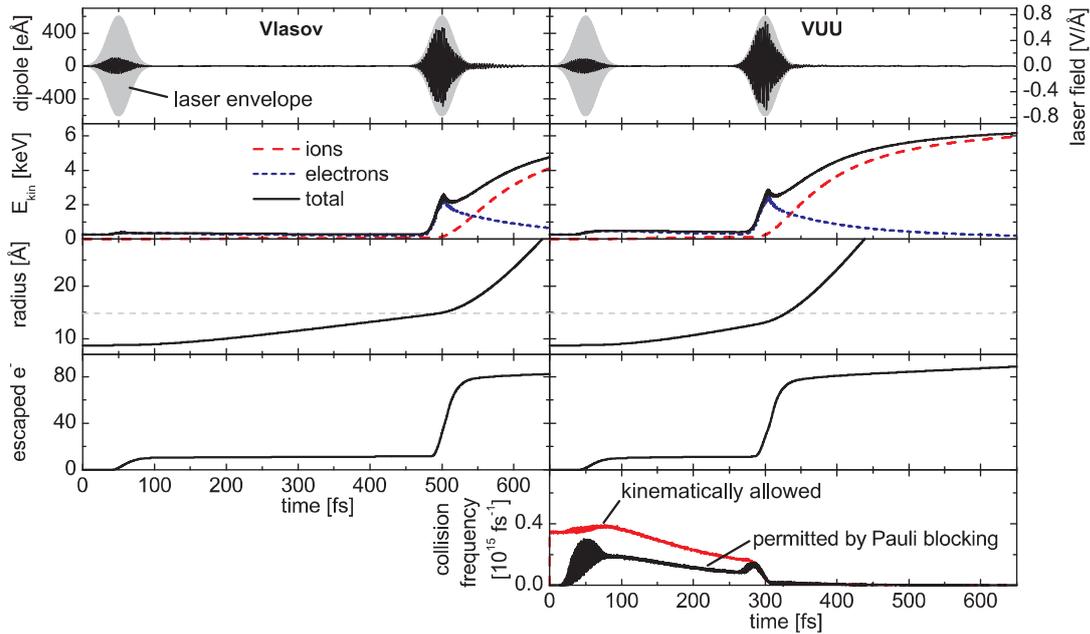
B1	Exciton matter in external potentials (1st and 2nd period)	Prof. Dr. Heinrich Stolz
B2	Microscopic description of quantum optics of many-body systems (1st period)	Prof. Dr. Werner Vogel, Prof. Dr. Klaus Henneberger
	Generation and detection of non-classical light in semiconductor lasers and nanostructures (2nd period)	Prof. Dr. Werner Vogel, Prof. Dr. Heinrich Stolz
B3	Excitonic clusters with strong coupling to light fields (1st period)	Prof. Dr. Holger Fehske*, Prof. Dr. Heinrich Stolz
B4	Possibilities and signatures of Bose Einstein condensation in structured electron hole systems (1st period)	Prof. Dr. Klaus Henneberger

B5	Collective excitonic phases in highly correlated electron hole systems (1st period)	Prof. Dr. Holger Fehske*, Prof. Dr. Gerd Röpke
	Optical signatures from excitons, bi-excitons, polaron-excitons and collective excitonic phases in strongly correlated electron-hole systems (2nd period)	Prof. Dr. Holger Fehske*
B6	Radiation-induced correlations in ultracold droplets (1st and 2nd period)	Prof. Dr. Karl-Heinz Meiwes-Broer
B9	Dynamics of correlated excitons in molecular aggregates (partially 1st, full 2nd period)	Prof. Dr. Stefan Lochbrunner
B10	Laser-driven multi exciton dynamics in molecular aggregates (partially 1st, full 2nd period)	Prof. Dr. Oliver Kühn
B11	Structural correlations in liquid Coulomb systems (2nd period)	Prof. Dr. Ralf Ludwig, Prof. Dr. Oliver Kühn, Prof. Dr. Stefan Lochbrunner
B12	Quantum correlations in light and matter: characterization and verification (2nd period)	Prof. Dr. Werner Vogel
MGK	Integrated Graduate School (2nd period)	Prof. Dr. Stefan Lochbrunner

\* Physics Department, University of Greifswald

### 3.1.2 Overview

In its first period (2005-2009) the SFB 652 comprised 13 research projects. 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 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 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

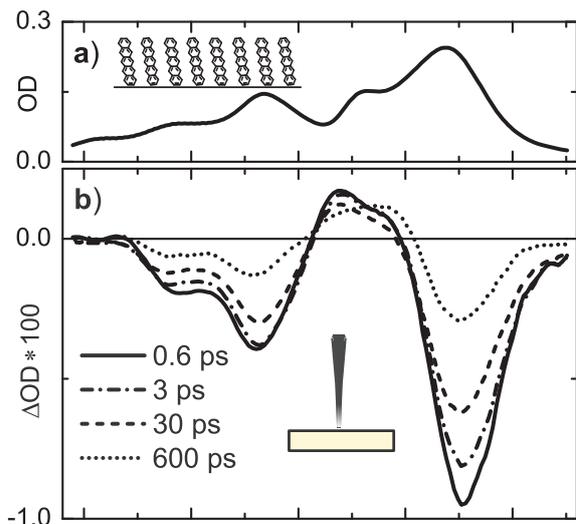


**Fig. 3.1:** Time evolution of the laser field envelope (upper row, right-hand scale), the dipole moment (upper row, left-hand scale), the electron and ion kinetic energies, the cluster radius, the total ionization, and the electron-electron collision frequency for the excitation of  $\text{Na}_{147}$  with dual 25 fs laser pulses at intensity  $I = 8 \times 10^{12}$   $\text{W}/\text{cm}^2$ . The left-hand column corresponds to the Vlasov calculations while the right-hand column represents the VUU results. Pulse delays are optimized for maximum energy absorption for the two cases, respectively. [J. Köhn et al., Phys. Rev. A **77**, 033202 (2008)]

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) will participate in first experimental campaigns at the LCLS X-ray free-electron laser in Stanford/USA by the end of 2010.

### 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-



**Fig. 3.2:** (a) Steady-state absorption spectrum of a microcrystalline pentacene film, (b) transient absorption spectra probed by a white light continuum at different delay times after photoexcitation at 670 nm. [Marciniak et al., Phys. Rev. B **79**, 235318 (2009)]

hole systems in semiconductors. The theoretical investigations in projects A1, A2, A4, and A6 (as well as A8, A9 from 2009 on) 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 the phase of the light in optically excited semiconductor structures (A7). 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, A7), linear response theory (A2, A4), density functional theory and quantum molecular dynamics simulations (A1, A2, A9) are applied.

Project complex B concentrates on the build-up of correlations in semiconductors, atom condensates, clusters, 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, however, can be tuned over a wide range by the choice of the material or tuning an external confinement potential. Corresponding studies are a major issue within the projects B1-B4. Excitons in mesoscopic potential wells are investigated in project B1, being very promising candidates in this context. Essential for the realization and the control of the light-induced correlations is the development of theoretical concepts that provide a consistent connection of quantum optics with many-particle theory. This is subject of the projects B2 and B4. In project B5 the formation of exciton-polariton quasiparticles through cooperative effects and the build-up of correlations at high pressures are investigated. Within 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 of the collaborative research centre. In the new funding period these activities are extended within the project B9 and B10.

For its second period (2009-2013) the SFB 652 could significantly be strengthened by the inclusion of several new aspects. 16 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 new 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. With the new projects A8, A9 and B12, methods of many-particle and density functional theory as well as problems of quantum correlations of light and matter are stronger emphasized within the SFB.

The two results sketched below give an impression of current collaborative activities in the SFB. The first example illustrates results of theoretical work of the strong laser field interaction with sodium clusters (A1, A2). In particular, the contribution of electron-electron collisions has been considered for the first time. Fig. 3.1 shows that without electron-electron collisions ('Vlasov') the maximum energy absorption occurs at around 450 fs whereas with collisions ('VUU') this situation is reached already at 250 fs.

The second example concerns experimentally investigated ultrafast dynamics in ordered molecular organic systems (B9). Organic materials have attracted strong scientific attention with respect to potential applications in photonics and electronics. In particular polyacenes are subject of intensive studies to understand the properties of organic crystals. The result in Fig. 3.2 demonstrates that the photoabsorption exhibits dramatic changes when tuning the delay between excitation and probing. This dynamics accelerates with increasing pump energy which is a strong indication for annihilation processes. By investigating these processes we study the exciton-exciton interaction in ordered organic systems.

## 3.2 DFG - Research Unit 485: “Quantum Optics in Semiconductor Nanostructures”

**Coordinator:** Prof. Dr. Heinrich Stolz

The goal of this research unit has been to combine the methods of Quantum Optics with the developments in Semiconductor Physics that have been made possible by advances in design and preparation of low dimensional semiconductor structures on a nanoscopic scale. This new and innovative field of Semiconductor Quantum Optics, which has emerged in the last few years, offers the possibility of both a fundamental understanding of matter-light interaction on a quantum level and the realization of unique devices for quantum optic experiments.

The research unit has been funded during the period 01.07.2002 - 30.06.2009 and was concentrated on the following areas:

- generation of squeezed light from semiconductors
- cavity Quantum Electrodynamics in the weak and strong coupling regime
- generation of entangled photons
- quantum dot laser structures with large spontaneous emission factor

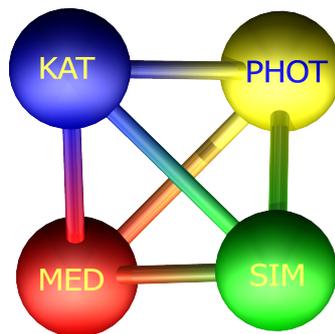
The research unit has been successful in looking for answers to questions on the physical mechanisms, demonstrate the various quantum optical effects in semiconductor structures and provide a thorough understanding by a quantum theoretical treatment of both semiconductor and light field. Besides these interests from basics physics, the developed concepts might be transferred into future applications such as high efficiency quantum light sources or single photon emitters.



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

## 4.1 Overview

In 2007, established within the Faculty of Interdisciplinary Research of the University of Rostock, the Department “Science and Technology of Life, Light and Matter” (LLM) has been founded. 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”, “Aging Sciences and Humanities” and “Knowledge - Culture – Transformation” together with LLM currently constitute the Interdisciplinary Faculty (INF), which is supported by the University and the state of Mecklenburg-Western Pomerania. 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 Life, Light and Matter aims at interdisciplinary research and training in the fields 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) as well as the Leibniz-Institute for atmospheric research (IAP) are significantly involved.

The scope of the investigations reaches from fundamental problems like the interaction of light with matter via the development of chemical and agricultural as well as biologically relevant drug design for biomedical applications. Smart materials play an important role in all of these areas. One backbone of the Department LLM is research on the impact of atomic and molecular properties onto macroscopic systems. In particular, microscopic mechanisms, i.e. those on the atomic or nanometer-scale will be interrogated and ultimately be used for the controlled development and modification of new materials. These may be of importance in far-future applications like quantum computing ('quantum matter') and the controlling of three-dimensional nerve cell growth as well as on current problems like biocompatibility. In several projects modern forms of light, e.g., laser pulses shaped in amplitude and phase, will be of use to reveal the microscopic dynamics and, at the same time, to steer the creation of desired structures.

The University of Rostock already has established competences at the intersection of natural, engineering and life sciences. They serve as solid basis for the Department LLM, being a condensation nucleus of an interdisciplinary high-technology field. Moreover, as the research has many links to technical applications it bears potential for a sustainable future growth sector.

Accompanied with the constitution of the department is the need for a specific education. Whereas the basic study period remains with the established departments of the university, the specialization on topics of LLM occurs during the master studies and the PhD theses. There will be opportunities for advanced training of scientific and technical personal. Besides its focus onto natural and engineering sciences and on medicine, the department provides many possibilities for interactions with topics of social sciences and economics. Thus there is much room for collaborations with the other departments within the Interdisciplinary Faculty.

### 4.3 Contribution of the Physics Institute to LLM

Among the over 35 research groups within LLM, 10 belong to the Physics institute. These are:

Prof. Dr. Thomas Gerber	Physics of Nano- and Biomaterials
Prof. Dr. Oliver Kühn	Molecular Quantum Dynamics
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. Heidi Reinholz	Spectral lines of dense plasmas
Prof. Dr. Christoph Schick	Polymer Physics
Prof. Dr. Heinrich Stolz	Semiconductor Optics

### 4.4 Current Activities

In the period under review one focal point of LLM has been the enhanced networking among the workgroups in different scientific disciplines. At first, partially language barriers had to be removed. At the same time the members had to recognize their own benefits when participating in this interdisciplinary effort. With strong support by the University and the local government PhD scholarship funds could be granted to 14 students. All of them work on interdisciplinary topics and are coached by two supervisors from separate institutes. Looking back it is a success that numerous personalities have made an application for admission in the department as well as have written down research subjects suitable to LLM. Members from 5 faculties as well as the IAP and LIKAT could be admitted thus after confirmation by the leading board of the Interdisciplinary Faculty and the rector of the University, Prof. Schareck.

LLM 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 ‘glue money’ to strengthen initiatives setting up new research projects. Some major 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 LLM. Approved by the German Council of Science and Humanities (Wissenschaftsrat) the scientific building “Complex Molecular Systems” will provide additional 2400 sqm of extensively equipped space. The topical focus of LLM and the high standard of the contributing research groups made it possible to acquire 20 Mio. EUR funding for the new building and for equipment. With this an appropriate environment will be established for the interdisciplinary research and education in the Department LLM. Activities within



**Fig. 4.2:** Computer aided design of the scientific building “Complex Molecular Systems”; drawing by Gerber Architekten GmbH.

the disciplines Physics, Chemistry, Biology, Medicine and Engineering will be bundled in order to pursue the research on complex molecular systems. A central topic is the analysis, control and design of systems which are governed through processes on the molecular level.

Further larger projects with the contribution of LLM research groups include:

- Collaborative Research Center DFG-SFB 652 “Strong correlations and collective effects in radiation fields: Coulomb systems, clusters and particles”, see the overview in this research report. This research is centered at the Institute of Physics, with one project leader being from the Chemistry Department of the University of Rostock and four project leaders from the Institute of Physics of the University of Greifswald.
- The Graduate School at the SFB 652 increases the communication among the PhD students within weekly colloquia, workshops, and other social activities. It strengthens the scientific abilities of the students by providing access to additional conferences, by being responsible for laboratory students, and by participating in the organization of the graduate school.
- Collaborative Research Center DFG-TR 37 “Micro- and nanosystems in medicine – reconstruction of biologic functions”. This center is a joint project between the universities of Aachen, Hannover and Rostock. The Rostock

side is mainly carried by the faculties of medicine, engineering and natural scientists. One project area comprises optical technologies, in particular laser technologies for the manipulation of cells and cell groups. Other projects include the generation, analysis and technical characterization of bioactive and nanostructured surfaces and particles to optimize their efficiency in the interaction with biological systems. Other central questions concern vascular illnesses and illnesses by eye and ear, and the development of new investigation methods in the areas of the microscopy and biocompatibility.

Furthermore, physics research groups and members of the department are 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.

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



# 5 Academic Qualifications, Colloquia, and Workshops

## 5.1 Academic Qualifications

### 5.1.1 Habilitations

- Dr. Michael Böhm, Analyse des Solitonengehalts von optischen Impulsen in Glasfasern, 05/2009

### 5.1.2 PhD Theses

<i>Author</i>	<i>Date</i>	<i>Title of PhD Thesis</i>
Christian Gocke	05.02.2007	Dekohärenz in offenen Quantensystemen am Beispiel eines Rydbergatoms im Plasma
Banaz Omar	05.02.2007	Spektrallinienverbreiterung von He I und Heliumartigen Ionen in dichten Plasmen
Markus Garczarczyk	29.03.2007	First Observations of the GRB Prompt and Early Afterglow Emission Phase at $\sim 100\text{GeV}$ Energy Regime with the 17m Diameter MAGIC Imaging Atmospheric Cherenkov Telescope (co-supervision with MPI Munich)
Armin Rudolf Schöch	02.04.2007	Temperatur-Struktur und Schwerewellen in der arktischen mittleren Atmosphäre über ALOMAR (69.3°N, 16°E)
Albert Sargsyan	02.04.2007	Quantification of the Immobilized Fraction in Polymer Inorganic Nanocomposites
Jens Berdermann	07.05.2007	Zustandsgleichung und Neutrino-Transport für supraleitende Quarkmaterie in Neutronensternen
Robert Thiele	21.09.2007	Thomsonstreuung in warmer und dichter Materie
Julia Hinkel	26.10.2007	Anwendung der Physik der stochastischen Prozesse auf Straßenverkehrsproblem

Alexander Kaukher	02.11.2007	A Study of Readout Electronics Based on Time-To-Digital Converters for the International Linear Collider TPC Detector
John R. Adams	28.11.2007	Magnetotransport Properties of Dense Plasma
Jens Lautenbach	29.11.2007	Experimentelle Untersuchungen mit einem Lidar zur thermischen Struktur der Mesospaunen-Region bei polaren und mittleren Breiten
Tomasz Denkiewicz	21.12.2007	Selected Aspects of the Conformally Invariant Cosmology
Monika Rauthe	18.01.2008	Lidarmessungen von Temperaturen und Schwebewellen zwischen 1-105 km über Kühlungsborn (54°N, 12°O)
Olof Zeller	20.06.2008	Einfluss der Variationen atmosphärischer Größen und der Ionisation auf mesosphärische Radarechos in polaren und mittleren Breiten
Mykhaylo Grygalashvylv	04.07.2008	Drei-dimensionale Modellierung chemischer Spurenstoffe in der Mesosphäre/unteren Thermosphäre
Andre Kietzmann	24.07.2008	Quanten-Molekulardynamik Simulation dichter Fluide
Patrick Ludwig	12.12.2008	Structure Formation in Strongly Correlated Few-Particle Systems in Traps
Carsten Fortmann	01.09.2008	Bremsstrahlung in Dense Plasmas: A Many-Body Theoretical Approach
Ivan Kuznetov	06.05.2009	Simulation of Oxygen Dynamics in the Baltic Sea Deep Water
Irina Strelnikova	08.05.2009	Messungen mesosphärischer Aerosolpartikel mit Höhenforschungsraketen und Radars
Dmytro Vasylyev	17.06.2009	Propagation of Nonclassical Light in Structured Media
Stefan Strauß	12.10.2009	Thermodynamics of Low-dimensional Light Front Gauge Theories
Nadine Nettelmann	13.11.2009	Matter Under Extreme Conditions: Modeling Giant Planets
Felix Richter	17.11.2009	Theory of Radiation for Bounded Media Systems With Highly Correlated Electron-Hole Plasmas
Mohamed Arafa Ali Mohamed Ismail	2009	Dynamics of the Immobilized Part of Semicrystalline Polymers and Polymer Inorganic Nanocomposites (co-supervision with Beni-Suef University, Egypt)

## 5.2 Physics and SFB Colloquia

<i>Date</i>	<i>Speaker, Affiliation, Title</i>
11.01.2007	Prof. Dr. Thomas Möller, Technische Universität Berlin: Cluster im Licht intensiver Synchrotronstrahlung
18.01.2007	Prof. Dr. Dieter Hoffmann, TU Darmstadt: Das CERN Axion Solar Telescope (CAST) Experiment
25.01.2007	Prof. Dr. Manfred Paulini, Carnegie Mellon University, Pittsburgh: Bs-Mesonen-Oszillationen
06.04.2007	Eric Suraud, Universität Toulouse: Dynamics of embedded and deposited clusters
12.04.2007	Prof. Dr. Florian Pfender, Institut für Mathematik: Obere Schranken für Codes durch lineare und semidefinite Programmierung
03.05.2007	Prof. Dr. Erich Becker, Institut für Atmosphärenphysik: Antrittsvorlesung
10.05.2007	Prof. Dr. Stefan Schael, RWTH Aachen: Das AMS Experiment - auf der Suche nach Dunkler Materie im Weltraum
24.05.2007	Prof. Dr. Joel H. Parks, The Rowland Institute at Harvard, Cambridge, USA: Electron diffraction of trapped clusters and biomolecules
21.06.2007	Prof. Dr. Jochen Schneider, DESY, Hamburg: Photon Science am DESY.
28.06.2007	Prof. Dr. Matthias Weidemüller, Universität Freiburg: Rydberg-Materie
05.07.2007	Prof. Dr. Stefan Richter, Institut für Biowissenschaften: Antrittsvorlesung
12.07.2007	Prof. Dr. Joachim Ullrich, MPI Heidelberg: Freie Elektronen Laser: Neue Werkzeuge für neue Wissenschaft
20.09.2007	Prof. Dr. Markus Siegrist, ETH Zürich, Institut für Quantenelektronik: Laser-spektroskopische Spurengasanalytik
04.10.2007	Prof. Dr. Gregor Rehder, Leibniz-Institut für Ostseeforschung Warnemünde: Antrittsvorlesung
16.10.2007	Prof. Dr. Charita Pattiaratchi, University of Western Australia: Tsunamis in the Indian Ocean
01.11.2007	Universitätskolloquium: Vorstellung der Interdisziplinären Fakultät INF
08.11.2007	PD Dr. Johanna Erdmenger, MPI für Physik, München: Ist die Stringtheorie experimentell überprüfbar?
15.11.2007	Prof. Dr. Roman Schnabel, MPI für Gravitationsphysik Hannover: Gequetschtes Licht für die Gravitationswellenastronomie

- 22.11.2007 Prof. Dr. Gustav Gerber, Universität Würzburg: Femtosekunden Spektroskopie und Quantenkontrolle molekularer Dynamik
- 06.12.2007 Prof. Dr. Stefan Lochbrunner: Antrittsvorlesung: Echtzeitspektroskopie ultraschneller molekularer Prozesse
- 13.12.2007 Prof. Dr. Martin Wolf FU Berlin: Zeitaufgelöste Elektronendynamik und Femtochemie an Festkörperoberflächen
- 20.12.2007 Prof. Dr. Hans Ruder, Universität Tübingen: Weihnachtskolloquium: Dunkle Materie, dunkle Energie (finstere Gedanken) - moderne Entwicklungen in der Kosmologie
- 10.01.2008 Prof. Dr. Hubert Ebert, Universität München: Elektronische Struktur und Magnetismus von Übergangsmetall-Clustern
- 24.01.2008 Prof. Dr. Christoph Keitel, MPI für Kernphysik Heidelberg: Hochenergetische Quantendynamik in extrem starken Laserpulsen
- 07.02.2008 Prof. Dr. Guido Dehnhardt, Institut f. Biowissenschaften: Lange verkannt: Die Bedeutung des Vibrissensystems mariner Säugetiere
- 29.02.2008 Schaltjahreskolloquium
- 06.03.2008 Prof. Dr. Markus Rapp, Leibniz-Institut für Atmosphärenphysik: Antrittsvorlesung: Die mittlere Atmosphäre - ein groß(artig)es Physikkolabor
- 03.04.2008 Oliver Kühn: Antrittsvorlesung: Molekulare Quantendynamik: Von Gasphasenclustern zu Biomolekülen
- 17.04.2008 Prof. Dr. Fritz Aumayer, TU Wien: Die Wechselwirkung hochgeladener Ionen mit Oberflächen und ihre Rolle für die Plasma-Wand-Wechselwirkung
- 24.04.2008 Für die interessierte Bevölkerung, Schüler und Studenten: Lange Nacht des Wissens
- 08.05.2008 Prof. Dr. Reinhard Schröder, Institut für Biowissenschaften: Antrittsvorlesung: Wie Embryonen wachsen. Signalwege in embryonalen Wachstumszonen
- 15.05.2008 Prof. Dr. Ralf Neuhäuser, Friedrich-Schiller-Universität Jena: Beobachtung extra-solarer Planeten und Planetenentstehung
- 05.06.2008 Prof. Dr. Mark Ediger, University of Wisconsin-Madison, USA: The glassy state
- 19.06.2008 Prof. Dr. M. Bellini, Istituto Nazionale di Ottica Applicata, Florenz: Probing the Quantum Nature of Light
- 03.07.2008 Prof. Dr. Ralf Zimmermann, Institut für Chemie: Antrittsvorlesung
- 10.07.2008 Prof. Dr. Matthias Kling, Max-Planck Institut für Quantenoptik, Garching: Attosecond dynamics in molecules and nanostructures
- 07.10.2008 Lange Nacht der kleinsten Teilchen
- 12.11.2008 Prof. Dr. John Schliemann, Uni Regensburg: Spins in niedrigdimensionalen Festkörpersystemen

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- 14.11.2008 Prof. Dr. Peter Schmelcher, Uni Heidelberg: Mesoskopische Physik mit ultrakalten Atomen
- 14.11.2008 Prof. Dr. Erich Runge, TU Ilmenau: Exzitonen, Plasmonen und Photonen
- 04.12.2008 Fakultätskolloquium: Vergabe des Fakultätspreises
- 09.12.2008 Richard Coleman, President of the Space Transportation Association, USA: Next steps to the moon: The CONSTELLATION- / ARES- / ORION-Program of the United States.
- 11.12.2008 Prof. Dr. Ian Brock, Universität Bonn: Beauty and Truth in Particle Physics (Atlas am LHC)
- 19.12.2008 Prof. Dr. V.E. Fortov and D.H.H. Hoffmann: Minisymposium Warm Dense Matter
- 08.01.2009 PD Dr. Joachim Gröger, Inst. für Biowissenschaften: Zentrale Probleme und moderne Verfahren der Fischereiwissenschaft
- 15.01.2009 PD Dr. Robert Wynands, PTB Braunschweig: Zeit messen mit Atomen
- 22.01.2009 Prof. Dr. Jasper Knoester, Rijksuniversiteit Groningen, Niederlande: Statistical and Dynamical Properties of Excitons in Disordered Molecular Aggregates
- 29.01.2009 Prof. Dr. Martin Garcia, Universität Kassel: Beschreibung laserinduzierter ultraschneller Strukturänderungen in kondensierter Materie
- 16.04.2009 Prof. Dr. Titus Beu, Universität Klausenburg, Rumänien: Soft matter simulations: Interfaces and Ion Channels
- 17.04.2009 Prof. Dr. Satoshi Hamagushi, Center for Atomic and Mol. Tech., Osaka: Plasma Surface Interactions for a Solid or Liquid
- 21.04.2009 Prof. Dr. Karl-Heinz Meiwes-Broer, Inst. f. Physik: Eröffnung der Ringvorlesung 'Leben, Licht, Materie': Vom Atom zur Atmosphäre
- 23.04.2009 Lange Nacht der Wissenschaften
- 05.05.2009 Prof. Dr. Nils Damaschke, Inst. für Elektrotechnik: Der Regenbogen im Labor
- 12.05.2009 Prof. Dr. Stefan Lochbrunner, Inst. f. Physik: Laserpulse für schnellste Vorgänge in der Natur
- 19.05.2009 Prof. Dr. Peter Leinweber, Inst. für Landnutzung: Massenspektroskopische und Synchrotron-Techniken in der Bodenanalytik
- 26.05.2009 Prof. Dr. Oliver Kühn, Inst. f. Physik: Moleküle in Bewegung
- 09.06.2009 Prof. Dr. Matthias Beller, LIKAT und Inst. für Chemie: Chemie: Vom Problemverursacher zur Schlüsseltechnologie
- 16.06.2009 Prof. Dr. Ursula van Rienen, Inst. für Elektrotechnik: Elektrische Impulse bringen Ohr, Hirn und Hüfte wieder auf Trab
- 23.06.2009 Prof. Dr. Rudolf Guthoff, PD Dr. Oliver Stachs, Augenklinik: Junge Augen für ältere Menschen

- 25.06.2009 Prof. Dr. Roderich Moessner, MPI für komplexe Systeme, Dresden: Magnetische Monopole in Spin Ice
- 30.06.2009 Prof. Dr. Franz-Josef Lübken, IAP Kühlungsborn: Die leuchtende Atmosphäre
- 07.07.2009 Prof. Dr. Olaf Keßler, Christoph Schick, Inst. Werkstofftechnik bzw. Inst. f. Physik: Aluminium - leicht und hochfest für Flugzeug und Automobil
- 09.07.2009 Prof. Dr. Volker Dohm, RWTH Aachen: Universalität und Diversität kritischer Phänomene
- 14.07.2009 Prof. Dr. Ralf Zimmermann, Inst. für Chemie: Quellen und Gesundheitswirkung von Feinstaub in der Atmosphäre
- 16.07.2009 Die Physik sagt dem Universitätshauptgebäude ade. Der SFB 652 startet in die 2. Förderperiode 2009-2013.
- 23.07.2009 Prof. Dr. Thomas Peter, ETH Zürich: Aerosole - schlecht für die Gesundheit, gut für das Klima?
- 30.07.2009 Prof. Dr. Steven C. Erwin, Center for Computational Materials Science, Naval Research Laboratory, Washington: Towards a theory of doping in semiconductor nanocrystals
- 02.11.2009 Prof. Dr. Dieter Weiss, Institut für Biowissenschaften: Sehen mit Auge und Gehirn
- 02.11.2009 Prof. Dr. Ludger Wöste, Freie Universität Berlin: Wunderwerkzeug Laser: Von Laborexperimenten zu Blitz und Hagel
- 05.11.2009 Dr. habil. Roland Heinz, Philips Lighting Academy Hamburg, und Institut für Chemische Technologie Anorganischer Stoffe, TU Graz: Moderne Lichtquellen: Von der Halogenlampe bis zur OLED
- 12.11.2009 Prof. Dr. Dieter Bauer, Inst. für Physik: Antrittsvorlesung: Materie im Lichte sehr starker Laser - von Quantenbahnen, Plasmonen und schnellen Elektronen
- 19.11.2009 Prof. Dr. Martina Havenith, Ruhruniversität Bochum: Ultrakalte Chemie: Höchstaufgelöste Spektroskopie in Helium-Nanotröpfchen
- 24.11.2009 Prof. Dr. Paolo Nussenzweig, Universität Sao Paulo: Three-Color Entanglement
- 26.11.2009 Prof. Dr. Andre Dieter Bandrauk, Sherbrooke University, Kanada: Femto-Atto-Zepto-second Science Technology: manipulating electrons with lasers
- 03.12.2009 Vergabe des Fakultätspreises: Goldenes Doktorjubiläum
- 10.12.2009 Prof. Dr. Udo Buck, MPI für Dynamik und Selbstorganisation, Göttingen: Natrium-Wasser Cluster als Nachweis für einen Ozean in einem Saturnmond
- 17.12.2009 Dr. Konrad Scheurmann, Dresden: Weihnachtsskolloquium: Der Stoff, aus dem die Farben sind

## 5.3 Scientific Meetings and Workshops

<i>Date</i>	<i>Title</i>
19.02.2007	Workshop des SFB 652: Berichte aus den Projekten
03.–04.05.2007	3rd Materials' Days: Functional Materials and Nanotechnology
16.–18.07.2007	390. Wilhelm und Else Heraeus-Seminar: Strongly correlated plasmas
13.–16.11.2007	Rostock: Alpha Condensation
26.–29.05.2008	International Conference: International Conference on Clusters at Surfaces ICCS2008
26.–29.05.2008	NOEKS 9 Workshop: International Workshop on Nonlinear Optics and Excitation Kinetics in Semiconductors
09.–12.06.2008	10th Lähnwitzseminar on Calorimetry: Calorimetry on a Nano Scale
26.–27.06.2008	4th Materials' Days: The development of new materials and their engineering on nanoscopic lengthscales is maturing to an important key technology of this decade
08.–10.09.2008	International Conference on "Correlations in Radiation Fields", SFB 652
09.–10.07.2009	5th Materials' Days: Functional Materials and Nanotechnology
15.–17.07.2009	Rostock: 3. Annual GIF-Workshop: Investigations of Ultra-High Magnetic Fields in Laser Produced and Z-Pinch Plasmas Using High Resolution Novel X-Ray and UV-Spectroscopy
05.–07.08.2009	Rostock: Alpha Condensation
17.–18.09.2009	Rostock: Miniworkshop on Stochastic Processes: Teaching, Research and Applications
11.–13.10.2009	Prerow: HIC for FAIR Workshop on Dense QCD Phases in Heavy-Ion Collisions and Supernovae
01.–02.10.2009	Wechselwirkung intensiver XUV-Impulse mit kondensierter Materie – Innovative Instrumentierung für Experimente bei FLASH





# Universität Rostock



Traditio et Innovatio

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