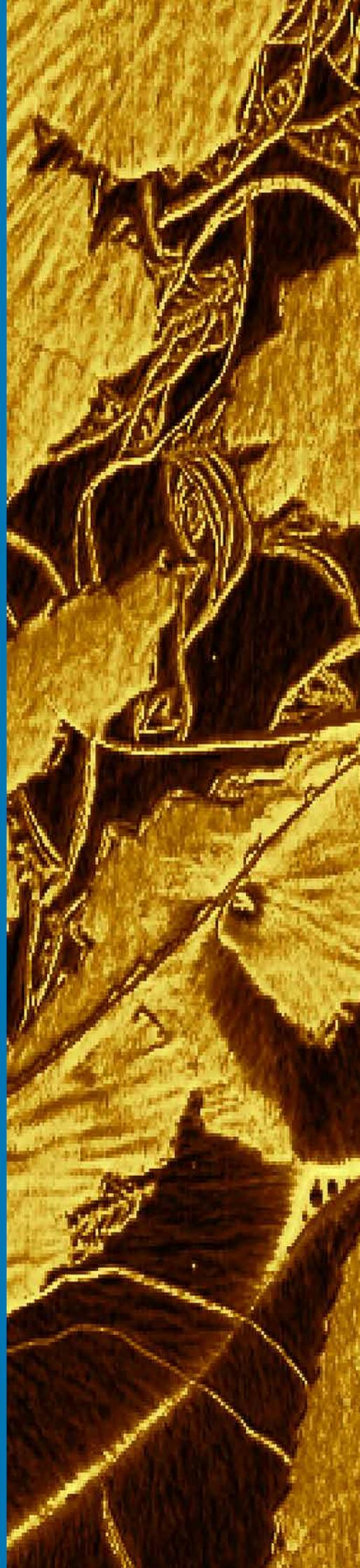


RESEARCH PORTFOLIO FACULTY OF NATURAL SCIENCES II 2022



MARTIN-LUTHER-UNIVERSITÄT
HALLE-WITTENBERG





Photos: Michael Deutsch | MLU

Research portfolio

Faculty of Natural Sciences II

Chemistry, Physics,
Mathematics

Research portfolio of the Faculty of Natural Sciences II (NF II)

With this research portfolio, we present an overview of the research topics pursued at our faculty, as represented by the different research groups in the institutes of Chemistry, Physics and Mathematics, research facilities and connected research institutes. With *Materials Science* being one of Martin Luther University's main research fields, our activities center on *Nanostructured Materials*. Concentrated on three research foci (Synthetic and Biological Macromolecules, Solid State Interfaces and Nanostructures and Materials for Energy Conversion and Storage), the faculty provides a vibrant, sustainable and attractive environment in education and research. The interconnectedness of the three research foci occurs via the topics Molecules, Materials and Models. There are many links to other main research areas at Martin Luther University, especially to *Molecular Biosciences*.

In each area, the individual groups' research is documented by large-scale collaborative projects, often funded by the German Research Foundation (DFG), the Ministry of Education and Research (BMBF), the Horizon 2020 of the European Union, and many other Third Party-Funders, including industry. Our dedication to educating young scientists and school teachers is reflected in a number of (under)-graduate and postgraduate-study programs, where students meet science early on in their studies.

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Local collaboration partners

A significant part of our research is performed in collaboration with the external partner institutions located on Halle's "Weinberg Campus." The close proximity enables quick and efficient exchange and personal interaction. A part of our faculty, named here, are co-appointed with our partner institutes.



Max-Planck-Institute of Microstructure Physics
Prof. Stuart Parkin
Prof. Joyce Poon



Interdisciplinary Center of Materials Sciences (IZM)
(central institution of Martin Luther University)
Prof. Georg Schmidt



Fraunhofer
IMWS
Fraunhofer Institute for Microstructure of Materials and Systems (IWMS),



Fraunhofer
CSP
Fraunhofer Center for Silicon-Photovoltaics (CSP), and Fraunhofer Pilot Plant Center for Polymer Synthesis and Processing (PAZ)



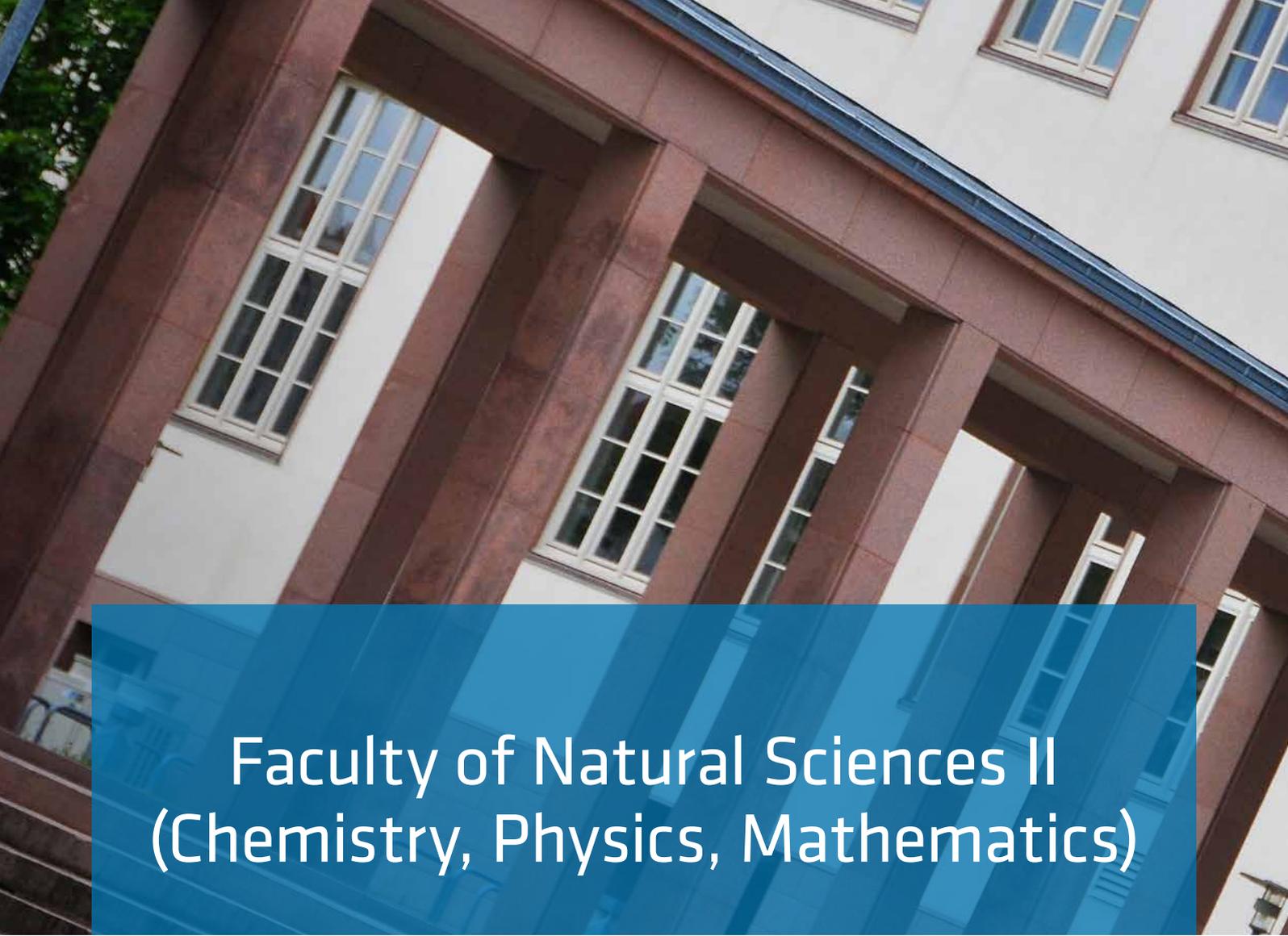
Beurlaubt: Prof. Ralf Wehrspohn (IMWS / CSP / PAZ)
Prof. Michael Bartke (PAZ)



Leibniz Institute of Plant Biochemistry
Prof. Ludger Wessjohann
Prof. Bernhard Westermann



Helmholtz Center for Environmental Research
Prof. Kai-Uwe Goss



Faculty of Natural Sciences II (Chemistry, Physics, Mathematics)

Address of the Dean

Halle as a bustling and modern city of $\frac{1}{4}$ million inhabitants hosts the Martin Luther University Halle-Wittenberg (MLU) together with many external research institutes. Located in the middle of Germany, MLU covers the full spectrum of science, philosophy and theology. Founded in the year 1502 MLU has a longstanding tradition in science and mathematics, with the Nobel Prize Laureates Gustav Hertz (Physics), Hermann Staudinger (Chemistry), Carl Ziegler (Chemistry) and the Mathematician Georg Cantor as prominent alumni.

Research at the Faculty of Natural Sciences II covers both, theoretical and experimental science in the areas of Chemistry, Physics and Mathematics. Striving to impact modern scientific research we address the growing and advancing needs of a dynamic society. Within the three main areas of research, solid materials interfaces, (bio-)macromolecules and energy storage, central aspects of materials science and molecular science are investigated. Together with 1000 students high-level research is conducted, in addition to many national and international collaborations.

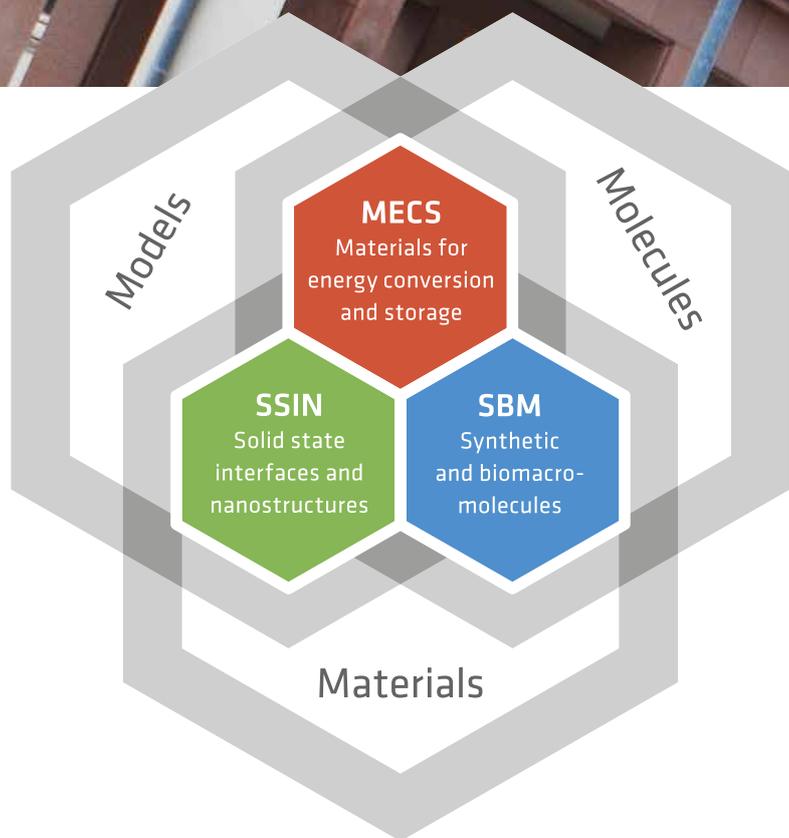
Located at a modern and integrative campus, students can experience education and science on one place, well connected to the historic, old town of Halle, also known as “Händelstadt”, Georg Friedrich Händel’s birthplace. Our study-programs address the Bachelor-, Master- and PhD-level, enabling students to either chose science programs in chemistry, physics or mathematics, or reach education in interdisciplinary fields such as medical physics, polymer materials science, renewable energies and economical mathematics. With this Research Portfolio we provide an overview on research-topics and the involved researchers, hoping to meet you here and stay in touch.



Prof. Dr. Wolfgang H. Binder, Dean



Photo: Michael Deutsch | MLU



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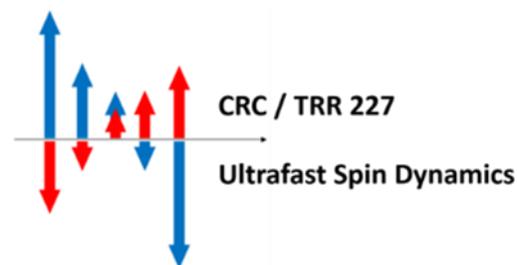
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www.natfak2.uni-halle.de/forschung

DFG Collaborative Research Center CRC/Transregio 227

Ultrafast Spin Dynamics

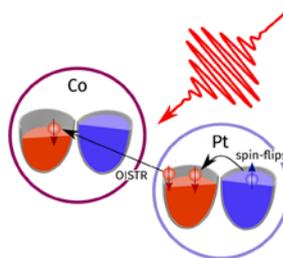


Project Description

The electron spin is one of the key quantum properties determining structure and dynamics of matter. It has large potential for applications in future magnetic memory and logic devices with simple architecture and reduced power consumption. Two fundamental spin-dependent interactions, exchange and spin-orbit coupling, allow for a spin response down to ultrafast time scales. Likewise, when reaching the nanoscale, electron and spin transport become ballistic and can occur ultrafast within femtoseconds. However, while future applications require such high speed and terahertz (THz) bandwidths, most spin-based magnetoelectronic devices are currently operating at 100-1000 times lower clock rates.

The goal of our CRC/TRR 227 is to establish a fundamental understanding of ultrafast spin dynamics, thereby laying the foundations for spin-based information technology that can be operated at THz clock rates. Our concerted research effort comprises cutting-edge experiments in ultrafast spectroscopy and multiscale theoretical modeling of spin dynamics. This science-driven approach promises a wealth of new results as well as the progress and buildup of our fundamental knowledge beyond technical applications. To study ultrafast spin dynamics, we will make use of the fastest stimuli and probes available: ultrashort optical and electromagnetic pulses with center frequencies ranging from the THz to the ultraviolet spectral range. Our research will focus on novel phenomena in state-of-the-art spintronic materials. In addition, we will address a few new, promising materials and explore nanoscale structures to localize and enhance incident electromagnetic fields. The analysis and control of ultrafast spin dynamics form the basis for our long-term goal: To transfer the understanding of femtosecond spin dynamics into novel functionalities for future ultrafast

spin-based technology. Our research consortium employs and develops a comprehensive portfolio of experimental and theoretical methods that is ideally suited to study ultrafast spin dynamics and train our graduate students in this scientifically exciting and technologically promising field of condensed matter physics.



Ultrafast optically induced inter site transfer of angular momentum

Participating Institutions

- › Freie Universität Berlin
- › Martin Luther University Halle-Wittenberg
- › Fritz-Haber-Institut der Max-Planck-Gesellschaft
- › Helmholtz Zentrum Berlin
- › Max Born Institut

Budget: 11 Mio € (4 Mio € Halle share)

Funding periods: January 2018 - December 2021



Projects and Project Leaders (First Funding Period)

- **A01: Ultrafast spin dynamics and its signature in the transient electronic structure**
Prof. Martin Weinelt (FU Berlin)
- **A02: Eisbitt Ultrafast spin dynamics in heterogeneous magnetic systems**
Clemens von Korff Schmising (Max Born Institute)
- **A03: Element-specific view on ultrafast spin and angular momentum redistribution**
Dr. Niko Pontius, Prof. Alexander Föhlisch (HZB)
- **A04: Theoretical simulation of the probe in pump-probe experiments: MOKE, MCD, and PES**
Dr. Sangeeta Sharma (MBI)
- **A05: Elementary terahertz spin interactions in magnetic solids**
Prof. Tobias Kampfrath (FU-Berlin)
- **A06: Nanometer-resolved ultrafast spin and electron dynamics at magnetic surfaces**
Dr. Chen-Tien Chiang, Prof. Wolf Widdra (MLU-Halle)
- **A07: Bridging the time scales between ultrafast and precessional magnetization dynamics**
Prof. Wolfgang Kuch (FU-Berlin)
- **A08: Multiscale modeling of ultrafast spin dynamics**
Dr. Unai Atxitia (FU-Berlin)
- **A09: Ultrafast magnetization dynamics and spin transport in magnetic oxide heterostructures**
Dr. Laurenz Rettig (FHI)

- **B01: Ultrafast spin currents and spin torques studied by (non-) linear magneto-optics**
Dr. Alexey Melnikov, Prof. Georg Woltersdorf (MLU-Halle)
- **B02: Ultrafast spintronic devices**
Prof. Tobias Kampfrath (FU-Berlin), Prof. Georg Woltersdorf, Prof. Georg Schmidt (MLU-Halle)
- **B03: Time-dependent spin dynamics and electron transport**
Prof. Piet Brouwer (FU-Berlin)
- **B04: Spin-dependent transport in inhomogeneous systems**
Prof. Ingrid Mertig, Dr. Jürgen Henk (MLU-Halle)
- **B05: Spin dynamics in atomically-precise nanostructures**
Prof. Katharina Franke, Prof. Tobias Kampfrath (FU-Berlin)
- **B06: Imaging and control of spatio-temporal spin dynamics in nanostructures**
Prof. Jamal Berakdar (MLU-Halle)
- **B07: Momentum-resolved dynamics of relaxation processes and control of spins and pseudospins in TMDC-based spintronic heterostructures**
Dr. Ralph Ernstorfer, Prof. Marin Wolf (FHI)
- **B08: Ultrafast spin transport at the interface between TMDCs and metals**
Prof. Kirill Bolotin, Dr. Cornelius Gahl (FU-Berlin)
- **B09: Real-time (pseudo-)spin transport and dynamics in transition metal dichalcogenides**
Prof. Miguel Marques (MLU-Halle)

Integrated Research Training Group (iRTG)

The iRTG offers a structured qualification program in scientific and key skills to all PhD students financed and associated to the CRC/TRR. Its training is divided into research training in several laboratories and in different research contexts, as well as an external training program, which offers courses for key skills. The PhD students have many occasions to actively learn about the works of their colleagues in the CRC, to communicate science and to discuss their own scientific results. The scientific exchange is fostered by a set of opportunities, such as training in other than their own labs, tutorials, seminars and a retreat.

Candidates are offered courses on transferable skills in collaboration with the Dahlem Research School Berlin (DRS) and the International Graduate Academy Halle (InGrA) RTG



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<https://www.trr227.de/>

DFG Collaborative Research Center SFB/Transregio 102:

Polymers under Multiple Constraints – Restricted and Controlled Molecular Order and Mobility



Third funding period: July 2019 – June 2023

Budget: 8,8 Mio. € (6,7 Mio. € Halle share)

Project Description

The rich versatility and the variable properties and functions of macromolecules are based on the one hand on a large variety of different monomers but on the other hand on the fact that polymers are able to self-assemble in organized structures, encoded in the chemical sequence of the polymer chains. In simple cases of self-assembly, the only constraint is the chain connectivity, leading to the existence of largely universal properties independent of the specific chemistry. But there are many important open and challenging problems in polymer science which are characterized by strong correlations between local structure and global conformation of the chain. In the CRC TRR 102 we investigate such processes of structure formation and self-assembly of chain molecules, for which the formation of molecular structures and the molecular dynamics are affected in addition to connectivity by constraints, such as specific internal interactions, external forces, geometrical confinement, crowding or topological restrictions.

Two prominent examples for such processes and central topics of the CRC are crystallization in the area of synthetic polymers and the formation of amyloids in the area of biopolymers. In both cases larger scale structures form, driven by the formation of local molecular order and constrained by the connectivity of the chains. The resulting structures are thus only partially ordered and of nanoscopic size in one or several directions. Both processes have universal features, but different from crystallization, amyloid formation is connected to specific interaction. In the CRC we study these and other related processes of structure formation and the properties of the resulting structures with the aim to work out and understand the fundamental, underlying physical principles. To achieve this aim we combine expertise from chemistry, experimental and theoretical physics, and biophysics using a large variety of experimental techniques and theoretical approaches based on simulations on different scales and levels of complexity.

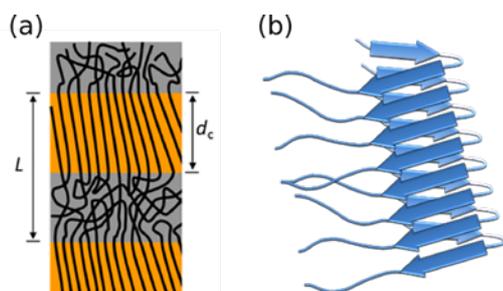


Figure 1: Central research topics of the CRC are the crystallization in synthetic polymers and the amyloid formation in proteins. There are obvious structural similarities between the semicrystalline morphology of a polymer (a) and the amyloid fibrils of peptides and proteins (b). Amyloids fibrils often feature a rigid β sheet motif in the core and mobile terminal chains. Within the SFB we attempt to connect both research fields by transferring methods and concepts.

Projects and Project Leaders

- **A1: Effects of topological constraints in polymer melts on crystallization and structure formation**
Prof. Thomas Thurn-Albrecht, Prof. Kay Saalwächter (Physics, MLU Halle)
- **A3: Crystallization and cooperativity in dynamic supramolecular polymers**
Prof. Wolfgang H. Binder (Chemistry, MLU Halle)
- **A6: NMR investigations of the self-organization and dynamics of amyloid protein fibrils**
Prof. Daniel Huster (Medicine, U Leipzig)
- **A7: Intra- and intermolecular structure formation in the presence of specific interactions**
Prof. Wolfgang Paul (Physics, MLU Halle)
- **A8: Organization and interactions of eye-lens crystallins: native states and cataract formation**
Prof. Kay Saalwächter, Prof. Jochen Balbach (Physics, MLU Halle)
- **A9: Structure formation and aggregation of solvated peptides and polymers in the presence of ions**
Prof. Daniel Sebastiani (Chemistry, MLU Halle)
- **A12: Assembly of PTH/polymer hybridmolecules**
Prof. Jochen Balbach (Physics, MLU Halle), Prof. Wolfgang Binder (MLU Halle)
- **B1: Aggregation and self-assembly of amyloid systems and functionalized peptides near interfaces - towards molecular mechanisms and smart materials**
Prof. Bernd Abel (Chemistry, U Leipzig)
- **B3: Substrate-induced molecular order and nucleation in thin films of semicrystalline polymers**
Prof. Thomas Thurn-Albrecht (Physics, MLU Halle)
- **B4: Nanopatterns of macromolecules**
Prof. Wolfhardt Janke (Physics, U Leipzig)
- **B7: Semicrystalline homopolymers and block copolymers at the air/water interface and in Langmuir-Blodgett films on solid supports**
Prof. Jörg Krefßler (Chemistry, MLU Halle)
- **B8: Refined infrared spectroscopy to study molecular orientation and order in heterogeneous polymer systems**
Prof. Friedrich Kremer (Physik, U Leipzig)
- **B10: Interactions of single polymer chains and amyloid fibrils in a thermophoretic trap**
Prof. Frank Cichos (Physics, U Leipzig)
- **B12: Mechanisms of early amyloid formation and the confining influence of macromolecular crowding**
Dr. Maria Ott (Biochemistry, MLU Halle)
- **B14: Structure formation in linear precision and comb-like polymers under external constraints: Influence of shear fields and interfaces**
Prof. Mario Beiner (Chemistry, MLU Halle and FhI Halle)



Figure 3: Group picture of the members of the CRC TRR 102 taken at the 6th retreat in Bad Schandau in March 2020.

Participating Institutions

Martin Luther University Halle-Wittenberg
University of Leipzig
Fraunhofer Institute for Mechanics of Materials Halle
Leibniz Institute of Surface Engineering Leipzig
Max Planck Institute of Colloids and Interfaces Potsdam

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SFB-TRR 102

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Prof. Kay Saalwächter (spokesperson iRTG)

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www.natfak2.uni-halle.de/sfbtrr102

blogs.urz.uni-halle.de/irtgpolymer/

- **B15: Dynamics and association in individualized macromolecules**

Dr. Martin Tress (Physics, U Leipzig)

- **B16: Crystallization of polymer chains under anisotropic confinement in liquid crystals**

Dr. Tiago Mendes Ferreira (Physics, MLU Halle)

- **B17: Force-induced α - β transitions in coiled coil structures**

Dr. Kerstin Blank (Biochemistry, MPIKG Potsdam)

- **Z1: Synthesis of labeled and unlabeled peptides with difficult sequences in large scales**

Dr. Sven Rothmund (Medicine, U Leipzig)

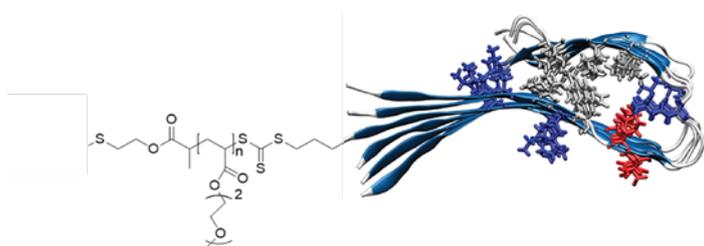


Figure 2: As a third class of materials, hybrid systems are studied in the CRC. The combination of elements typical for synthetic polymers and proteins in one hybrid macromolecule leads to new functions and material properties.

Integrated Research Training Group “Polymers: Random Coils and Beyond”

The graduate program provides in-depth training in interdisciplinary soft matter research, including the design and preparation of specific materials, their characterization, and their theoretical understanding. A thorough command of the basic principles of chemistry, physics and engineering of polymers and soft matter are aims of the training within our graduate school. Common projects, mutual support by, e.g., measurements in other research groups and seminars lead to active exchange between the doctoral students. Highlights are full two-days advanced training modules giving an introduction to selected research methods. In addition, the faculty offers lectures on several polymer topics and lecture series by international guest researchers. Besides the scientific education, doctoral students are supported in their transferable skills, such as writing publications and giving persuasive talks. The scientific progress and the current research activities are discussed regularly during meetings with supervisor and mentor. The English language is the common basis for communication within the graduate school.



Figure 4: In the integrated Research Training Group “Polymers: random coils and beyond” about 30 doctoral students obtain additional training in (bio)polymer science. In this interdisciplinary research field, questions related to physical, biophysical, chemical and materials science are in the focus, combining experiments and theory of synthetic and biological polymers.

DFG Research Training Group (RTG/GRK) 2670

Beyond Amphiphilicity:

Self-Organization of Soft Matter Via Multiple Noncovalent Interactions



First funding period: 2021-2025 (4.5 years)

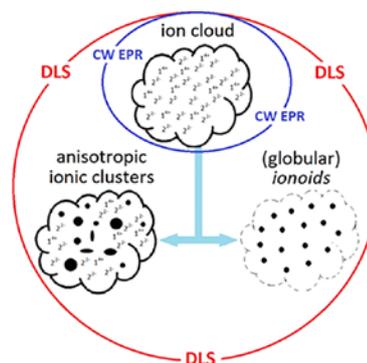
Budget: 4.53 Mio. €

Project Description

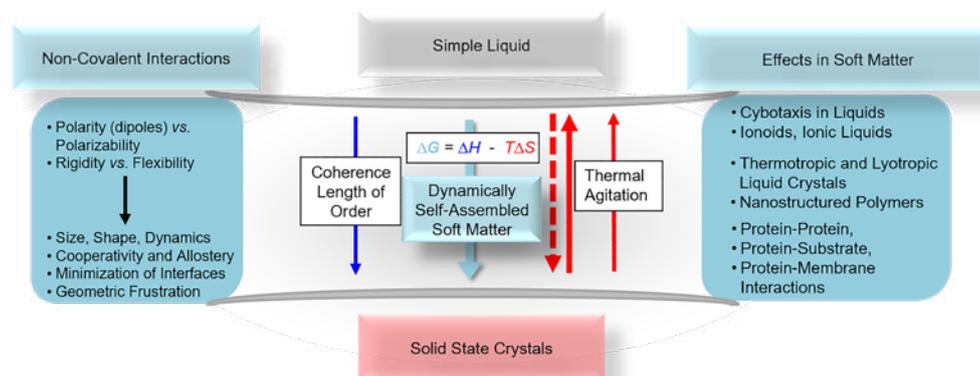
Amphiphilicity is a well-established qualitative concept contributing to the understanding of self-assembly processes of molecules composed of two inherently incompatible units (hydrophilic and hydrophobic) in aqueous systems. Polyphilic molecules are more complex molecules, from small molecules to macromolecules, that have interaction patterns with at least two types of interactions, one of them based on amphiphilicity. Self-assembled soft matter systems attain their complexity through noncovalent interaction patterns of their molecular constituents with their environment, solvents, biomolecules, membranes, and surfaces.

With this RTG “Beyond Amphiphilicity” (BEAM), we aim at a research and training consortium that takes the vast and scattered knowledge and work on noncovalent interactions further to develop a research training that centers on dynamic structuring of polyphilic soft matter through multiple non-covalent interactions. The relevant self-assembly is dynamic on the pico- to microsecond scale but may often dominate the macroscopic length scale and time scales. This translates into the creation of order on multiple length scales in the presence of dynamics. We want to advance the understanding of the emergence of complexity in molecular systems, in the long run we aim at uncovering design principles for nanostructured materials or aspects of self-assembly in biological systems. All studied systems are in or close to thermodynamic equilibrium or at least in long-lived metastable states. From the training perspective for our students, it is highly illustrative to build research on complex structuring on soft matter on the often-used and seemingly simple concept of amphiphilicity. We then go beyond amphiphilicity as a concept by extending the interaction patterns to understand and finally design complexity in soft matter.

This RTG combines existing competencies in simulation, design and synthesis, characterization and understanding of new materials and their properties. The research and educational concepts of the RTG go beyond the classical division into disciplines of chemistry and will offer doctoral researchers an excellent and broad education combining many facets of modern chemical, physical and mathematical methods. The RTG’s educational program will empower its doctoral researchers to become well-qualified scientists in academia and industry alike – with a unique combination of scientific training, professional training and strategic research training elements.



Schematic of structure formation to ionoids and anisotropic ionic clusters starting from ion clouds, as studied in project A2. It also shows the main methods of characterization of the ten-day incubation period in ion clouds (CW EPR) and after ten days (DLS).



Structure and dynamics during self-assembly through multiple interactions of soft matter that has properties between simple (ideal) liquids and solid-state crystalline materials. On the left-hand side, different types of interactions and physical-chemical properties that lead to effective interactions (or forbid certain others) are exemplified. These interactions cause dynamic structuring in soft matter systems depicted on the right-hand side.

Projects and Project Leaders

Project area A – Self-organization of small and medium-sized synthetic molecules through multiple interactions

- **A1: Systematic multidimensional quantification of multiple interaction patterns between polyphilic molecules**
Prof. Dr. Daniel Sebastiani (Chemistry, MLU Halle)
- **A2: Dynamic yet defined self-assembly of small molecules in solution: colloid-like ionic clusters (ionoids)**
Prof. Dr. Dariush Hinderberger (Chemistry, MLU Halle; HALOmem), Prof. Dr. Daniel Sebastiani (Chemistry, MLU Halle)
- **A3: Design of liquid quasicrystals and their approximants**
Prof. Dr. Carsten Tschierske (Chemistry, MLU Halle), Prof. Dr. Rebecca Waldecker (Mathematics, MLU Halle)
- **A4: Characterizing the interaction of proteins with polyphilic detergents and lipids and their impact on membrane self-assembly**
Prof. Dr. Carla Schmidt (Biochemistry and Biotechnology, MLU Halle; HALOmem)
- **A5: Studying amino acid interactions with non-natural polyphilic substrates**
Prof. Dr. Martin Weissenborn (Chemistry, MLU Halle and IPB)

Project area B – Self-organization of (bio-)polymeric polyphilic molecules through multiple interactions

- **B1: Thermodynamics of fluorophilicity, lipophilicity, hydrophilicity, and their combination in polymers**
Prof. Dr. Jörg Krefßler (Chemistry, MLU Halle)
- **B2: Cluster-formation and interfacial function in polymeric ionic liquids**
Prof. Dr. Wolfgang H. Binder, (Chemistry, MLU Halle)
- **B3: Tuning protein and nanocolloid diffusion and (transient) assembly through polyphilic interactions: the role of patchiness and charges**
Prof. Dr. Kay Saalwächter, (Physics, MLU Halle)
- **B4: Diffusional and co-diffusional analysis of polyphilic protein–protein and protein–membrane Interactions**
Prof. Dr. Kirsten Bacia, (Chemistry, MLU Halle; HALOmem)

Molecules of different philicity (regular, semi-fluorinated and perfluorinated alkanes and alcohols), simulated in a lipid bilayer and studied as in project A1.

Participating Institutions

Institute of Chemistry, Institute of Physics, Institute of Mathematics (all of Faculty of Natural Sciences II at MLU)
Institute of Biochemistry and Biotechnology (Faculty of Natural Sciences I at MLU)

HALOmem: Interdisciplinary Research Center ZIK HALOmem

IPB: Leibniz Institute of Plant Biochemistry

Contact

GRK 2670

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Institute of Chemistry

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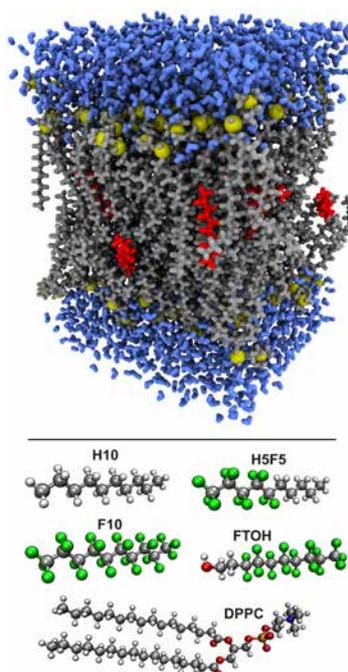
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BMBF Center for Innovation Competence (ZIK):

SiLi-nano – Silicon and Light: from Macro to Nano



Budget of current funding period (2016-2021): 7,07 Mio EUR
 Additional strategic Investments (2020-2021): 3,998 Mio. EU

Project Description

Light-matter interaction is the basis for many interesting and technologically relevant processes, and the ability to create nanostructures with dimensions on the order and below the wavelength of light allows now to manipulate this interaction in new and fascinating ways. Therefore, the Centre of Innovation competence SiLi-nano (ZIK SiLi-nano) was established in 2009 with the two junior research groups “Light to Silicon” and “Silicon to Light”. During the first period the research mainly focused on the interaction of light with silicon – especially the generation of electricity by silicon based photovoltaics and the control of light emission, transformation and propagation in silicon photonic circuits. Adapting to new research challenges and with the addition of the two new groups “Light-for-High-Voltage-Photovoltaics” and “Light-for-Hydrogen” in 2016 the range of investigated material systems broadened. However the focus of the research on light-matter interaction in nanostructures for technologically relevant processes and applications remained. Today the research at the ZIK SiLi-nano includes topics ranging from laser ablation and hybrid photonics to ferroelectric photovoltaics and photocatalytic water splitting.

Publications

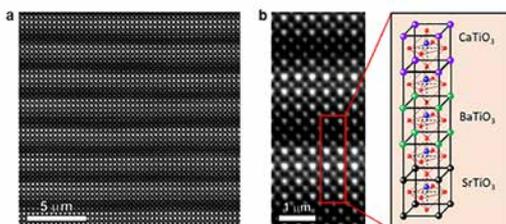
D.S. Knoche, Y. Yun, NR. Gowda, L. Mühlenbein, X. Li and A. Bhatnagar:

Domain and Switching Control of the Bulk Photovoltaic Effect in Epitaxial BiFeO₃ Thin Films. Scientific Reports 9, 13979 (2019)

H. Zhang, X. Li, A. Hähnel, V. Naumann, C. Lin, S. Azimi, S.L. Schweizer, A.W. Maijenburg and R.B. Wehrspohn: **Bifunctional heterostructure assembly of NiFe LDH nanosheets on NiCoP nanowires for highly efficient and stable overall water splitting.** Advanced Functional Materials 28, 1706847 (2018)

V. Rutckaia, F. Heyroth, A. Novikov, M. Shaleev, M. Petrov, and J. Schilling: **Quantum Dot Emission Driven by Mie Resonances in Silicon Nanostructures.** Nano Lett. 17, 6886 (2017)

M. Muchow, T. Buchner, A. Sprafke, G. Seifert: **Femtosecond laser-written high-efficiency blazed phase gratings in the volume of soda lime glass for light management in solar modules.** OPTICS EXPRESS 23, 33540-33549 (2015)



High resolution transmission electron microscope image and model of atomic ordering of a ferroelectric superlattice cell.

Project Groups

Silicon-to-Light

Although silicon represents a formidable material for integrated photonics due to its high refractive index, light emission and non-linear optical processes are largely impeded by its indirect bandgap, centrosymmetric crystal structure and high two-photon absorption. The research of the group “Silicon-to-Light” aims to overcome these challenges by either modifying the optical properties of silicon itself or combining silicon with different materials of desired optical functionality creating hybrid photonic devices for “optics on the chip”. This includes the generation of a second order nonlinearity ($\chi^{(2)}$) in silicon based on symmetry breaking by an applied electric field, third order nonlinear optical processes in hybrid photonic devices, Purcell luminescence enhancement in Mie-resonances and plasmonic metamaterials for ultra-tight focussing and SERS.

Light-to-Silicon

Femto- and picosecond laser ablation offers the possibility for selective layer removal without causing thermal damage to the surrounding material. Currently spatial and temporal pulse shaping techniques are studied to optimize areal ablation and material selectivity. Furthermore focussing intensive femtosecond laser pulses inside materials like glass starts an interplay of nonlinear defocusing and refocusing resulting in long intensity “filaments” and a local internal refractive index change. Extended periodic index gratings could be “written” into glass in this way. Short pulse laser irradiation is also used to locally melt-ablate nano-volumes of different materials, which then form perfectly smooth spheres due to the surface tension in the liquid state before re-solidifying and re-depositing at a new substrate.

Light-for-High-Voltage-Photovoltaics

The anomalous photovoltaic effect (APV) in ferroelectric / multiferroic materials results in an open circuit voltage (V_{oc} , in volts) which is far greater than the bandgap (in eV) of the illuminated material. This distinguishes the effect from junction based classic semiconductor photovoltaics. However the generated photocurrent of the APV is usually far smaller than in traditional solar cell materials. The research of the group aims to improve on this point and is actively pursuing the following strategies:

1. Growth of multiferroic and complex oxide material systems in the form of Superlattices, and heterostructures.
2. Band gap engineering of oxides via substitutional doping and strain from the substrate.

Furthermore the interplay between photovoltaic and ferroic properties are investigated.

Light-for-Hydrogen

When specific photocatalytic materials are immersed in water and irradiated with sunlight the photo(electro) chemical water splitting reaction occurs resulting in the formation of hydrogen gas in an environmentally friendly way. The group aims to develop specifically designed nanostructures to increase the light-to-hydrogen efficiency for this photocatalytic water splitting reaction. In particular Metal Organic Frameworks (MOFs), template based nanostructures as well as electrospun photocatalytic nanofibers are investigated. The investigation of the physical and chemical suitability of different types of nanostructures and their combination in photocatalytic cells for improved photoelectrochemical and autonomous water splitting completes these studies.

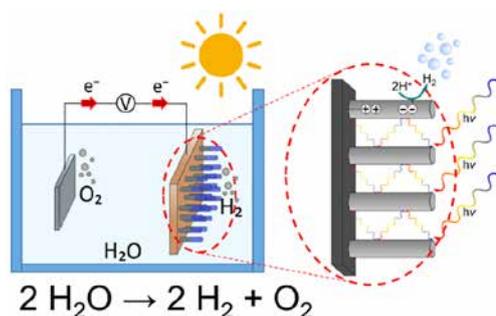


Illustration of optimized photoelectrochemical water splitting device using quasi one-dimensional nanostructures: a maximum of solar light can be absorbed over the nanowire length, while the nanowire diameter is small enough for efficient electron and hole diffusion.

Project Leaders

- **Prof. Jörg Schilling**
Since 2009 leader of the group “Silicon-to-Light”
Email: joerg.schilling@physik.uni-halle.de
- **Dr. Paul Miclea**
Since 2017 leader of the group “Light-to-Silicon”
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- **Dr. Akash Bhatnagar**
Since 2016 leader of the group “Light-for-High-Voltage-Photovoltaics”
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- **Jun. Prof. Wouter Maijenburg**
Since 2016 leader of the group “Light-for-Hydrogen”
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Project Partners

Local:

Fraunhofer CSP
Fraunhofer IMWS
Max Planck Inst. of Microstructure Physics
Smart Membranes GmbH
Interdisciplinary Centre for Materials science (IZM) of the MLU
Several Research groups at the Institutes of Physics and Chemistry of the MLU

National:

Laserzentrum Hannover/FH Bremen
Fraunhofer IST Braunschweig
Fraunhofer IKTS Hermsdorf
MPI for Solid State Research Stuttgart
Leibniz Inst. für Oberflächen Modifikation Leipzig
Fraunhofer ISIT Itzehoe
Friedrich Schiller University Jena
TU Darmstadt
University Leipzig
University Bochum
University Köln
University Giessen

International:

University of Warwick (UK)
University Twente (NL)
University of Pennsylvania (USA)
IBM/Lumiphase Zürich (Switzerland)
ICMAB Barcelona (Spain)
IIT Banaras (India)
ITMO St. Petersburg (Russia)
IMP RAS Nishni Novgorod (Russia)
Chungnam Nat. Univ. (South Korea)
University Donhua (China)

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BMBF Center for Innovation Competence (ZIK):

HALOmem – Membrane Protein Structure and Dynamics

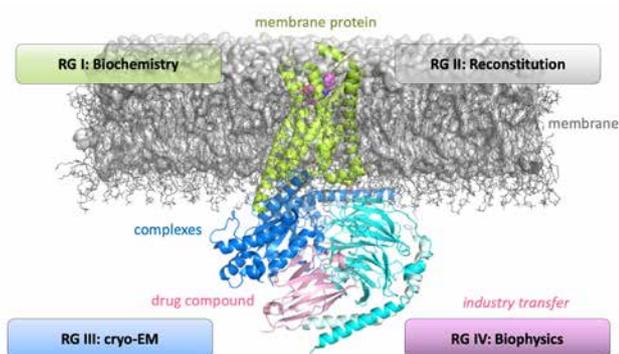


Budget: 24 Mio. €

Funding period: 2009 - 2022

Project Description

HALOmem is an interdisciplinary research center at the Martin Luther University Halle-Wittenberg (MLU). We focus on the structure of membrane proteins and their interactions with the surrounding membrane. Membrane proteins direct and regulate a wide range of essential cellular functions, being responsible for such diverse processes as inter- and intracellular communication, neurotransmission, transport of nutrients and generation of energy. Their vital nature is reflected by the fact that up to 70% of current drug targets are membrane proteins.



Four junior research groups (RG I – IV) investigate molecular details of membrane proteins and their complexes by various methods of basic research and for drug industry transfer.

HALOmem was founded by Prof. Dr. Milton T. Stubbs and Prof. Dr. Jochen Balbach as a joint effort of the Institute of Biochemistry & Biotechnology (Faculty of Natural Sciences I) and the Institutes of Physics and Chemistry (Faculty of Natural Sciences II). The research center brings together resources and special expertise from those institutes, such as recombinant protein production, biophysical methods for studying membranes, and protein structure determination by mass spectrometry, cryo-electron microscopy, crystallography and NMR. Within the first phase of funding of the HALOmem research center (2009 - 2015), the two independent tenure-track junior research groups Membrane Protein Biochemistry (RG I Dr. Mikio Tanabe) and Biophysical Chemistry of Membranes (RG II Prof. Dr. Kirsten Bacia) were established. In 2015, Kirsten Bacia became a full professor (W2) of Biophysical Chemistry at our faculty. Within the second phase of funding (2016 – 2022), two additional independent tenure-track junior research groups joined HALOmem: Cryo-Electron Microscopy of Membrane Complexes (RG III Jun.-Prof. Dr. Panagiotis L. Kastiris) and Biophysical Characterisation of Medically Relevant Proteins (Jun.-Prof. Dr. Carla Schmidt). They extended the experi-

mental methods of HALOmem by cryo-EM and mass spectrometry and the scientific focus towards membrane protein complexes supported by substantial investments into instrumentation by the BMBF and the state Sachsen-Anhalt. In 2020, HALOmem associated Prof. Dr. Dariush Hinderberger from our Institute of Chemistry for EPR spectroscopic studies of complex self-organization of membrane proteins.

Collaboration Partners

- **Protein crystallography**
Prof. Dr. Milton T. Stubbs, Institute of Biochemistry and Biotechnology, MLU
- **NMR and protein dynamics**
Prof. Dr. Jochen Balbach, Institute of Physics, MLU
- **Fluorescence correlation spectroscopy**
Prof. Dr. Kirsten Bacia, Institute of Chemistry, MLU
- **Protein mass spectrometry**
Jun.-Prof. Dr. Carla Schmidt, HALOmem
- **Cryo-Electron microscopy**
Jun.-Prof. Dr. Panagiotis L. Kastiris, HALOmem

Contact

Center for Innovation Competence HALOmem

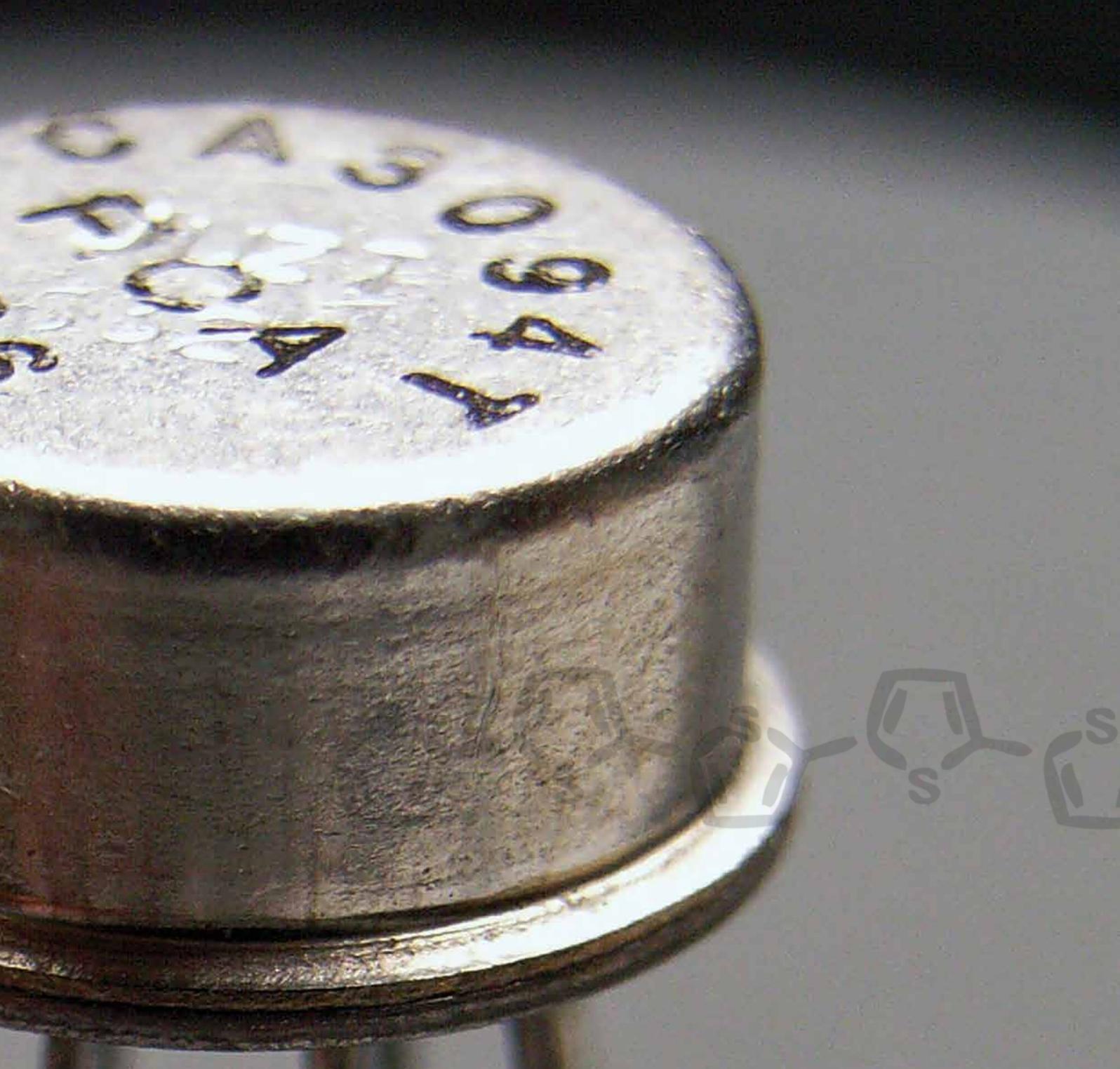
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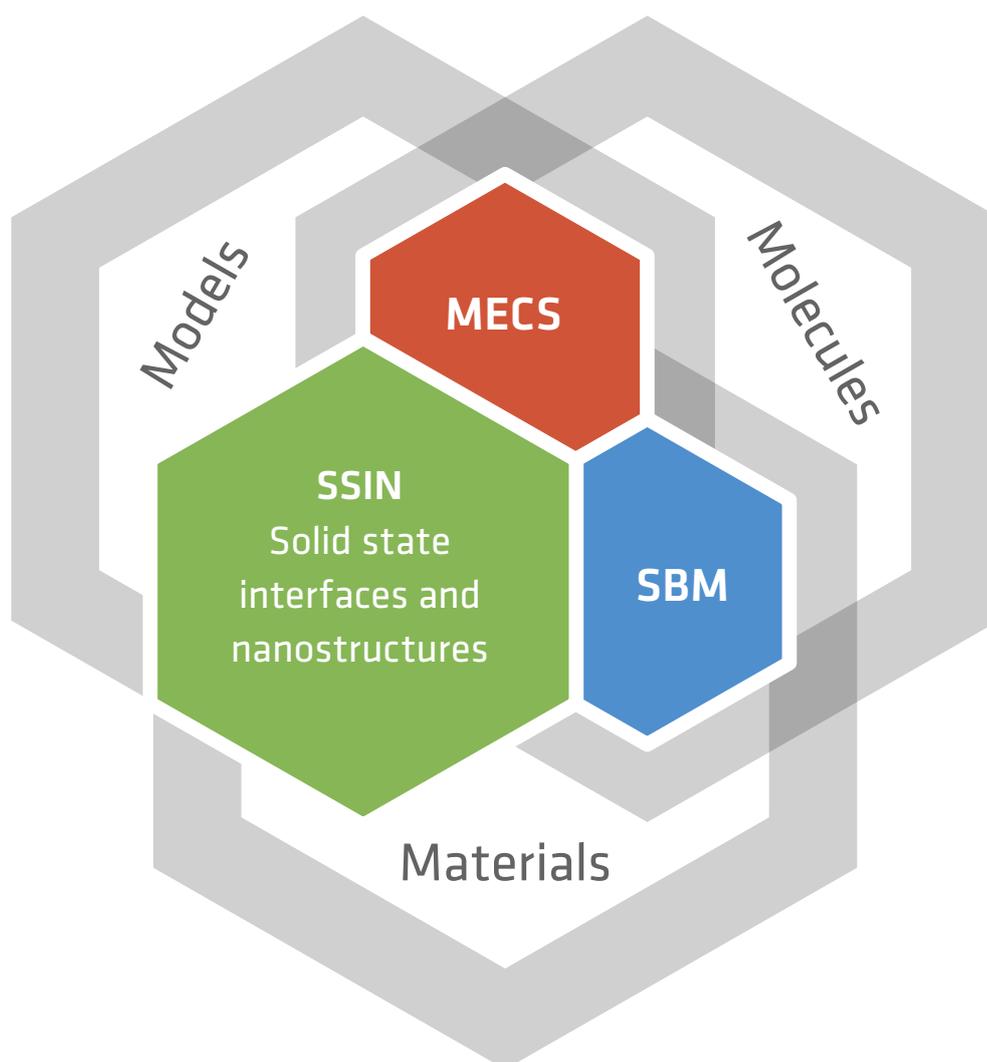
Solid state interfaces and nanostructures

Gaining control over structure formation on the nanoscale opens tremendous possibilities to enhance, alter or even create new materials properties. These can be employed for future applications ranging from chemical synthesis to new nano-optical and -electrical devices. Moreover in composite- and super-structures with individual elements of nanoscale dimensions the surface and interface regions start to play a crucial role affecting basic electronic transport properties and giving rise to unexpected new phenomena.

Our investigated nanostructures range from individual carbon based complexes and metal-organic/anorganic clusters to solid state oxides. Besides the natural structure formation and self-assembly of the nanostructures their particular chemical and physical properties are

studied. This involves research in their catalytic, electronic and optical properties as well as their impact on electronic/spintronic transport, photonic, magnonic and plasmonic wave propagation and the associated switching and modulation dynamics. Nanostructures and surfaces of ferromagnetic and ferroelectric materials are of particular interest in this respect.

These activities are supported by mathematical modeling and several network initiatives like the SFB "Functionality of oxidic interfaces", the SFB "Ultra fast spin dynamics", the international Max-Planck-research school for "Science and Technology of Nano-Systems" and the Centre of innovation competence (ZIK) SiLi-nano have been and are continuing to foster the research in this field.

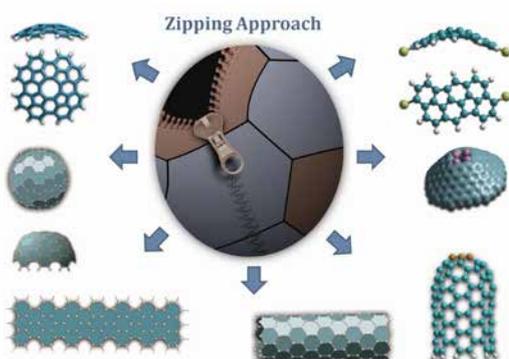


Institute of Chemistry

Organic Chemistry

Fields of Research:

Our main goal is to find and to develop alternative synthetic approaches suitable for preparative production of various carbon based nanostructures in isomerically pure form. Our research group is working on the rational synthesis of sp^2 -carbon based nanostructures which includes the rational synthesis of higher and non-classical fullerenes, geodesic polycyclic hydrocarbons, buckybowls, graphene nanoribbons, nanographenes, carbon nanotubes and other related systems. Our synthetic strategy is based on the synthesis of precursor molecules – polycyclic aromatic hydrocarbons, containing the carbon framework required for the formation of the target nanostructure. The respective precursor molecule can be transformed to the desired carbon nanostructure by intramolecular Aryl-Aryl domino-coupling. For this purpose specially designed precursor molecules are synthesized and investigated for controlled synthesis of the respective carbon nanostructures. The characteristic feature of the approach is a zipper mechanism of cyclization (regiospecific condensation in a domino fashion) by which the regiospecificity of each condensation step is unambiguously predefined by the specially “designed” precursor structure.



Current Projects and Future Goals:

Carbon-carbon bond formation

The development of effective technique allowing effective intramolecular carbon-carbon (carbon-heteroatom) bond formation is one of the main focus of the current research. Particular interest lies in the field of intramolecular Aryl-Aryl coupling reactions which can be performed in domino fashion. This include investigation in the field of C-F bond activation (cyclodehydrofluorination), surface assisted cyclodehydrogenation and dehydrative π -extension (DPEX).

synthesis of carbon based nanostructures

Currently we also working on development of alternative synthetic approaches allowing effective C-C coupling on metal oxide surfaces. The respective synthetic methods will open facile asses to the synthesis of carbon based nanostructures directly on technologically relevant non-metallic templates. We believe that our synthetic approaches will provide many interesting carbon based material in relevant for further investigation amounts.



Prof. Dr.
Konstantin Amsharov

2002

Ph.D from the Institute of Macromolecular Compounds, Russian Academy of Science

2005

Max-Planck Institute for Solid State Research, Stuttgart

2012

habilitation in Organic chemistry at the Institute of Organic Chemistry, University of Stuttgart

2014-2019

FAU Erlangen-Nürnberg leading an independent research group

Since 2019

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Selected publications:

M. Kolmer, A.K. Steiner, I. Izydorczyk, W. Ko, M. Engelund, M. Szymonski, A.P. Li, K. Amsharov. Rational synthesis of atomically precise graphene nanoribbons directly on metal oxide surfaces. *Science* 2020, 369, 571-575.

M. Kolmer, R. Zuzak, A.K. Steiner, L. Zajac, M. Engelund, S. Godlewski, M. Szymonski, K. Amsharov. Fluorine-programmed nano-zipping to tailored nanographenes on rutile TiO₂ surfaces. *Science* 2019, 363, 57-60.

J. R. Sanchez-Valencia, T. Dienel, O. Gröning, I. Shorubalko, A. Mueller, M. Jansen, K. Amsharov, P. Ruffieux, R. Fasel. Controlled synthesis of single-chirality carbon nanotubes. *Nature* 2014, 512, 61-64

K. Amsharov, M. A. Kabdulov, M. Jansen. Facile Bucky-Bowl Synthesis by Regiospecific Cove-Region Closure by HF Elimination. *Angew. Chem. Int. Ed.* 2012, 51, 4594-4597.



Prof. Dr. Martin Arnold

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PhD in Numerical Mathematics,
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1991-1997

PostDoc and Assistant Professor,
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Research Scientist, DLR German
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Selected publications:

S. Hante, M. Arnold, RATTLie: A variational Lie group integration scheme for constrained mechanical systems, *Journal of Computational and Applied Mathematics*, 2020 (in press), DOI: 10.1016/j.cam.2019.112492.

M. Arnold, O. Brüls, A. Cardona, Error analysis of generalized- α Lie group time integration methods for constrained mechanical systems, *Numerische Mathematik*, 2015, 129, 149-179.

H. Lang, J. Linn, M. Arnold, Multibody dynamics simulation of geometrically exact Cosserat rods, *Multibody System Dynamics*, 2011, 25, 285-312.

M. Arnold, Numerical methods for simulation in applied dynamics. In: M. Arnold, W. Schiehlen (eds.): *Simulation Techniques for Applied Dynamics*. Springer Wien New York, 2009.

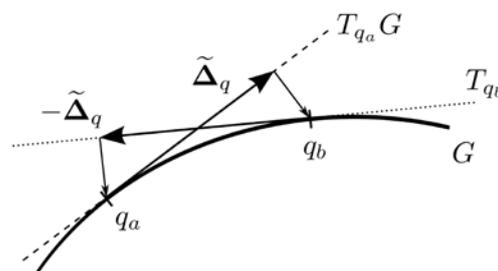
Institute of Mathematics**Numerical Mathematics****Fields of Research:**

- › Time integration of constrained and coupled systems of differential equations
- › Geometric integration, Structure preserving coarse grid discretizations of differential equations
- › Model based simulation and optimization in science and engineering
- › Numerical methods and software for time dependent problems: Interfaces, constraints, multi-disciplinary applications

Multi-disciplinary and multi-scale aspects of complex phenomena and processes in science and engineering result typically in mathematical models of some specific structure that is exploited by problem adapted numerical methods to improve robustness, numerical stability and efficiency. Such specially tailored numerical solution methods are the backbone of model based simulation and optimization in various fields of application.

Our group focusses on time integration methods for coupled systems of differential equations and on the numerical solution of constrained systems that result from the use of redundant coordinates in network approaches for modelling complex systems. We study typical problem classes in science and engineering to design specially adapted time integration methods for constrained systems that combine numerical stability with numerical efficiency in terms of computing time. Software aspects include numerical issues as well as the standardization of interfaces in (commercial) simulation software.

Recently, the preservation of structural properties in coarse grid discretizations of differential equations has found special interest. We construct and analyse Lie group time integration methods for flexible multibody systems that are modelled by differential equations on a manifold with Lie group structure. This novel approach helps to avoid singularities in the simulation of systems with large rotations.

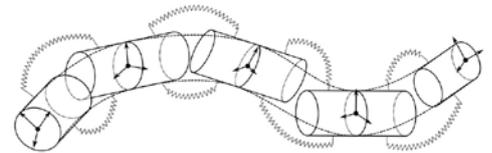


Differential equations on manifolds:
Interpolation in Lie groups.

Current Projects and Future Goals:

■ **Numerical Modelling of Highly Flexible Structures**

Highly flexible slender structures like yarns, cables, hoses or ropes are essential parts of high-performance engineering systems. The complex response of such structures in real operational conditions is far beyond the capabilities of current modelling tools that are at the core of modern product development cycles. In the framework of Horizon 2020, we coordinate the interdisciplinary network THREAD of 26 European universities, research organisations and industrial partners who will develop mechanical models and numerical methods for designing highly flexible slender structures. This Marie Skłodowska-Curie ITN is one of the first research projects that applies systematically the novel mathematical concept of geometric numerical integration in industrial settings.



Coarse grid discretization of a geometrically exact beam model.

■ **Time integration of non-smooth problems**

Design, analysis and implementation of time integration methods are based on mathematical smoothness assumptions that are frequently violated in applied problems from science and engineering. We investigate alternative approaches being based on precise localization of discontinuities, on analytical regularization of non-smooth model components or on a numerical regularization by so-called time-stepping methods. In a joint project with the University of Rijeka (G. Jelenić), these numerical results are validated by test rig experiments for a rigid body rocking on a flexible structure.

■ **Modular time integration of coupled and constrained systems**

The modular structure of complex coupled systems in science and engineering may be exploited in time integration combining different time integration methods (with different, problem adapted time step sizes) for different subsystems and restricting the data exchange between subsystems appropriately. For stiff and for constrained systems, the numerical stabilization of these methods is a topic of active research.

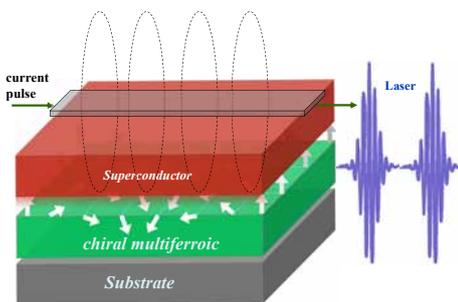
Institute of Physics

Nonequilibrium Many-Body Systems

Fields of Research:

- › Nanophysics
- › Photonics
- › Nanomagnetism
- › Ultrafast Optics

We develop theoretical concepts and numerical codes to understand the behavior of matter under external driving fields. The goal is to control materials properties in a spatio-temporal way or even to generate new features by specific engineering of the fields and/or the material under study. We are particularly interested in magnetically active structures at the nanoscale driven by shaped laser pulses, magnetic fields, elastic deformations or heat gradients. With a focus on technological applications we study how classical or quantum information can be stored, transmitted, and retrieved in terms of certain magnetic phases. One goal is to design fast and reliable electronic devices that offer new functionalities and operate with low energy consumption. On the other hand, we study the influence of material structuring and modifications of its physical properties on the propagation of electromagnetic waves with the aim to identify suitable optical materials for polarization shaping and wave-front structuring of light fields. We use the structured laser fields as building blocks for optical communication devices and ultrafast science with a particular emphasis on low-dimensional quantum structures such as waveguides, quantum dots, and molecular aggregates.



With external fields such as a magnetic field generated by a current pulse or the electric field of a short laser pulse we calculate, analyze, and seek to control the behavior of nanostructured materials and their compositions such as superconductor/ferromagnetic or ferroelectrics with a magnetic response (called multiferroics). The aim is to identify new fast, efficient and energy-saving ways to store and process classical and quantum information.

Current Projects and Future Goals:

■ Superconductor-magnetic heterostructures

Superconductors have a wide-range of applications in energy-saving devices, sensorics, and quantum information circuits. Multilayers composed of magnetic materials deposited on superconductors show in addition to the superconducting and magnetic properties, further emerging features that can be exploited in superconducting/magnetic tunnel junctions and superconductor-based quantum information science. We are developing new approaches capable of predicting the physical properties of meso- and macroscopic samples of magnetic/superconducting nanostructures.

■ Magnonics and ultrafast spintronics

Instead of optical signals, excitations in a magnetic system (called magnons) also serve as a very effective carrier of information and can be generated and detected at very low energy cost. We seek ways to increase the bandwidth and the efficiency of such information channels by material design and/or by shaping the input signals. In addition, we also study the possibility of using the spin as a key element for the operation of electronic circuits, in particular we study such spintronic systems driven by short optical fields to achieve a swift operational speed.

■ Photonics and non-linear optics

In addition to the temporal structuring of laser pulses, a control on the polarization state as well as on the phase of the wave front opens the way for new applications of lasers. We study how polarization and wave-front structuring affect the interaction of laser fields with matter in general. In addition, we study the propagation of intense laser pulses in optical devices with the goal of realizing efficient and reliable optical logic gates.

■ Topology and geometry in quantum matter

We study how the space-time structure leads to the emergence of stable phases or resonances. A particular focus is put on the influence of topology and geometry of the system on the stability of the formed states in field-free environment or for driven systems.



Prof. Dr. Jamal Berakdar

1994

Dr. rer.nat in Theoretical Physics, University of Freiburg, Germany

1995

Research associate, Royal Holloway University of London, UK

1995–1997

Feoder-Lynen Humboldt fellow and research fellow at the Institute of Advanced Studies, Australian National University, Canberra, Australia

1997–2006

Scientific member of the Max-Planck Institute of Microstructure Physics, Halle, Germany

Since 2006

Full professor of Theoretical Physics, Martin Luther University Halle-Wittenberg, Halle, Germany

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Selected publications:

Yu, D., Kang, J., Berakdar, J. et al., Nondestructive ultrafast steering of a magnetic vortex by terahertz pulses. *NPG Asia Mater* 12, 36 (2020).

De Ninno G., Wätzel J., Ribič P.R. et al. Photoelectric effect with a twist *Nature Photonics* 14, pp 554 (2020).

Wätzel J., and Berakdar J., Open-Circuit Ultrafast Generation of Nanoscopic Toroidal Moments: The Swift Phase Generator, *Advanced Quantum Technologies* 2, pp 1800096 (2019).

Jia, C., Ma, D., Schäffer, A.F., Berakdar, J., Twisted magnon beams carrying orbital angular momentum, *Nat Commun* 10, 277 (2019).

Pursehouse J., Murray A. J., Wätzel J., Berakdar J., Dynamic Double-Slit Experiment in a Single Atom, *Phys. Rev. Lett.* 122, pp 053204 (2019).

Jandieri V., Khomeriki R., Berakdar J., Erni D., Theory of soliton propagation in nonlinear photonic crystal waveguides, *Optics Express* 27, pp 29558 (2019).



Prof. Dr. Tomáš Dohnal

2005

PhD in Applied Mathematics,
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Habilitation in Applied Mathematics,
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Selected publications:

T. Dohnal and L. Wahlers. Coupled Mode Equations and Gap Solitons in Higher Dimensions. *J. Differ. Equations* (2020), 269, 2386–2418.T. Dohnal and D. Pelinovsky. Bifurcation of nonlinear bound states in the periodic Gross-Pitaevskii equation with PT-symmetry. *Proc. R. Soc. Edinb. A* (2020), 150, 171–204.T. Dohnal and H. Uecker. Bifurcation of Nonlinear Bloch Waves from the Spectrum in the Gross-Pitaevskii Equation. *J. Nonlin. Sci.* (2016), 26, 581–618.T. Dohnal, A. Lamacz, and B. Schweizer. Dispersive homogenized models and coefficient formulas for waves in general periodic media. *Asymptotic Analysis* (2015), 93, 21–49.T. Dohnal, M. Plum and W. Reichel. Surface gap soliton ground states for the nonlinear Schrödinger equation. *Comm. Math. Phys.* (2011), 308, 511–542.

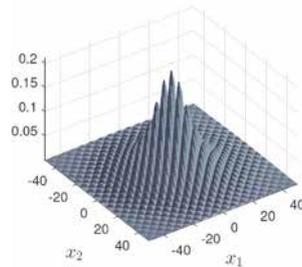
Institute of Mathematics

Applied Mathematical Analysis

Fields of Research:

- › Wave-packets in heterogenous media
- › Rigorous asymptotics of wave-packets, envelope equations
- › Bifurcation of nonlinear waves
- › Waves in periodic media and at interfaces

Propagation of waves in heterogenous media, along interfaces or through media with defects is of importance in various physical applications ranging from electromagnetic waves (e.g. in photonic crystals) to elastic waves or density waves. Physically most relevant are finite energy waves. These can exist in the form of pulses, i.e. wave-packets.

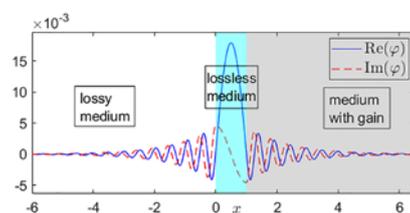


wave-packet in a 2D periodic medium,

(T. Dohnal and D. Rudolf, *Appl. Ana.* 99, 1685–1723, 2020)

Wave propagation is typically dispersive which leads to a delocalization of wave-packets. This can be, however, balanced by an intrinsic nonlinearity. A typical task in the analysis of nonlinear wave-packets is their approximation on asymptotically large time scales via a slowly varying envelope ansatz. A rigorous justification of such an approximation involves proving a well-posedness of the (nonlinear) error equation and careful estimates of the residual.

In special cases standing or moving solitary waves exist. These correspond to a balance between the dispersion and the nonlinearity. Their existence can be typically shown via a bifurcation analysis or via variational methods, e.g. energy minimization via concentration compactness. Such solitary waves are usually found in spectral gaps and are then called gap solitons. Their bifurcation analysis from spectral edges relies on a restriction to a symmetry subspace, like, e.g., the parity-time-symmetric subspace: $\varphi(-x) = \overline{\varphi(x)}$.



PT-symmetric solution of the Gross-Pitaevskii eq

Current Projects and Future Goals:

Surface Plasmon Wave-Packets in Nonlinear Media

Surface plasmons are electromagnetic waves at interfaces of metal and dielectric material layers. Due to the extremely tight localization to the interface these are often applied in nano-photonics and could once play a role as bit carriers in optical computing. In the presence of nonlinearity surface plasmon pulses are possible.

Being governed by the (vector valued) quasi-linear Maxwell equations in two or three dimensions, it is of importance to find simpler approximate envelope equations for such pulses. This is typically the Ginzburg-Landau equation.

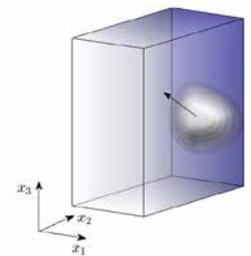
The justification of the approximation requires showing long time well-posedness of the quasi-linear Maxwell problem. Moreover, the response of the metal to the field is time-delayed as well as lossy, resulting in the Maxwell system being non-local in time and the spatial operator being non-self-adjoint. A boot strap argument can be used for the well-posedness on large time intervals for small initial data.

Spectral Analysis of Surface Plasmons

Eigenvalues of the Maxwell problem in frequency domain for the metal dielectric interface correspond to linear surface plasmons. For the bifurcation analysis it is necessary to understand the whole spectrum of the problem. The analysis of the essential spectrum is an open problem. The spectral properties also depend on the geometry of the interface.

Gap Solitons in Maxwell Equations for Two Dimensional Photonic Crystals

In dielectric photonic crystals the spectrum is obtained by the Bloch analysis and typically includes spectral gaps. No bounded linear waves exist in these gaps but nonlinear gap solitons may be found. The bifurcation of these from spectral edges is governed by coupled mode equations describing the coupling of modulated linear Bloch waves at the spectral edge. The proof of the bifurcation can be obtained using a fixed point iteration for the Maxwell system in a suitable function space and a restriction to a symmetric subspace in order to avoid the kernel of the coupled mode linearization operator.

surface plasmon pulse
illustration

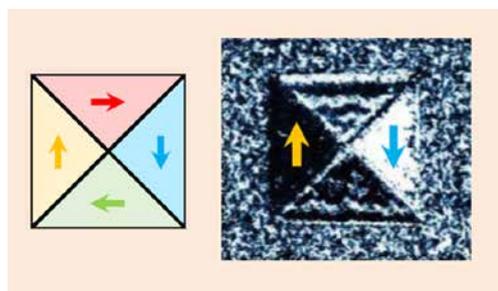
Institute of Physics

Functional Oxide Interfaces

Fields of Research:

- › Thin film epitaxy of oxide materials
- › Physics of transition metal oxides
- › Magnetism and Ferroelectricity
- › Domains in ferroelectric materials

Our research is aimed at the fundamental understanding of ferroic ordering and switching in thin films, at interfaces, in nanostructures and bulk materials. Ferroics are materials with a switchable magnetic, electric or elastic polarization. They find wide-spread application in data storage, as sensors and actuators. The properties of thin films can be controlled utilizing interface effects and elastic strain. One major goal of our research is the discovery of strain-driven effects. In-situ dynamic strain control is realized by using piezoelectric monocrystalline substrates. The approach gives access to direct measurements of strain-dependent electronic and optical properties. Thin films are grown by pulsed laser deposition (KrF 248 nm). Structural analysis is done by (in-house or synchrotron-based) x-ray diffraction.

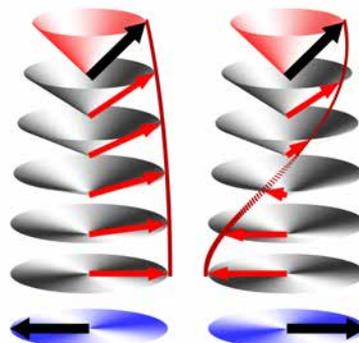


Ferroelectric Landau domain pattern of in-plane polarization written mechanically in a P(VDF-TrFE) polymer film on graphite. Writing with a force microscopy tip is based on the ferroelastic effect.

Current Projects and Future Goals:

■ Non-collinear interface magnetism in oxides

Interfaces of ferromagnetic oxides of ABO₃ (perovskite) type are promising for the formation of non-trivial spin textures. An example of a spin spring is shown in Fig.1. Strong exchange coupling and lattice distortions govern magnetic anisotropy and spin textures in ways unknown from metals. Novel transport phenomena beneficial for spintronics applications are expected from such oxide thin film systems with engineered interface magnetism.



Switchable spin spring at an epitaxial interface of ferromagnetic oxides (Das 2019).

■ Ferroelastic domain manipulation in polymers

The flexibility of ferroelectric polymers has recently been discovered to enable domain manipulation by tip-induced mechanical strain in a force microscope (Roth 2018). Strain-driven alignment of electric polarization vitally improves the electric performance parameters such as piezoelectric and dielectric coefficients. Fig.2 shows a Landau domain with in-plane polarization aligned in four directions in a P(VDF-TrFE) film.

■ Oxide interfaces with strong spin orbit coupling

Antiferromagnetic oxides offer fascinating options for ultrafast optical spin control using light / electromagnetic radiation from the visible to the THz range. While early experiments relied on single-crystalline samples, the advances of oxide epitaxy open pathways for domain control and for the growth of materials previously inaccessible in required quality.



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Selected publications:

S. Das et al., Low-field switching of non-collinear spin texture at La_{0.7}Sr_{0.3}MnO₃-SrRuO₃ interfaces, Phys. Rev. B 99, 024416 (2019).

A. Herklotz et al., Designing morphotropic phase composition in BiFeO₃, Nano Lett. 19, 1033 (2019).

R. Roth et al., Aligning in-plane polarization multiplies piezoresponse in P(VDF-TrFE) films on graphite, New J. Phys. 20, 103044 (2018).

E. J. Guo et al., Ferroelectric 180° domain wall motion controlled by biaxial strain, Adv. Mater. 27, 1615 (2015).

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1987

Dr.-Ing. in Chemical Process Engineering, Universität Karlsruhe (TH), Germany

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Selected publications:

F. Marske, J. Martins de Souza e Silva, R. B. Wehrspohn, T. Hahn, D. Enke, Synthesis of monolithic shape-stabilized phase change materials with high mechanical stability via a porogen-assisted in situ sol/gel process RSC Adv., 10 (2020), 3072.

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Institute of Chemistry

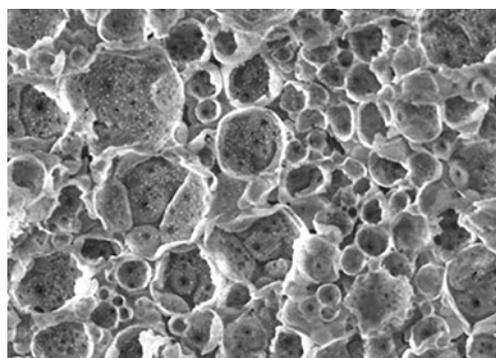
Industrial Chemistry

Fields of Research:

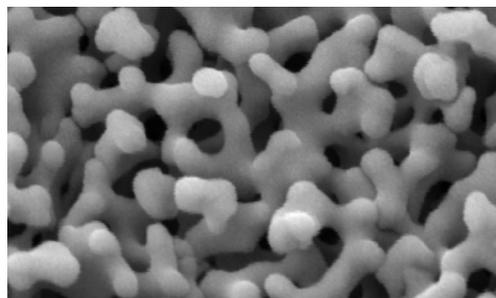
- › Preparation and characterisation of porous materials and catalysts
- › Reaction engineering – coupling of transport properties and chemical reaction

More than 85% of the products of chemical industry are made in catalytic processes. Especially solid catalysts are indispensable for fuel production, bulk and fine chemicals and abatement of pollution in end-of-pipe processes.

Our activities in the field of catalysis starts with the synthesis of nanoscale catalytically active materials but also includes the formulation and shaping of different porous solids and catalysts for use in an industrial reactor, their functional characterisation and the assessment of transport and reaction kinetics. We explore novel processing options experimentally and by using modeling and simulation tools. Reactions under study are diverse, however, (partial) oxidation and acid-base reactions play a major role.



shape-stabilized PCM



Controlled pore glass CPG (Enke, Dirk: "Über die anwendungsbezogene Charakterisierung von Katalysatorträgern", Habilitationsschrift, Martin Luther University Halle-Wittenberg, 2005)

Current Projects and Future Goals:

■ Oxygen transfer reactions

Preparation of solid single or multi-component catalysts for partial/total oxidation reactions in gas or liquid phase especially for aromatic substrates, assessment of reaction kinetics (activity, selectivity, time on stream) and reaction networks for gas-phase reactions with/without oxygen spillover. In-situ characterization of active components by solid-electrolyte-potentiometry.

■ Optimisation of heterogeneous catalysts

Preparation, characterization and testing of nano- and mesoporous aluminate spinels for high-temperature reactions, for example dry reforming of methane.

■ Catalyst deactivation

Using local lignite for catalytic cracking with solid acid catalysts can only be cost-effective if the deactivated catalysts can be reactivated a sufficient number of times. Dependent of cracking conditions the physical blocking of the catalyst by "coke" mainly takes place at the outer surface of the catalyst body and/or inside the porous structure. This can be differentiated by use of physical characterization and model reactions with substrates of different molecule size to give hints for an optimized regeneration procedure.

■ Thermal energy storage materials

Monolithic shape-stabilized phase change materials (ss-PCMs) are one of the most promising materials to store large amounts of solar energy, waste heat and off-peak electricity as heat in energy-saving buildings, photovoltaics and water-heating systems. However, more than 15 wt% PCM in ss-PCMs leads to a loss of the monolithic form, low mechanical stabilities and PCM leakage problems. To overcome these problems, over 60 wt% PCM are incorporated in situ in a highly mechanical stable silica matrix by a sol-gel synthesis. Pore size effects on physicochemical properties are analyzed.

■ Investigation of phase formation in silica-free glasses and glass-ceramics in the Na₂O-B₂O₃-M_xO_y (M = Fe, Ti) system

Fundamental studies of the Na₂O-B₂O₃-M_xO_y (M = Fe, Ti) system concerning the complex relationships between initial glass composition, crystallization conditions, structure formation mechanisms and properties of the resulting porous glass-ceramics. The aim is to prepare porous and mechanically stable titanium oxide- and/or iron oxide-based glass-ceramic monoliths. Further systematic investigations regarding the control of morphology and the crystallizing species.

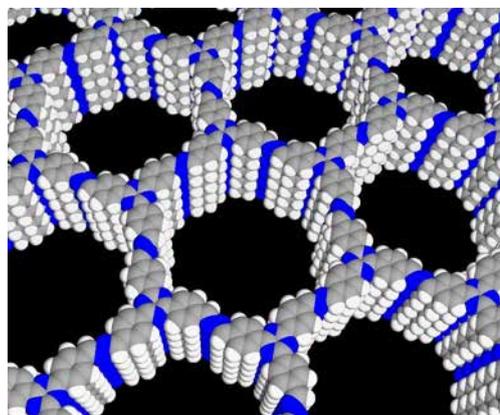
Institute of Chemistry

Reticular Materials

Fields of Research:

- › Preparation and characterization of crystalline and porous organic and hybrid materials.
- › Characterization of disorder and real structure
- › Solid state transformations

Typical solid-state chemistry is dominated by crystalline materials that are typically formed directly from the elements under thermodynamic equilibrium. This critically limits rationally approaching the design and synthesis of new materials. In our group we work on a class of materials, where exceptional control over the material structure and composition is possible due to a netlike structure. These reticular materials are built from organic building blocks that are either combined with metal organic nodes to form metal organic frameworks (MOFs) or with reversible covalent linkages to form covalent organic frameworks (COFs). By using rigid building blocks with strong directional bonding between them crystalline porous and highly functional materials can be obtained.



Example of a covalent organic framework constructed from a trialdehyde building block and hydrazine.

Our focus is on controlling and understanding the assembly pathways leading to higher crystallinity or to introduce new functionality. The structures of reticular materials can be directly traced back to the geometry, shape and properties of the organic building blocks. We therefore use creative chemistry, to design new building blocks and thereby structures. Due to the difficulty growing single crystals of reticular materials we also extensively rely on characterization techniques to solve the structures of reticular materials such as powder X-ray diffraction, single crystal X-ray diffraction and collaborate for transmission electron microscopy and solid-state NMR.

Current Projects and Future Goals:

Frustrated assembly

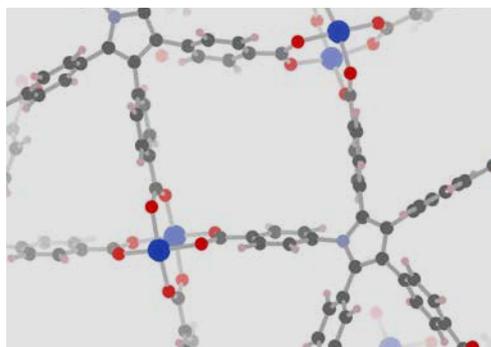
The excellent building block control in reticular materials are normally used to design clearly determined assembly pathways towards designing synthesis outcomes. The opposite approach is also possible where we create intentionally frustrated systems, which lead to emergent behavior and complexity that can be used as a design tool itself. Frustration is achieved by designing building blocks whose local geometry or symmetry is not compatible with forming extended structures.

Topochemical reactions

Reticular materials are typically porous materials and therefore their internal structure is accessible to perform reactions on the pore walls and linker backbones. Together with a straightforward design process, this enables the modification of the structures after their synthesis. By chemically manipulating the backbone of reticular materials the structure and properties of the material can be strongly affected leading to highly stable materials.

Novel pathways to covalent solids

Covalently bonded materials are interesting materials due a range of properties such as chemical, mechanical and thermal stability, electronic properties, and their variability and design. While these properties are inherent to covalent materials, in materials available through current synthesis pathways many of these properties are lost. Therefore, novel synthesis pathways for covalent materials are needed to fully reap their potential.



Detail of a frustrated metal organic framework constructed from copper ions and organic pseudo-five-fold-symmetrical building blocks



Prof. Dr. Frederik Haase

2018

PhD in Chemistry with Prof. B.V. Lotsch at the Max-Planck Institute for Solid State Research, Stuttgart, Germany and Ludwig-Maximilians University of Munich, Germany

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JSPS Postdoctoral fellow with Prof. S. Furukawa at Kyoto University, Japan

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Selected publications:

F. Haase et al., Pseudo-5-Fold-Symmetrical Ligand Drives Geometric Frustration in Porous Metal-Organic and Hydrogen-Bonded Frameworks *J. Am. Chem. Soc.* 2020, 142, 32, 13839-13845

F. Haase and B. V. Lotsch, Solving the COF trilemma: towards crystalline, stable and functional covalent organic frameworks *Chem. Soc. Rev.*, 2020, 49, 8469-8500

F. Haase et al., Topochemical conversion of an imine- into a thiazole-linked covalent organic framework enabling real-structure analysis *Nat. Comm.* 2018, 9:2600.



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Selected publications:

Maria Soledad Aronna, Joseph Frédéric Bonnans, and Axel Kröner, Optimal control of PDEs in a complex space setting; application to the Schrödinger equation, *SIAM Journal on Control and Optimization*, 57(2), 1390-1412, 2019.

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Axel Kröner, Athena Picarelli, and Hasnaa Zidani, Infinite horizon stochastic optimal control problems with maximum cost, *SIAM Journal on Control and Optimization*, 56(5), 3296-3319, 2018.

Axel Kröner, Karl Kunisch, and Boris Vexler, Semismooth Newton methods for optimal control of the wave equation with control constraints, *SIAM Journal on Control and Optimization*, Vol. 49(2), 830-858, 2011.

Institute of Physics

Optimization

Fields of Research:

- › Optimization of PDEs
- › Optimal control of fluid-structure interactions
- › Feedback control
- › Numerical simulation

Optimization/optimal control with partial differential equations (PDEs) and systems of PDEs has many applications in physics and engineering. A classical problem formulation is to identify a control which drives the state of a underlying physical process close to a desired one, as, e.g., when controlling the temperature during a cooling process or when reducing and controlling the vibration of a plate. That means mathematically, one tries to minimize a cost functional under a constraint given by a PDE or coupled system. Often the cost functional contains a tracking type term for the state and a second term representing the cost for using the control. Additionally further constraints on the state or the control might be imposed as well as additional terms inducing, e.g., sparsity. Main challenges in the theoretical analysis of these problems are the derivation of existence of solutions, to prove differentiability properties of control-to-state mappings, optimality conditions of first and second order for characterizing optimal controls as well as to develop and analyze efficient numerical algorithms to solve these problems taking the specific structure of the problem into account.

Current Projects and Future Goals:

■ **Optimal control of fluid-structure interaction problems**

This research topic addresses fluid-structure interaction problems when a fluid flows in a channel around an elastic obstacle which deforms under the flow.

By controlling the inflow the hydrodynamic pressure at the elastic body should be minimized. Challenges in the theoretical analysis arise here in particular due to corners in the flow domain and in the analysis of the unsteady case.

■ **Data-driven optimization with hybrid partial differential equations**

When the full physical understanding of a problem is unknown, data-driven models allow to include further information in the model to improve the mathematical description of the underlying process. Moreover, in contrast to mathematical models based on first principles, these hybrid models often allow a less complex and less time consuming adaptation to other problem settings. In this research project we consider optimal control problems for these type of systems and analyze them theoretically as well as their numerical performance.

■ **Feedback control of nonsmooth processes**

From an engineering perspective often one is less interested in finding an optimal control for a specific setting but rather to find a control in feedback form which can react to changes in the data or perturbations of the system which have not been included in the model a priori. While for smooth problems many contributions have been made, less is available for nonsmooth problems. In this project we consider a special problem class, namely nonsmooth processes given as (parabolic) variational inequalities. The aim is to derive feedback controllers and analyze their properties theoretically and numerically.

Institute of Mathematics

Numerical Methods for Stochastic Differential Equations

Fields of Research:

- › Numerical analysis of stochastic evolution equations
- › Galerkin finite element methods for stochastic partial differential equations
- › Randomized schemes for rough differential equations
- › Monte Carlo methods for non-smooth problems
- › Stability, complexity and error analysis

Evolution equations are a powerful and well-established tool to model highly complex phenomena in physics, chemistry, biology, medicine and the engineering disciplines. Important examples include the porous media equation in fluid mechanics, the Cahn-Hilliard equation in metallurgy, or the FitzHugh-Nagumo equation in neuroscience. Stochastic evolution equations have attracted a lot of attention in various mathematical fields such as stochastic analysis, numerical analysis and PDE theory over the last decades. In Uncertainty Quantification, for instance, one introduces random coefficients or stochastic perturbations into evolution equations to model incomplete knowledge of parameter values or measurement errors. Other processes, such as the motion of a Brownian particle suspended in a moving fluid or the production, transport and consumption of renewable energy, are intrinsically random and directly modeled by stochastic differential equations.

In most cases, the presence of stochastic noises leads to a low regularity of the exact solution. In particular, a solution to a stochastic differential equation is typically nowhere differentiable. Their mathematical solution therefore requires the development of novel analytical tools. In addition, the accuracy and performance of numerical methods is often affected severely. Due to the low regularity, standard approaches to construct efficient numerical methods, e.g. Runge-Kutta methods, are often intractable and their speed of convergence is typically reduced drastically.

The overall goal of the research activities therefore consists in the design and the analysis of more efficient numerical methods for the simulation of evolution equations with random or stochastic perturbations.

Current Projects and Future Goals:

■ Galerkin finite element methods for stochastic evolution equations

Numerical methods for stochastic evolution equations in infinite dimensions (such as the stochastic heat or wave equation) are investigated. The goal is to design more efficient methods by better intertwining different strategies, which are used for the discretization of the evolution equation with respect to the spatial or temporal variables. For instance, we aim to better integrate the Euler-Maruyama method and Galerkin finite element methods with Monte-Carlo methods by making use of adaptive strategies, the multi-level Monte Carlo approach or sparse grid techniques.

■ Quasi-linear stochastic partial differential equation

In recent years, there has been a considerable progress in the analysis of quasi-linear stochastic partial differential equations, e.g., the stochastic porous media equation, based on the application of variational methods. We examine if these analytical tools can be adapted to also perform an error and stability analysis of associated numerical methods for these problems.

■ Randomized numerical methods for rough differential equations

It is already well-known that by randomizing quadrature rules one can combine the benefits of Monte Carlo methods with those of classical numerical integration methods. For instance, the randomized Riemann sum has a higher order of convergence than the deterministic Riemann sum or the standard Monte Carlo method without increasing the smoothness requirements on the integrand. In this project we study how this result can be extended to develop novel numerical methods for non-smooth, stochastic or rough differential equations.



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2008

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Selected publications:

M. Eisenmann, M. Kovács, R. Kruse, S. Larsson, On a Randomized Backward Euler Method for Nonlinear Evolution Equations with Time-Irregular Coefficients. *Found Comput Math* 19, 1387–1430 (2019).

W.-J. Beyn, E. Isaak, R. Kruse, Stochastic C-Stability and B-Consistency of Explicit and Implicit Milstein-Type Schemes. *J Sci Comput* 70, 1042–1077 (2017).

R. Kruse, Consistency and stability of a Milstein-Galerkin finite element scheme for semilinear SPDE. *Stoch PDE: Anal Comp* 2, 471–516 (2014).

R. Kruse, Strong and Weak Approximation of Semilinear Stochastic Evolution Equations. *Lecture Notes in Mathematics*, Vol. 2093, Springer, (2014).



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Selected publications:

B. Göbel, A. Mook, J. Henk, and I. Mertig, Antiferromagnetic skyrmion crystals: Generation, topological Hall, and topological spin Hall effect. *Phys. Rev. B* 96, 060406(R) (2017).

A. Mook, J. Henk, and I. Mertig, Edge states in topological magnon insulators. *Phys. Rev. B* 90, 024412 (2014).

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M. Fechner, I. V. Maznichenko, S. Ostanin, A. Ernst, J. Henk, P. Bruno, and I. Mertig, Magnetic phase transition in two-phase multiferroics predicted from first principles. *Phys. Rev. B* 78, 212406 (2008).

V. V. Maslyuk, A. Bagrets, V. Meded, A. Arnold, F. Evers, M. Brandbyge, T. Bredow, and I. Mertig, Organometallic benzene-vanadium wires: A one-dimensional half-metallic ferromagnet. *Phys. Rev. Lett.* 97, 097201 (2006).

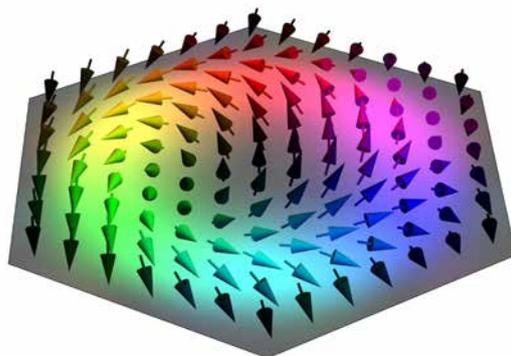
Institute of Physics

Quantum Theory of the Solid State

Fields of Research:

- › **Multiferroics and magnetoelectric coupling**
- › **Spintronics**
- › **Topological properties in solids**

Our activities are attached to the quantum theoretical description of solids based on density functional theory. This means that we start to model our systems at the atomic level, do not take any free parameter into account, and solve the Schrödinger and other relevant equations to obtain finally a macroscopic property that can be measured. To support the experimental developments, to predict new materials for future applications, and to optimize the effects under consideration, first-principle electronic structure calculations are the most powerful tool. In this way, we gain insight into the microscopic origin of macroscopic properties of metals, semi-conductors, and insulators in their 3D bulk formation or as 2D surfaces and interfaces and 1D wires. The underlying methods are particularly useful to describe nanostructures of realistic dimension up to thousands of atoms. The formalism is based on Green functions for the equilibrium and the non-equilibrium state. We are particularly qualified for the ab initio description of transport properties in the coherent limit based on Landauer theory and in the diffusive limit based on Boltzmann theory. In general, our theory is material specific and has a strong overlap with experiments.



Bloch skyrmions – magnetic whirls in a solid

Current Projects and Future Goals:

■ **Multiferroics and magnetoelectric coupling**

Multiferroic materials are particularly interesting since they show a spontaneous magnetisation and a spontaneous polarisation in one and the same system. The interaction of magnetisation and polarisation is called magnetoelectric coupling which offers the opportunity that magnetic information can be influenced by an electric field and vice versa. This is a very attractive concept for memory technology. We consider in particular multiferroic interfaces which occur in artificially grown heterostructures and separate a ferroelectric from a ferromagnetic layer.

■ **Spintronics**

Spintronics is an emerging field based on the transport properties of electrons exploiting both their charge and spin degree of freedom. Most of the spintronic effects like giant magnetoresistance and tunneling magnetoresistance occur in magnetic materials and are widely used. The next step is the search for spintronic devices manipulating pure spin currents. They would play an important role in the next generation of low-energy-consumption electronics. Pure spin currents are generated by the spin Hall effect. We are looking for alloys with giant spin currents.

■ **Topological properties in solids**

The next generation of spintronic effects is based on spin currents which occur in metals as well as in insulators, in particular in topologically non-trivial materials. Spin currents are a response to an external stimulus – for example an electric field or a temperature gradient. Topological properties are always related to spin-orbit interaction and cause a whole zoo of transversal transport coefficients: the trio of Hall, Nernst, and quantum Hall effects, all in their conventional, anomalous, and spin flavour. They offer the possibility for future low-energy-consumption electronics.

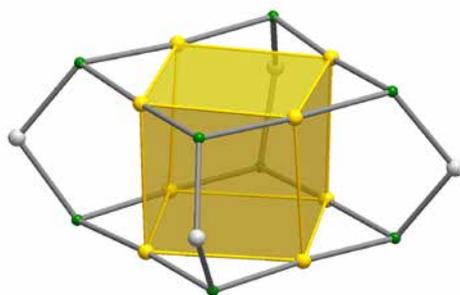
Institute of Chemistry

Molecular and Structural Chemistry

Fields of Research:

- › Main group element chemistry
- › Coordination and cluster chemistry
- › X-Ray crystal structure analysis
- › Metal complexes and clusters with functionalized silylamido ligands
- › Structural chemistry of metal amides
- › Donor-functionalized 2,4-pentandionate ligands

A main part of our research interests is located at the interface between main group and transition metal chemistry. At the beginning, the research was focused on mixed main group/transition metal cluster compounds like $[(\text{Cp}(\text{CO})_2\text{Fe})_4\text{Sn}_4\text{E}_6]$ ($\text{E} = \text{S}, \text{Se}, \text{Te}$) and the employment of the related thioannates $\text{R}_2\text{SnS}_3^{3-}$ as building blocks for heteronuclear clusters like $[(\text{R}_2\text{SnS}_3)_2(\text{CuPR}'_3)_2]$. In order to extend and thus generalize this approach of cluster synthesis, analogous trifunctional silylamido ligands $\text{RSi}(\text{NR}')_3$ and difunctional derivatives $\text{R}_2\text{Si}(\text{NR}')_2$ were applied. This led to the discovery of hitherto unknown copper(I) silylamido clusters with up to 12 copper atoms, e.g. $[\text{Cu}_8\{\text{Me}_2\text{Si}(\text{NPh})_2\}]$, $[\text{Cu}_9\{\text{MesSi}(\text{NPh})_2(\text{PhCO}_2)\}]$, and $[\text{Li}(\text{THF})_4]_2[\text{Cu}_{12}\{\text{MeSi}(\text{NPh})_2\}_4]$. Generally, Cu(I) silylamides exhibit extreme air and moisture sensitivity along with very low thermal stability. In order to improve the thermal stability and to ease the accessibility of Cu(I) and other metal derivatives, silylamido ligands bearing auxiliary donor groups were developed. Particularly the introduction of thioether functionalities opened the door to new types of silylamido cluster compounds. Ligand improvement and optimization is by no means limited to the silylamido area. The concept of side-arm functionalization can be also applied for classical ligands like amides, amidines and acetylacetonates in order to design new coordination patterns. Some years ago this approach was used to modify acetylacetonato ligands with chiral amino acid units. Furthermore, donor-functionalized amides of alkali metals and copper(I) were studied.



Central core of the cluster
 $[\text{Cu}_8\{\text{Me}_2\text{Si}(\text{NPh})_2\}]_4$

Current Projects and Future Goals:

Metal complexes and clusters with functionalized silylamidoligands

Currently, this work concentrates on the investigation of low valent Cr(II), Mo(II) and V(II) compounds. The first results in the case of Mo(II) have shown, that silylamido ligands support the formation of Mo-Mo multiple bonds along with Mo clusters, depending on the nature of the silylamido ligand. According to preliminary tests, Mo(III) silylamides display catalytic activity towards cyclotrimerization of isocyanates. The field of Cr(II) and V(II) complexes with $\text{R}_2\text{Si}(\text{NR}')_2$ ligands is practically unexplored, probably due their extreme air and moisture sensitivity. The goal of this project is to provide an access to this class of compounds using "tailor made" silylamido ligands with OR, NR_2 , PR_2 and N-heterocyclic carbene (NHC) functionalities. Apart from the synthetic challenge, this study is designed to give insight into the magnetic behavior of low-valent Cr and V complexes and the formation of metal-metal bonds.

Structural chemistry of metal amides

Nitrogen ligands like amides and imides are of considerable interest in coordination chemistry, both of main group and transition metals. In the case of main group elements our research is focused on alkali metal and group 14 element (Ge(II), Sn(II)) derivatives of anilides bearing additional donor functions OR, NR_2 , SR and PR_2 . Typically, the solid state structure of sodium and potassium anilides are characterized by extended 3D structures, and in contrast to this Ge(II) and Sn(II) derivatives tend to form molecular heterocubane-type clusters $[\text{M}_4(\text{NR})_4]$. In the case of related Cu(I) compounds, cluster complexes like $[\text{Cu}_6\text{X}_2(\text{NHR}')_4]$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}; \text{R}' = \text{C}_6\text{H}_4\text{-}2\text{-PPh}_2$) dominate. Currently, the investigation of the structure directing influence of the OR, SR, NR_2 and PR_2 functionalization is in focus.

Donor-functionalized 2,4-pentandionate ligands

Acetylacetonate ligands are widely used in coordination chemistry. The reaction of 3-formylacetylacetonone with OR, SR or PR_2 functionalized anilines provides a synthetic path to novel tridentate ligands with N,O,X donor sets ($\text{X} = \text{O}, \text{S}, \text{P}$). First studies on this type of N,O,P-ligands revealed a pincer-type coordination mode in octahedral complexes of Fe^{2+} , Mn^{2+} , Ni^{2+} . In the last years, pincer type ligands have attracted growing interest due to their application in homogenous catalysis. A future goal in this project is the synthesis of pincer-type hybrid ligands combining the coordination properties of acetylacetonates and N-heterocyclic carbenes (NHC).



Prof. Dr. Kurt Merzweiler

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 PhD in Inorganic Chemistry,
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 Habilitation, University of
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 Full Professor (C3) of Inorganic
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Selected publications:

U. Morgenstern, C. Wagner, K. Merzweiler. Dinuclear Molybdenum(II) Complexes with Thioether Functionalized Silylamido Ligands. *Z. Anorg. Allg. Chem.* 2019, 645, 1.

R. Albrecht, P. Liebing, U. Morgenstern, C. Wagner, K. Merzweiler. Ni(II) complexes with thioether-functionalized silylamido ligands. Synthesis and crystal structures of $[\text{Ni}\{\text{Me}_2\text{Si}(\text{N-C}_6\text{H}_4\text{-}2\text{-tBu})_2\}]$, $[\text{Ni}\{\text{Ph}_2\text{Si}(\text{N-C}_6\text{H}_4\text{-}2\text{-SMe})_2\}]$ and $[\text{Ni}\{\text{Ph}_2\text{Si}(\text{N-C}_6\text{H}_4\text{-}2\text{-SPh})_2\}]$. *Z. Naturforsch. B.* 2019, 74, 233.

U. Morgenstern, C. Wagner, K. Merzweiler. Synthesis and crystal structure of the copper silylamido cluster compound $[\text{Cu}_8\{\text{MesSi}(\text{NPh})_2(\text{PhCO}_2)\}]$. *Z. Naturforsch. B.* 2018, 11, 953.

P. Liebing, K. Merzweiler. Gold(I) and Silver(I) Complexes with Thioether Functionalized Silylamido Ligands. *Z. Anorg. Allg. Chem.* 2017, 643, 1220

C. Wagner, K. Merzweiler. Novel Dinuclear Tin(II) and Lead(II) Compounds with 2-Pyridyl Functionalized Silylamido Ligands. *Z. Anorg. Allg. Chem.* 2017, 643, 938.

P. Liebing, J. Freudenberg, C. Heiser, K. Merzweiler. Novel Copper(I) Clusters with 2-(Diphenylphosphanyl)anilide Ligands. Synthesis and Crystal Structures of $[\text{Cu}_4\text{X}_2(\text{NHR}')_4]$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}; \text{R}' = \text{C}_6\text{H}_4\text{-}2\text{-PPh}_2$). *Z. Anorg. Allg. Chem.* 2017, 643, 203.



Prof. Dr. Stuart Parkin
Alexander von Humboldt Professor

1981
PhD in Physics (University of Cambridge, UK)

1980-1981
PostDoc (Université Paris-Sud, France)

1981
PostDoc (IBM San Jose Research Laboratory, USA)

1982-2014
IBM Almaden Research Center, San Jose, USA
- Research Staff Member
- IBM Fellow (since 1999)
- Manager of Magnetoelectronics Group (since 1999)

since 2014
Director (Max Planck Institute of Microstructure Physics, Halle, Germany) and Alexander von Humboldt Professor (MLU)

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Selected publications:

J. Jeong, N. Aetukuri, T. Graf, T. D. Schladt, M. G. Samant, and S. S. P. Parkin; Suppression of Metal-Insulator Transition in VO₂ by Electric Field-Induced Oxygen Vacancy Formation *Science* 339, 1402 (2013)

H. Yang, S.-H. Yang, S. Takahashi, S. Maekawa, and S. S. P. Parkin; Extremely long quasiparticle spin lifetimes in superconducting aluminium using MgO tunnel spin injectors *Nat. Mater.* 9, 586 (2010)

S. S. P. Parkin, M. Hayashi, and L. Thomas; Magnetic Domain-Wall Racetrack Memory *Science* 320, 190 (2008)

L. Thomas, M. Hayashi, X. Jiang, R. Moriya, C. Rettner, and S. S. P. Parkin; Oscillatory dependence of current-driven magnetic domain wall motion on current pulse length *Nature* 443, 197 (2006)

S. S. P. Parkin; Systematic variation of the strength and oscillation period of indirect magnetic exchange coupling through the 3d, 4d, and 5d transition metals *Rev. Lett.* 67, 3598 (1991)

Max Planck Institute of Microstructure Physics

Experimental Department II

Fields of Research:

- › Spintronics
- › Oxides and Interfaces
- › Atomically engineered materials
- › Computational Materials Discovery
- › Cognitive Devices and Bio-Inspired Materials

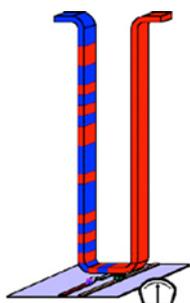
Current Projects and Future Goals:

Spintronics

Spintronics is a field of research that comprises the generation, manipulation and detection of spin-polarized electrons in a wide range of materials including metals, insulators, and semiconductors. The most important spintronic materials are composed of artificially engineered atomically layered magnetic thin film structures with spin-dependent transport properties. The use of both spin-polarized charge currents and pure spin currents, generated by electric voltages, temperature gradients and / or optical means, to excite and manipulate magnetic moments is of great interest from both fundamental and technological perspectives. Spin-orbit interaction is a principle driving mechanism behind many topical phenomena including spin-orbit torques, current driven domain-wall motion, perpendicular magnetic anisotropy, spin Hall effect, anomalous and topological Hall effects, and topological magnetic structures including skyrmions.

Oxides and Interfaces

Complex oxides display an enormous variety of properties, ranging from insulators to metals and superconductors, from anti-ferromagnetism to ferromagnetism, and ferroelectric to paraelectric to name just a few. By forming heterostructures between thin films of distinct oxides, novel materials can be engineered with functionalities that are not otherwise seen in the individual materials. One example are magneto-electric phenomena in which magnetic fields can influence ferroelectric behavior or electric fields can control magnetic behavior.



A vertical-configuration racetrack offers the highest storage density by storing the pattern in a U-shaped nanowire normal to the plane of the substrate.

Atomically engineered materials

Experimental methods to deposit layers just one atom or one unit cell thick include physical methods, such as molecular beam epitaxy, pulsed laser deposition and magnetron and ion beam sputtering, as well as chemical methods such as atomic layer deposition and chemical vapor deposition. Theoretical methods to simulate the growth of such materials and to calculate their properties are powerful and accurate enough that, by using these methods in tandem with experiment, rapid advances in atomically engineered materials with novel and technologically relevant properties is currently possible. Atomically engineered materials underpin the fields of spintronics, oxide electronics, cognitive devices and routes to room temperature superconductors.

Computational Materials Discovery

The theoretical modelling of structure-property relationships from the nano- to the meso-scale requires the synergistic use of various simulation methodologies. Electronic and magnetic properties of, e.g., molecules, nano-wires or oxide layers are studied by quantum mechanical methods, via the development and application of electronic density functional techniques. Molecular arrangements and properties on longer length scales of, e.g., macromolecules or magnetic model systems, are studied by Molecular Dynamics and Monte Carlo techniques. Heterogeneous structures on still larger scales are mapped onto field-theoretical descriptions and treated with tools of numerical mathematics. Different techniques are used to bridge multiple time- and length-scales to characterise and understand the functions of complex structures. The use of such computational methods to explore and predict the properties of novel, engineered materials is an emerging discipline of considerable current interest.

Cognitive Devices and Bio-Inspired Materials

It is clear that nature has devised methods of preparing materials that we can't yet replicate and with properties that we can't yet match. However, the very existence of such biological materials and functionalities serves as inspiration for research into novel ways of manufacturing materials and fabricating devices with such properties. A very important area of research is the development of cognitive computing devices that could support novel computing architectures that could carry out computations a million times more efficiently than conventional charge based devices.

Institute of Mathematics

Applied Stochastics

Fields of Research:

- › Numerical Approximations to Rough/ Stochastic Partial Differential Equations
- › Lévy Processes
- › Stochastic Differential Equations/Stochastic Evolution Equations
- › Model Reduction for Stochastic Systems
- › Galerkin Schemes for Controlled Stochastic Partial Differential Equations with Lévy Noise

The focus of our research is on stochastic (partial) differential equations (S(P)DEs) and at the interface of analysis, numerics and stochastics.

In particular, efficient solution algorithms for S(P)DEs are investigated and applications with uncertainties in other natural sciences are modeled by S(P)DEs. This provides links to other disciplines like chemistry and physics as, e.g., in the field of molecular dynamics or in materials science (data-based modeling and simulation of phenomena under uncertainties: optimization of model parameters; high-dimensional simulation; model reduction).

Current projects of this group deal with the analysis and the numerical approximation of stochastic (partial) differential equations that can, e.g., be used in the context of modeling materials and their properties.

Current Projects and Future Goals:

■ Discretizing Rough/Stochastic (Partial) Differential Equations

Rough/Stochastic (Partial) Differential Equations can be used to model applications in different areas. Usually they cannot be solved analytically. Therefore, we investigate and generalize numerical approximation schemes (like finite element methods or Runge-Kutta methods) for these equations and subsequently run simulations.

■ Model Order Reduction for Stochastic Systems

In many real life applications, large dimensional problem occur, especially when stochastic PDE models are discretized in space. We investigate and study methods to reduce the dimension of the problem leading to a lower computational complexity. We are mainly interested in non-linear stochastic systems which are reduced using, e.g., are the proper orthogonal decomposition, reduced basis methods or system-theoretic model reduction.

■ Option Pricing

We develop and study efficient algorithms to price, e.g., Bermudan or American options. We are particularly interested in problems where existing methods fail since they do not provide sufficiently accurate results. Moreover, we apply model order reduction to large-scale asset price models which allows to apply option pricing algorithms to the problem that are usually not feasible in high dimensions.

■ Solving High-Dimensional Partial Differential Equations

These equations have applications, e.g., in molecular dynamics and it is usually very complicated to solve them since finite element methods cannot be applied due to the curse of dimensionality. We aim to approximate high-dimensional PDEs by ones of low order. Here, model reduction for stochastic nonlinear systems becomes the key, because stochastic representations for the PDE solutions can be used.

The project deals with high dimensional partial differential equations that play a role in molecular dynamics and in finance, too.



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2012–2016

PhD student in mathematics, Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg

2016–2019

Postdoctoral researcher in mathematics, Weierstraß Institute for Applied Analysis and Stochastics in Berlin

2018–2019

Interim Professor, University of Southern Denmark (Odense): Department of Mathematics and Computer Science

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Selected publications:

M. Redmann, S. Riedel, Runge, Kutta methods for rough differential equations, Submitted 2020.

C. Bayer, D. Belomestny, M. Redmann, S. Riedel, J. Schoenmakers, Solving linear parabolic rough partial differential equations, *Journal of Mathematical Analysis and Applications*, 2020.

M. Redmann, Type II balanced truncation for deterministic bilinear control systems, *SIAM Journal on Control and Optimization*, 2018.

M. Redmann, Type II singular perturbation approximation for linear systems with Lévy Noise, *SIAM Journal on Control and Optimization*, 2018.

P. Benner and M. Redmann, Model Reduction for Stochastic Systems, *Stochastic Partial Differential Equations: Analysis and Computations*, 2015.

P. Benner, T. Damm, M. Redmann, and Y. R. Rodríguez Cruz, Positive Operators and Stable Truncation, *Linear Algebra and its Applications*, 2014.



Prof. Dr. Joachim Rieger

1988

PhD in Singularity Theory,
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1988–1989

Royal Society Fellowship,
University of Warwick, England

1989–1991

Postdoc, University of Karlsruhe

1992–1995

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Selected publications:

Baumers, H. and Dachs-Cadefau, F., Computing jumping numbers in higher dimensions, *Manuscripta Math.* 161 (2020), 35–59.

Domitrz, W. and Rieger, J.H., Volume-preserving subgroups of A and K and singularities in unimodular geometry, *Math. Annalen* 345 (2009), 783–817.

Rieger, J.H. et al., M -deformations of A -simple germs from \mathbb{R}^n to \mathbb{R}^{n-1} , *Math. Proc. Cambridge Phil. Soc.* 142 (2008), 181–195.

Carter, J.S., et al., A combinatorial description of knotted surfaces and their isotopies, *Advances Math.* 127 (1997), 1–51.

Rieger, J.H., On the complexity and computation of view graphs of piecewise smooth algebraic surfaces, *Phil. Trans. Royal Soc. London Ser. A* 354 (1996), 1899–1940.

Rieger, J.H., Families of maps from the plane to the plane, *J. London Math. Soc.* 36 (1987), 351–369.

Institute of Mathematics

Geometry

Fields of Research:

- › Singularities of mappings and of varieties (classification, deformations and invariants)
- › Applications of singularity theory (e.g. to differential geometry, topology and enumerative geometry)
- › Bifurcations in families of mappings on real algebraic sets, stratifications of bifurcation varieties
- › Computational aspects of invariants of ideals and modules

Singularity theory is concerned both with singularities of smooth mappings between (real or complex) manifolds and with singular points of varieties. Some of the principal questions in this field are the classification of singularities (up to various notions of equivalence), the study of invariants associated with a singularity, and the study of deformations of singularities (which singularities are stable and persist under small deformations, which stable singularities can appear in a deformation of a given unstable singularity?). The most classical singularities are the stable critical points of a smooth real-valued function on a manifold: by a non-linear change of coordinates (a diffeomorphism) the function near each critical point can be transformed to a sum of squares in the variables (with coefficients +1 and -1), and it is known from Morse theory that the critical points provide a lot of information about the manifold. The more recent work on singularities arising in the more general context of smooth mappings and varieties has similar applications in other areas of mathematics.

Our group is working on the classification of singularities of mappings, on subgroups of the group of diffeomorphisms preserving some additional structure (e.g. some volume form), on the use of invariants for equisingularity problems, and on deformations of singularities. We are also interested in applications of singularity theory to differential geometry, to low dimensional topology (knotted surfaces) and to enumerative questions in projective algebraic geometry.

Current Projects and Future Goals:

Classification of singularities

Most of the classifications of mappings from n -space to p -space have been carried out for particular pairs (n, p) of dimensions, and either list the A -orbits up to a certain codimension or up to a certain modality (first the 0-modal, deformation finite, singularities, also known as simple singularities, next the uni-modal singularities, and so on). We want to extend these classifications in two directions. (1) We can relate the A -orbits of modality 0 for dimension pairs (n, p) on certain lines by three operations called extensions, suspensions and embedding. (2) We consider a certain subgroup $A(E)$, which replaces the right diffeomorphisms in the group A by diffeomorphisms preserving the exceptional divisor of the blowing-up of the source.

Invariants and deformations of singularities

For singularities of complex analytic mappings there are analytic and topological invariants describing the geometry and topology of the image or the discriminant of a stable deformation of an unstable singularity. And one wants to find formulas for these invariants e.g. in terms of certain multiplicities and also formulas relating various invariants. The constancy of these invariants in families plays a key role in equisingularity problems. Related are also invariants of complex (analytic and algebraic) varieties. For example, the jumping numbers associated to multiplier ideals of rational surface singularities.

Projections of algebraic surfaces

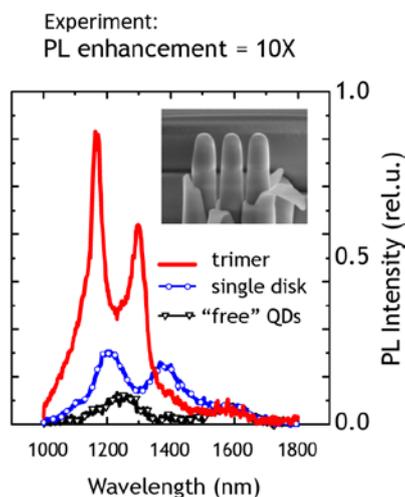
The projection of an algebraic surface M in a projective space P from a point c in M (or more generally from a linear subspace L which intersects M) is a map from the blow-up of M , rather than from M itself. In order to compactify the space of all projections of a given surface M one has to admit such inner projections of M from points c in M . Outer projections of M , from points c in the complement of M , are classified by A -equivalence. Inner projections, from points c in M , are classified by the refined $A(E)$ -equivalence. And the space P has a natural stratification by equisingularity strata of projections (the complement of M is stratified by A -types and M by $A(E)$ -types). And for a generic algebraic surface M of a given degree d one can study the enumerative geometry of this stratification of P .

Institute of Physics

Nonlinear Nanophotonics

Fields of Research:

The miniaturisation of light propagation on-chip and integration of a wide variety of optical processes in micro- and nanostructures represent an intriguing possibility for future optical information technology and sensing (“optics on the chip”). The research of the group focuses especially on the integration of active processes into silicon photonic structures by either trying to mould the optical properties of silicon itself or combining silicon with other materials resulting in hybrid photonic elements. For this, fundamental questions like light concentration, light-matter interaction in resonators and the control of optical dispersion in nanostructures play an important role. Furthermore plasmonic nanostructures consisting of more or less regular arrays of metal discs and wires are investigated as basis for surface enhanced Raman spectroscopy (SERS) and hyperbolic metamaterials offering the possibility to create artificial optical properties not found in nature. The design and simulation of the optical properties of the involved structures is based on commercial finite-element software. For experimental realisation and investigation the following methods are applied: electron beam lithography, focused ion beam milling, reactive ion etching, electrochemical etching and deposition, cw- and time resolved micro-photoluminescence spectroscopy, nonlinear measurements in reflection and transmission (e.g. SHG), angular resolved transmission spectroscopy. The group has strong connections and overlapping activities with the Centre of Innovation Competence (ZIK) SiLi-nano at the Martin Luther University.



Enhancement of the luminescence of Ge-quantum dots embedded in silicon Mie-resonators. Strongest enhancement is observed for higher Q collective Mie-resonances in trimer structure.

Current Projects and Future Goals:

Luminescence enhancement in nanostructure resonators

An increased density of photonic states (Purcell effect) and increased outcoupling of light from cylindrical Silicon- Mie resonators is used to enhance the luminescence of embedded Germanium quantum dots. Current research focuses on the further increase in Q-factor of the resonances by coupling several closely spaced Mie-resonators resulting in collective resonances (Fig. 1) enhancing the luminescence further with the aim to construct a miniaturised light source on-chip.

Nonlinear wavelength conversion in micro- and nanophotonic platforms

Using SiN-coated silicon waveguides a remarkable increase of the SHG signal can be observed due to the symmetry breaking introduced by the inhomogeneously strained Si-lattice as well as by the electric fields, which are generated by fixed charges at the SiN/Si. Furthermore degenerate four wave mixing is enhanced in silicon slot waveguide ring resonators, which are infiltrated with a chalcogenide glass by a newly developed nano-injection moulding process. In the future intentionally applied electric fields will be used to increase the generated $\chi(2)$ in silicon and hybrid nanostructures further, so that efficient wavelength conversion processes can be integrated on-chip.

Hyperbolic (wire) Metamaterials

Dense arrays of parallel aligned nanowires represent metamaterials for light in the visible and infrared, which exhibit a negative dielectric constants for electric fields parallel to the wires and a positive one for fields perpendicular to them. This leads to an unusual hyperbolic dispersion relation for light propagating through this metamaterial featuring very large wavevectors (very small wavelengths). It is currently investigated how these properties can be used to create hyperlenses, which could be used for nanofocussing light or subwavelength imaging.

Plasmonic nanostructures for SERS

Arranging metal nanodiscs in strictly periodic arrays allows to intensify the overall plasmonic oscillation by forming lattice resonances. When these resonances are tuned to the emission wavelength of a molecule or the Raman laser wavelength, the luminescence or SERS-intensity can be enhanced. The combination of these lattice resonances with near field hot spots is currently studied. The goal is the creation of regular nanostructures, which offer a reproducible, high and uniformly distributed Raman enhancement.



Prof. Dr. Jörg Schilling

2002

PhD in Physics from Martin Luther University Halle-Wittenberg for research on Photonic Crystals carried out at Max Planck Institute of Microstructure Physics, Halle

2002–2005

Postdoc at California Inst. Of Technology, Pasadena, USA with Prof. Axel Scherrer

2005–2009

Royal Society University Research Fellow at the Queen's University Belfast, UK

Since 2009

Group leader at Centre for Innovation Competence (ZIK) SiLi-nano, MLU

2011–2017

Juniorprofessor at MLU

Since 2017

Full Professor for Nonlinear Nanophotonics, Institute of Physics, MLU

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Selected publications:

V. Rutckaia, F. Heyroth, A. Novikov, M. Shaleev, M. Petrov, and J. Schilling. Quantum Dot Emission Driven by Mie Resonances in Silicon Nanostructures. *Nano Lett.* 17, 6886 (2017).

I. Staude and J. Schilling. Metamaterial-inspired silicon nanophotonics. invited Review article in *Nature Photonics* 11, 274–284 (2017).

C. Schriever et al. Second order optical nonlinearity in silicon waveguides – inhomogeneous stress and interfaces. *Advanced Optical Materials* 3, 129 (2015).

J. Kanungo, J. Schilling. Experimental determination of the principal dielectric functions in silver nanowire metamaterials. *Applied Physics Letters* 97, 021903 (2010).



Prof. Dr. Georg Schmidt

1996

PhD Physics, RWTH Aachen, Germany

1999–2008

PostDoc at Würzburg University, Germany, Prof. Laurens W. Molenkamp

2004

Habilitation in experimental physics, Universität Würzburg, Germany

Since 2009

Full professor (W3) of Physics, Group of Nanostructured Materials and director of the Interdisciplinary Center for Materials Science, Martin Luther University, Halle-Wittenberg, Germany

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Selected publications:

F. Heyroth et al., Monocrystalline Freestanding Three-Dimensional Yttrium-Iron-Garnet Magnon Nanoresonators, *Physical Review Applied* 12 (5), 054031 (2019).

C. Hauser et al., Yttrium Iron Garnet Thin Films with Very Low Damping Obtained by Recrystallization of Amorphous Material, *Scientific Reports* 6, 20827 (2016).

O. Wid et al., Investigation of the unidirectional spin heat conveyor effect in a 200 nm thin Yttrium Iron Garnet film, *Scientific reports* 6, 28233 (2016).

M Grünewald et al., Vertical organic spin valves in perpendicular magnetic fields, *Physical Review B* 88 (8), 085319 (2013).

M. Grünewald et al., Tunneling anisotropic magnetoresistance in organic spin valves, *Physical Review B* 84 (12), 125208 (2011).

B. Pigeau et al., A frequency-controlled magnetic vortex memory, *Applied Physics Letters* 96 (13), 132506 (2010).

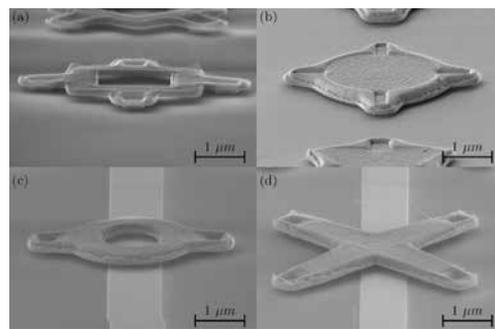
Institute of Physics & Interdisciplinary Center of Materials Sciences

Nanostructured Materials

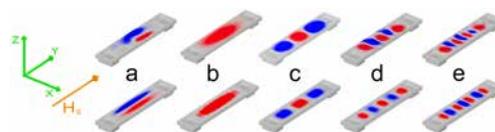
Fields of Research:

- › Magnonics and spin transport in nanostructures
- › Complex oxide electronics and spintronics
- › Organic spintronics
- › Nanolithography

Spintronics and magnonics both make use of the electron spin to replace the charge of the electron in novel Post-CMOS electronics. While spintronics mainly relies on the transport of electrons for the transfer of spin information, magnonics uses elementary excitations namely spin waves in ferromagnetic materials for information transfer and processing. Our group makes use of metals, organics, and complex oxides to investigate the basic physics of spin transport like spin pumping or the inverse spin Hall effect on one hand. On the other hand, new devices are tailored by sophisticated methods of 3D nanofabrication that may allow to couple spin waves, photons, and phonons for possible use in quantum information processing. The three pillars of the work are thin film deposition (Pulsed laser deposition, evaporation, magnetron sputtering and organic molecular beam deposition), Nano fabrication (electron beam lithography, lift-off, and dry etching), and characterization. The characterization ranges from magnetic characterization (SQUID, MOKE) to magnetotransport and ferromagnetic resonance at low temperature down to mK.



Free standing YIG resonators



Standing spin waves detected by MOKE (top) and simulated patterns (bottom)

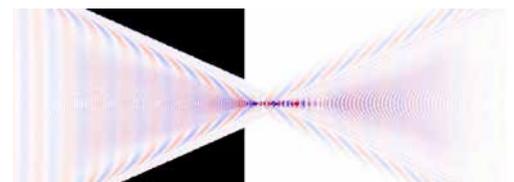
Current Projects and Future Goals:

Oxide interfaces

The interface between the two insulating oxides LaAlO_3 and SrTiO_3 is known to exhibit an electron gas with reasonable mobility at low temperature. We were able to show that at low temperature the electrons are located at domain walls which appear due to a structural phase transition in the SrTiO_3 substrate. In nanostructures which are fabricated in a proprietary nano patterning process this leads to anomalies in the temperature dependence of the conductivity and in magnetotransport.

3D magnonics

Using a new deposition and patterning process for yttrium iron garnet (YIG) we are able to fabricate suspended or free standing YIG nanostructures. These unique structures can be used for experiments ranging from low temperature magnonics like coupling between superconducting micro resonators to YIG nano structures to coupling between mechanical resonances and magnons, both areas which can be relevant for quantum information processing. A similar patterning process can also be used to create 3D YIG structures for magnon optics which can act as optical elements for focusing spin waves to high intensities.



Simulated spin wave focusing in a YIG based micro device

Spin dynamics and spin pumping

Spin pumping is a reliable method to create pure spin currents. These can be converted into real currents by the inverse spin-Hall effect. We investigate the spin pumping efficiency in various material systems ranging from all-metal multilayers to oxide hybrid structures and organic/ferromagnet hybrids. Using these pure spin currents spin dynamics can be detected but also spin-currents induced by the spin-Hall effect can be used to reduce the damping in ferromagnetic resonance and to create nano-sized high frequency oscillators for the GHz regime.

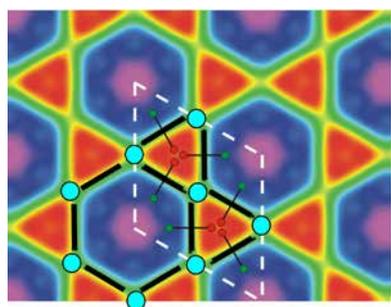
Institute of Chemistry

Supramolecular Chemistry and Liquid Crystals

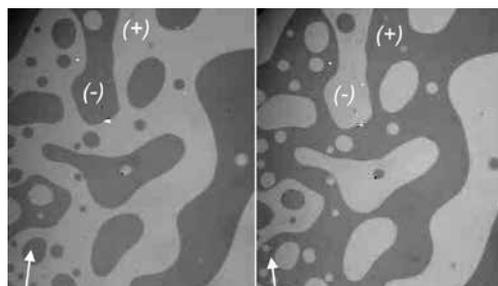
Fields of Research:

- › Design and investigation of new liquid crystals (LCs)
- › Dynamic network formation by liquid state self-assembly (liquid organic frameworks)
- › Spontaneous mirror symmetry breaking in soft matter
- › Emergence of complexity by soft self-assembly
- › Development of polar order and ferroelectricity in LCs
- › Photoisomerizable and other functional LCs

Liquid crystals represent a state of matter uniquely combining fluidity with order. This combination is essential for numerous technological applications, the commonly known is the LC display; but this state of matter is also of importance in numerous other fields, as for example for the complex self-assembly in biosystems. Our group deals with the synthesis of new materials capable of forming such self-assembled ordered fluids with high structural complexity and new emergent functionalities. We perform the design, the synthesis and the characterization of new liquid crystalline molecules. For the investigations various complimentary methods are employed, among them polarizing microscopy, calorimetric analysis, X-ray diffraction methods and electro-optical investigations. Further studies are performed in cooperation with partners from all over the world.



Electron density map of the liquid crystalline kagome pattern (B. Glettner et al.).



Chiral conglomerate of a mirror symmetry broken liquid, observed with polarized light (C. Dressel et al.).

Current Projects and Future Goals:

Complex fluid nanostructures of polyphilic mesogens

Division of space into distinct subspaces is a central feature of life as exemplified by cells and organelles. Our goal is to understand the fundamental basic principles of self-assembly of simple molecules into highly complex compartmented LC superstructures. An example is shown in Fig. 1, where the molecules form the walls of a honeycomb composed of hexagonal and triangular cells (the Kagome), which are filled by different materials, the red triangles by hydrocarbons and the larger blue hexagons by perfluorinated hydrocarbons. Both are separated by walls with only one molecule in diameter (black lines). Our future aim in this area is to find new tiling patterns with increased complexity, finally leading to quasi-crystalline tilings (see S. Poppe 2015, X. Zeng et al.).

Dynamic Supramolecular Networks

Networks are the basis of intelligence, metabolic cycles and the open-end development of complex systems. We design molecules capable of self-assembly into dynamic networks with cubic symmetry, connected by three-, four- and higher valence junctions into single nets and double or multiply interwoven networks (see S. Poppe et al. 2020). These networks are of interest for photonic applications and can provide conduction pathways in all three dimensions, which is of importance for applications in photovoltaics, as ion carriers and for other functionalities.

Spontaneous mirror symmetry breaking in fluids and the origin of biochirality

Homogeneous chirality is one of the basic features of life and its origin is still unclear. We have demonstrated that achiral molecules can spontaneously develop conglomerates composed of two chiral liquids with opposite chirality, which are immiscible and form separate phases (dark/bright in Fig. 2, see C. Dressel et al., T. Reppe et al., M. Alaasar et al.). This synchronization of enantiomeric molecular conformers is supported by the cooperativity provided by the formation of highly dynamic helical networks in these percolated liquids. We work on the fundamental understanding of these phenomena and their possible implications for the emergence of uniform chirality in prebiotic liquids.



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Selected publications:

C. Tschierke et al. Mirror Symmetry Breaking in Liquids and Their Impact on the Development of Homochirality in Abiogenesis: Emerging Proto-RNA as Source of Biochirality? *Symmetry*, 2020, 12, 1098.

T. Reppe et al. Spontaneous mirror symmetry breaking in benzil-based soft crystalline, cubic liquid crystalline and isotropic liquid phases. *Chem. Sci.* 11, 2020, 5902-5908.

S. Poppe et al. Liquid Organic Frameworks: The Single-Network "Plumber's Nightmare" Bicontinuous Cubic Liquid Crystal. *J. Am. Chem. Soc.* 2020, 242, 3296-3300.

M. Alaasar et al. Isothermal Chirality Switching in Liquid-Crystalline Azobenzene Compounds with Non-Polarized Light. *Angew. Chem. Int. Ed.* 2017, 56, 10801-10805.

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C. Dressel, et al. Chiral Self-sorting and Chirality Amplification in Isotropic Liquids of Achiral Molecules. *Nature Chemistry*, 2014, 6, 971-977.

X. Zeng, et al., Complex Multicolor Tilings and Critical Phenomena in Tetrphilic Liquid Crystals. *Science*, 2011, 331, 1302-1306.

B. Glettner et al. Liquid-Crystalline Kagome. *Angew. Chem. Int. Ed.* 2008, 47, 9063-9066.



Prof. Dr. Rebecca Waldecker

2007

PhD in Mathematics, University of Kiel, Germany

2007-2009

Honorary Lecturer and Research Fellow, University of Birmingham, UK

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Junior Professor for Groups and Geometries, Martin Luther University Halle-Wittenberg

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Selected publications:

P. Salfeld and R. Waldecker, The occurrence of finite simple permutation groups of fixity 2 as automorphism groups of Riemann surfaces. *Journal of Algebra* 561 (2020), 402-420.

Chr. Jefferson, M. Pfeiffer and R. Waldecker, New refiners for permutation groups search. *J. of Symb. Comp.* 92 (2019), 70-92.

Chr. Jefferson, Eliza Jonauskaitė, M. Pfeiffer and R. Waldecker, Minimal and canonical images. *J. of Alg.* 521 (2019), 481-506.

K. Magaard and R. Waldecker, Transitive permutation groups with trivial four point stabilizers. *J. Group Theory* 18 (2015), no. 5, 687-740.

K. Magaard and R. Waldecker, Transitive permutation groups where nontrivial elements have at most two fixed points. *J. of Pure and Appl. Alg.* 219, Issue 4 (2015), 729-759.

I. Toborg and R. Waldecker, Finite simple 3'-groups are cyclic or Suzuki groups. *Archiv der Mathematik* 102, No. 4 (2014), 301-312.

R. Waldecker, Isolated involutions in finite groups. *Memoirs of the AMS*, Volume 226, Number 1061 (2013).

Institute of Mathematics

Algebra

Fields of Research:

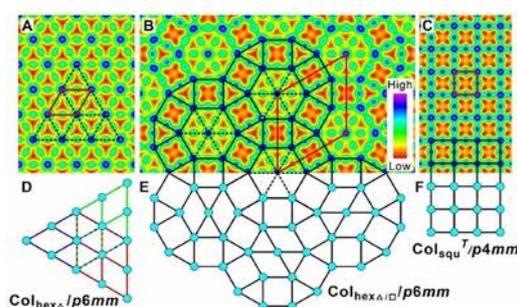
- › Abstract theory of finite groups
- › Applications of the classification of finite simple groups
- › New algorithms in computational permutation group theory
- › Algebraic and geometric methods in chemistry and physics

Groups arise naturally wherever symmetry is present, which is why group theory and algebraic methods have applications far beyond mathematics. Using the language of group theory helps to understand the structure and symmetry of curves and surfaces, it plays a role for virus models, for modelling the self-assembly of molecules or for calculating energy levels of electrons, and recently group theory has played a role in solving difficult algorithmic problems.

Algebraic methods have made it possible to develop new algorithms for computer algebra software that have substantially changed the state of the art. While some problems can be solved using elementary techniques and arguments from geometry or group theory, others need deep knowledge about the abstract theory of finite groups. For some applications we need an inductive approach which often leads to an investigation of the smallest building blocks of abstract groups: the finite simple groups.

Their classification is of crucial importance not only for group theory, and much is still left to understand in greater detail.

Many open research problems have been (and still are) solved by direct use of this classification result, and much inspiration for further research into even more details stems from applications within and outside of mathematics.



Development of the dodecagonal supertiles at the transition from triangular to square tiling patterns. (M. Poppe, et al., *A Periodic Dodecagonal Supertiling by Self-assembly of Star-shaped Molecules in the Liquid Crystalline State*, *Communications Chemistry* volume 3, Article number: 70 (2020), 5).

Current Projects and Future Goals:

Groups acting with low fixity

In a number of interesting open problems there is some group action involved on a mathematical object with high symmetry, for example a network, a curve or a surface. Then the goal is to use the interplay between the structure of the object and the structure of its symmetry group in order to understand the object better.

For instance, a compact Riemann surface of genus at least 2 has a finite automorphism group, and fixed points of non-trivial automorphisms can be used to understand the structure of the surface better.

This leads to questions about permutation groups acting with low fixity. In ongoing research, it has been possible to prove classification results about finite groups acting with fixity 2 or 3, partial results for fixity 4 are available and there is much work in progress in order to classify the Riemann surfaces that exhibit such groups as groups of automorphisms, along with ramification data. This work will continue and all results will not only be published, but will also be made available in computer algebra software.

Algorithms

For many search problems in permutation groups, a backtrack search method is used. While often good enough in practice, the worst-case performance is so bad that there is a desperate need for new ideas that help to prune the search tree quickly and substantially.

After the introduction of new refiners around orbital graphs, there is now a new approach that instead of partitions used stacks of labelled digraphs for the organisation of the search procedure (collaboration with Computer Science, St Andrews). We have also developed new methods for the calculation of canonical images, and future projects include combining our new ideas for even better algorithms and extending the graph stack method in order to solve even harder problems.

Further applications

Using symmetry, we intend to better understand the tessellations that model the self-assembling behaviour of liquid quasi-crystals.

Institute of Mathematics

Functional Analysis

Fields of Research:

- › Topological Methods in Nonlinear Analysis
- › K-theoretic Methods in Bifurcation Theory
- › Selfadjoint Fredholm Operators and the Spectral Flow
- › Index Bundles for Families of Fredholm Operators

Topological methods have been used in nonlinear analysis from the very beginning of its systematic study. The usual task is the search for solutions of nonlinear equations in Banach spaces that are obtained from differential equations. A common strategy is to construct indices that can be assigned to such equations and whose non-triviality predicts the existence of solutions. When constructed by topological methods, such indices sometimes turn out to be invariant under certain deformations of the equations, making them well suited for such an application.

A related problem is the setting of bifurcation theory, where families of nonlinear equations are considered that are parametrized by one or several parameters. All of these equations are assumed to have a “trivial” solution that we already know. Here the above topological methods can be used to find parameter values where new solutions branch off from the known ones.

We mostly study two related kinds of topological indices for bifurcation problems. Firstly, we consider K-theory classes for families of Fredholm operators that were introduced by Jänich and Atiyah in the sixties in connection to family versions of the Atiyah-Singer Index Theorem. Their applicability in bifurcation theory was pointed out in the late eighties and this link has since then steadily been developed. Secondly, we focus on selfadjoint Fredholm operators and consider the spectral flow, which is an invariant that was introduced by Atiyah, Patodi and Singer in the seventies. The spectral flow was first linked to bifurcation theory in the late nineties and we have made substantial contributions to this active field of research. We have in particular developed methods to estimate spectral flows, which are often good enough for applications to bifurcation problems.

Current Projects and Future Goals:

■ The equivariant spectral flow and bifurcation theory

Differential equations often have symmetries, which can be described as invariances under the action of a group. Unfortunately, such symmetries can ruin the topological approach when they cause the vanishing of the invariants. The aim of this project is to introduce an equivariant spectral flow as an element of the representation ring of the group of symmetries. Like the ordinary spectral flow, which is an integer, its equivariant version can be estimated by using a partial order on the representation ring. The ultimate goal of this project is to show that a non-vanishing equivariant spectral flow yields bifurcation just as for the ordinary spectral flow in the non-equivariant case. Moreover, we apply our theorem to study bifurcation phenomena for periodic Hamiltonian systems having symmetries which cause the ordinary spectral flow to vanish.

■ Exponential Dichotomies

We have previously studied topological bifurcation invariants for various discrete and continuous dynamical systems that were assumed to be asymptotically hyperbolic, i.e., that converge in forward and backward time to a special kind of system. The aim of this project is to lift this restrictive convergence assumption and to require instead the existence of exponential dichotomies, which is a common setting in the theory of dynamical systems. This is a joint project with R. Skiba (Torun) which is funded by a DAAD grant (2020–2021).

■ Several parameter bifurcation invariants for variational problems

Many differential equations are induced by variational problems. This makes their representing operators selfadjoint and so the spectral flow is a convenient invariant for studying bifurcation phenomena in this setting. Unfortunately, the spectral flow is only defined for problems depending on a single parameter. The aim of this project is to obtain K-theoretic invariants for several parameter bifurcation problems that generalize the spectral flow. These invariants will be used to study bifurcation of periodic solutions of autonomous Hamiltonian systems, where one parameter is necessarily reserved for the length of the period.



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PhD in Mathematics, University of Göttingen

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DAAD PostDoc Fellow at Politecnico di Torino, Italy

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Selected publications:

N. Doll, H. Schulz-Baldes, N. Waterstraat, Parity as \mathbb{Z}_2 -valued spectral flow, *Bull. Lond. Math. Soc.* 51 (2019), 836–852

N. Waterstraat, Spectral flow and bifurcation for a class of strongly indefinite elliptic systems, *Proc. Roy. Soc. Edinburgh Sect. A* 148 (2018), 1097–1113.

N. Waterstraat, Spectral flow, crossing forms and homoclinics of Hamiltonian systems, *Proc. Lond. Math. Soc.* (3) 111 (2015), 275–304.

N. Waterstraat, A family index theorem for periodic Hamiltonian systems and bifurcation, *Calc. Var. Partial Differential Equations* 52 (2015), 727–753.

A. Portaluri, N. Waterstraat, A Morse-Smale index theorem for indefinite elliptic systems and bifurcation, *J. Differential Equations* 258 (2015), 1715–1748.

N. Waterstraat, A K-theoretic proof of the Morse index theorem in semi-Riemannian geometry, *Proc. Amer. Math. Soc.* 140 (2012), 337–349.



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Selected publications:

L. K. Scarbath-Evers, R. Hammer, D. Golze, M. Brehm, D. Sebastiani, and W. Widdra, *From Flat to Tilted: Gradual Interfaces in Organic Thin Film Growth*, *Nanoscale* 12, 3834 (2020).

K. Gillmeister, D. Golež, C.-T. Chiang, N. Bittner, Y. Pavlyukh, J. Berakdar, P. Werner, and W. Widdra, *Ultrafast coupled charge and spin dynamics in strongly correlated NiO*, *Nature Comm.* 11, 4095 (2020).

A. Trüttschler, M. Huth, C.-T. Chiang, R. Kamrla, F. O. Schumann, J. Kirschner, and W. Widdra, *Band-Resolved Double Photoemission Spectroscopy on Correlated Valence Electron Pairs in Metals*, *Phys. Rev. Lett.* 118, 136401 (2017).

S. Förster et al., *Observation and Structure Determination of an Oxide Quasicrystal Approximant*, *Phys. Rev. Lett.* 117, 095501 (2016).

S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Quasicrystalline structure formation in a classical crystalline thin-film system*, *Nature* 502, 215 (2013).

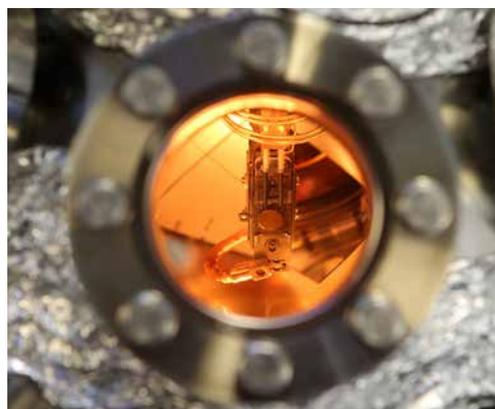
Institute of Physics

Surface and Interface Science

Fields of Research:

- › Surface properties of oxides
- › Growth and properties of oxide quasicrystals
- › Electronic structure of organic thin films
- › Surface vibrational spectroscopy
- › Femtosecond laser spectroscopy
- › Ultrafast photoelectron microscopy

Surface science is a modern research area within solid-state physics. The nanometer-controlled material science, where interfaces and surfaces dominate device performance, inspires novel material concepts for future applications in information and sensor technologies. For the understanding of such new concepts, atomically controlled surfaces and interfaces provide an ideal research environment: Nanostructures are assembled atom-by-atom or atomic layer-by-layer; new structures are atomically resolved by scanning tunneling microscopy (STM) in-situ under ultraclean vacuum conditions, and state-of-the-art surface-sensitive spectroscopies directly analyze the new physical or chemical properties. At the MLU, we developed a variety of methods as scanning tunneling microscopy, high-resolution inelastic electron scattering (HREELS), electron diffraction (LEED), angle-resolved photoelectron spectroscopy (ARPES), photoemission electron microscopy (PEEM) and laser-based two-photon photoemission (2PPE). Their combinations allow exceptional resolution in space, time, energy as well as momentum to address novel interface phenomena.



View onto a quasicrystal in an ultra-high vacuum chamber.

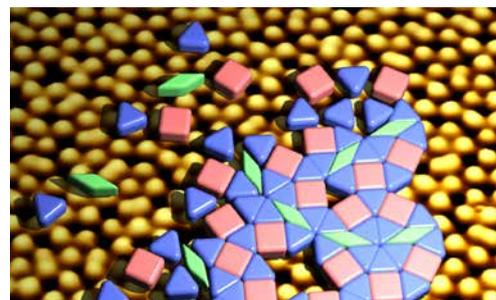
Current Projects and Future Goals:

Oxide nanostructures

Growth of oxide thin films and oxide heterostructures and their characterization by in-situ microscopy and spectroscopy has been leading the SFB-762 in the past decade. Emerging electronic properties, new bonding schemes, lattice dynamics and femtosecond dynamics of excited electrons are investigated by complementary techniques.

Quasicrystals

Peculiarities and unexpected physical properties of oxide quasicrystals – highly ordered monolayer films with self-similar structures, but without periodicity – define the focus of this research field since the discovery of oxide quasicrystals in 2013 in Halle. We address the fundamental aspects of quasicrystal physics, but also aim at application for quasicrystal thin film coatings.



Square-triangle-rhomb tiling of a dodecagonal oxide quasicrystal with STM image as background.

Laser-based spectroscopy and microscopy

Femtosecond lasers enable the observation of dynamic processes of electrons on femtosecond time scales. Within the SFB/TRR-227, we advance this field by the use of widely tunable lasers and laser-based high-harmonics generation at high repetition rates. With this instrumentation, we identify electron decay and transport on intrinsic time scales. Ultimate goal is combination of femtosecond spectroscopy and nanometer microscopy via laser-based electron microscopy.

Organic electronics

Polymer and organic thin films on solid surfaces are key elements in the field of organic electronics. Understanding of their self-organization as well as their electronic properties is our goal by combination of STM and photoemission. The assignment of local electronic states to specific interface-induced structures leads to deeper understanding for charge injection in organic devices.

Institute of Physics

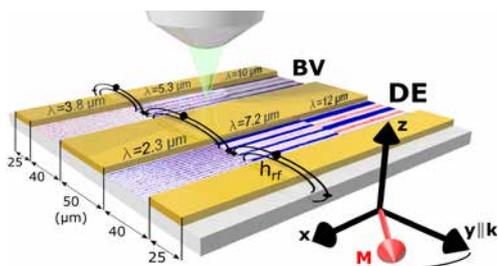
Optics and time resolved spectroscopy

Fields of Research:

- › Spin dynamics and spin transport
- › Ultrafast spin dynamics
- › Time resolved microscopy
- › Magnetic hetero and nano structures
- › Spintronics

The electron spin is a quantum property and determines structure and dynamics of matter. It has a strong influence on light emission and absorption, allows controlling charge transport processes, and is essential for the emergence of magnetic order. Consequently, spin physics has a broad impact on everyday life. Examples are the usage of electron spins to store digital information in nanoscale bits and the magnetization dependence of electronic transport in nanoscale sensors. Employing the electron's spin degree of freedom has large potential for advanced electronic device concepts with simple architecture and reduced power consumption. The field of spin electronics (spintronics) has enjoyed enormous interest in last three decades due to the discovery of numerous effect linking electrical currents to the spin and its dynamics. These phenomena allow controlling the magnetization state by charge currents and vice versa.

The research activities in the optics group focus on understanding spin dynamics and spin transport on small time (femtoseconds) and length scales (nanometers). Most of the experiments involve ultrafast optical methods for the detection of spin dynamics. In addition to the time resolved optical experiments our group also prepares of the most samples (growth and nano-fabrication processes). The goal of our research is an improved understanding of fundamental processes facilitating the development of novel spin electronic devices.



Time resolved magneto-optic imaging of spin waves in a ferrimagnetic material at a frequency of 5 GHz.

Current Projects and Future Goals:

Nanoscale magnetization dynamics

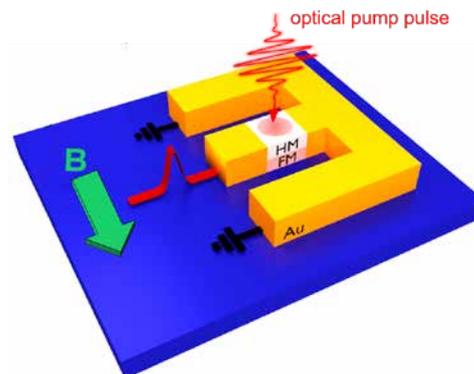
We use time resolved magneto optic microscopy to obtain snapshots the spin dynamics (spin waves) in magnetic nanostructures. Here the interaction of the magnetic excitations with electrically driven spin currents is of particular interest as spin transfer torque and spin orbit torque effects allow control the dynamics. In order to overcome the diffraction limit we currently develop an optical near field method.

Spin to charge conversion

Spin currents may be created without a ferromagnetic material using the spin orbit interaction. This effect is known as the spin Hall effect. We use this phenomenon to generate spin transfer torques in metallic multilayer systems and sample the effect by time resolved microscopy. In our experiments, we would like to understand and maximize this effect.

Ultrafast spin dynamics

We use ultrafast (femtosecond) laser pulses to generate ultrashort and intense spin current pulses in spintronic hetero-structures. One aim is to use these pulses to excite ultrafast spin dynamics in ferrimagnets and achieve ultrafast spin switching. Alternatively, a material with large spin orbit interaction is used to convert the ultrafast spin current pulses into intense charge current pulses with THz bandwidth via the inverse spin Hall effect. Thereby creating on chip THz source with vast applications ranging from THz imaging to antiferromagnetic spintronics.



On-chip generation of THz current pulses with a spintronic emitter.



Prof. Dr. Georg Woltersdorf

2004

PhD Physics at Simon Fraser University, Canada with Prof. Bretislav Heinrich

2004–2007

Postdoc at the University of Regensburg with Prof. Christian Back

2007–2013

Staff scientist at the University of Regensburg with Prof. Christian Back

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Habilitation at the University of Regensburg

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Selected publications:

S. Poellath et al., Ferromagnetic Resonance with Magnetic Phase Selectivity by Means of Resonant Elastic X-Ray Scattering on a Chiral Magnet, *Phys. Rev. Lett.* 123, 167201(2019).

T.S. Seifert et al., Femtosecond formation dynamics of the spin Seebeck effect revealed by terahertz spectroscopy, *Nature Communications* 9, 2899 (2018).

S. Baierl et al., Terahertz-Driven Nonlinear Spin Response of Antiferromagnetic Nickel Oxide, *Phys. Rev. Lett.* 117, 197201(2016).

H.G. Bauer, P. Majchrak, T. Kachel, C.H. Back, and G. Woltersdorf, Nonlinear spin-wave excitations at low magnetic bias fields, *Nature Communications* 6, 8274 (2015).

D. Wei, M. Obstbaum, M. Ribow, C. H. Back, and G. Woltersdorf, Spin Hall voltages from a.c. and d.c. spin currents, *Nature Communications* 5, 3768 (2014).



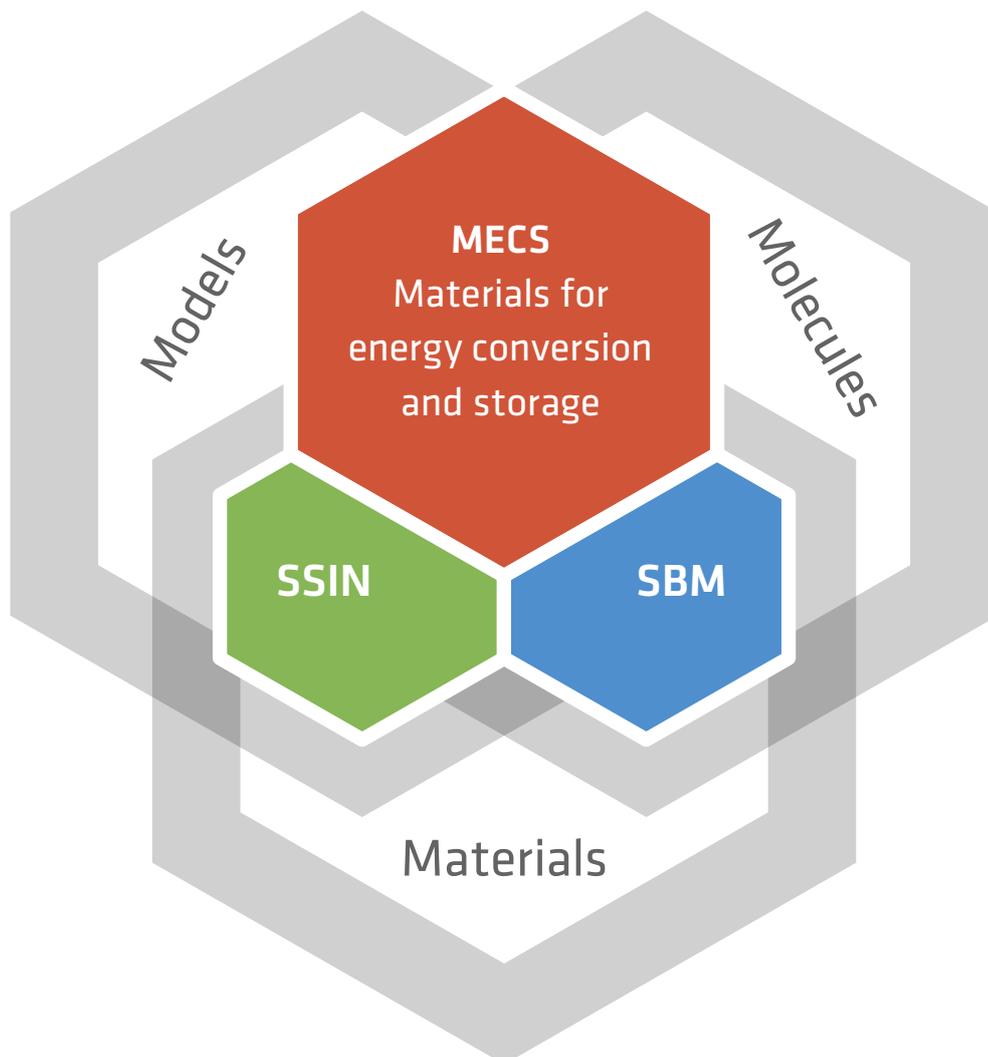


Materials for energy conversion and storage

Considering the challenges of climate change and the associated transformation towards an environmentally friendly energy supply technology our research theme on “Materials for Energy Conversion and Storage” focuses on a highly relevant topic for current and future generations. The aim is the development of a sustainable and efficient energy supply for the future.

Within the research theme experimental and theoretical projects are combined, which represent an advancement on prior topics formerly investigated within the areas of functional solid state interfaces and photovoltaics/

renewable Energy. Current network initiatives include the research cluster Solarvalley Mitteldeutschland (since 2009) as well as the consortium HYPOS: Hydrogen Power Storage (since 2014) and the ZIK SiLi-nano (since 2009). The research theme was recently strengthened by two new professorships within the area. Future perspectives for development– especially with the aim to establish new cooperative research networks – lie in the fields of CO₂-fixation, novel lithium-free battery systems, closed material cycles and chemical hydrogen storage and usage.



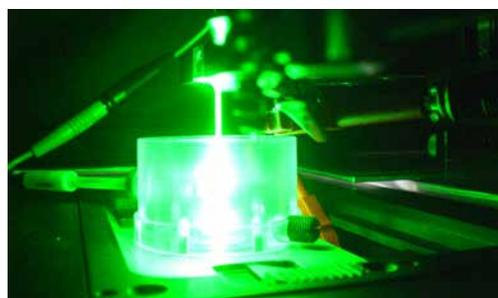
Institute of Chemistry

Materials for Energy

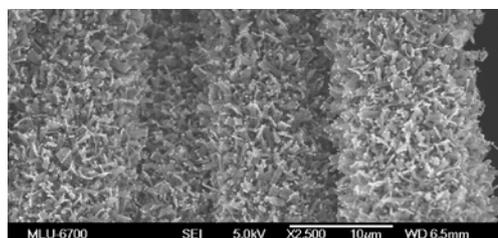
Fields of Research:

› Nanostructured Materials for Electrochemical Energy Conversion

The conversion of electrical into chemical energy and vice versa is a key process in a renewable energies-scenario, and allows excess electrical energy e.g. from wind and solar to be converted and stored, and made available when needed. Electrochemical energy conversion devices rely heavily on nanostructured materials, at which the relevant electrochemical reactions take place. Our group is focusing on the development of such materials, their characterization, and an in-depth understanding of the processes taking place at these materials and the parameters determining their activity and stability. We are using advanced synthesis approaches including colloidal synthesis, microwave assisted synthesis and chemical vapor deposition to prepare materials with distinct properties. A detailed ex situ characterization using e.g. TEM, XRD, and XPS on the one hand and an electrochemical characterization using advanced techniques like impedance spectroscopy helps to establish structure-property-relationships which in turn may be used to develop novel materials. Furthermore, we are actively developing novel experimental techniques including in situ-IR- and Raman spectroscopy as well as micro-electrochemical methods to unravel processes occurring during electrochemical energy conversion. Finally, to evaluate the properties of new materials under realistic conditions and to transfer the gained knowledge from basic studies to application, we are performing cell tests at our fuel cell, electrolysis and battery test benches.



Novel setup for in situ-Raman measurements of electrode surfaces under potential control



Current Projects and Future Goals:

■ Carbon-based materials for vanadium redox-flow batteries (VRFB)

In redox flow batteries chemical energy is stored in redox reactions of dissolved materials instead of the electrodes (e.g., vanadium ions). However, for efficient catalysis of the redox reactions, catalytically active electrode materials are needed. We are synthesizing and investigating a variety of carbon materials (carbon nanotubes, graphene, carbonized polymers, composites of these, etc.) toward their activity and stability as electrodes in VRFB with a focus on the influence of functional surface groups as well as porosity.

■ Nickel-based materials for alkaline water electrolysis

The efficiency of water electrolyzers is strongly influenced by over-potentials required to run the electrochemical reactions at reasonable rates. NiFe oxides are known active materials for the oxygen evolution, while NiMn compounds catalyze the hydrogen evolution with low over-potentials. Both types of materials are investigated towards the respective reaction with a focus on structure-activity relationships, including influence of composition and surface structure.

■ CO₂ electroreduction

CO₂ may be electrochemically reduced to valuable products, including CO and lower hydrocarbons. However a major issue is the low selectivity and high amount of (in this case unwanted) hydrogen produced during electroreduction. We are synthesizing size-selected Au-, Ag-, and Cu-nanoparticles for this reaction to unravel particle size/structural effects and their influence on activity and selectivity. Electronic effects and support effects are investigated as well.

■ Fuel cell catalysis

Current fuel cell related research in our group is motivated by recent advances in alkaline exchange membranes, which might preplace the currently used acid membranes. We are investigating the oxygen reduction reaction over carbon based materials as well as the oxidation of ethylene glycol and glycerol over Pt and Au. Besides activity, a major focus is on the long-term stability of the materials, which is crucial for later application.

Polyaniline deposited on carbon cloth as high-surface-area fuel cell electrode



Prof. Dr. Michael Bron

1998

PhD in Physical Chemistry, TU Chemnitz, Germany

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2002–2009

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Selected publications:

M. Steimecke et al., Higher-Valent Nickel Oxides with Improved Oxygen Evolution Activity and Stability in Alkaline Media Prepared by High-Temperature Treatment of Ni(OH)₂. ACS Catal. 10 (2020) 3595–3603.

X. Lu et al., Titanium as a Substrate for Three-Dimensional Hybrid Electrodes for Vanadium Redox Flow Battery Applications. ChemElectroChem 7 (2020) 737.

X. Lu et al., Plasma-etched Functionalized Graphene as a Metal-free Electrode Catalyst in Solid Acid Fuel Cells. J. Mater. Chem. A 8 (2020) 2445–2452.

M. Steimecke et al., In situ Characterization of Ni and Ni/Fe Thin Film Electrodes for Oxygen Evolution in Alkaline Media by a Raman-coupled Scanning Electrochemical Microscope Setup. Anal. Chem. 89 (2017) 10679–10686.

A.B.A.A. Nassr et al., Rapid Microwave-Assisted Polyol Reduction for the Preparation of Highly Active PtNi/CNT Electrocatalysts for Methanol Oxidation. ACS Catal. 4 (2014) 2449–2462.



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Selected publications:

M. Breitenbach et al. Magnetolectric and HR-STEM Investigations on Eutectic CoFe_2O_4 - $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ Composites, *Journal of Physics and Chemistry of Solids* (2019), 135, 109076.

N. Quandt et al. Spin Coating of Epitaxial $\text{BaTiO}_3/\text{CoFe}_2\text{O}_4$ Thin Films on Single Crystalline (001)- SrTiO_3 , *Materials Chemistry and Physics* (2019), 229, 453–459.

R. Köferstein et al. Investigations of Nano-crystalline $\text{Sr}_{0.5}\text{Ba}_{0.5}\text{Nb}_2\text{O}_6$ and Bulk Ceramics Synthesized by a Polymerization Method Using PEG400, *Journal of the European Ceramic Society* (2019), 39, 1156–1163.

J. Jacobs et al. Structure, Optical and Photocatalytic Properties of Oxynitride Solid Solutions $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_2\text{N}$, $\text{CaNb}_{1-x}\text{Ta}_x\text{O}_2\text{N}$, and $\text{SrNb}_{1-x}\text{Ta}_x\text{O}_2\text{N}$ Prepared from Soft-Chemistry Precursors, *Zeitschrift für Anorganische und Allgemeine Chemie* (2018), 644, 1832–1838.

T. Walther et al. Novel Magnetolectric Composites of Cobalt Iron Alloy and Barium Titanate, *Journal of the American Ceramic Society* (2017), 100, 1502–1507.

F. Oehler et al. Preparation and Dielectric Properties of CaTaO_2N and SrNbO_2N ceramics, *Journal of the European Ceramic Society* (2017), 37, 2129–2136.

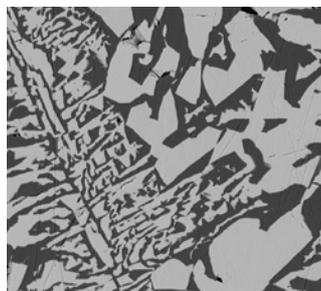
Institute of Chemistry

Solid State Chemistry

Fields of Research:

- › Preparation, structure and physical properties of complex oxides
- › Soft-chemistry synthesis of nanoparticles, processing and characterisation of ceramics, single crystal growth
- › Structure determination by X-ray and neutron diffraction
- › Magnetic, (di-)electric and thermal transport properties

Complex oxides are key functional materials for various applications like data storage devices, solid oxide fuel cells, thermoelectric converters, (photo-) catalysts, sensors, capacitors etc. Our group deals with the synthesis and comprehensive characterisation of new oxides with various morphologies including crystals, ceramics, powders, thin films, and nano particles. The applied synthesis methods comprise classical solid state reactions, sintering techniques, single crystal growth, plasma-assisted reactions as well as soft-chemistry approaches like sol-gel synthesis, decomposition of precursors, spray drying/spray pyrolysis and spin coating. The materials properties are affected by the complex interplay of composition, crystal structure, particle sizes and interfaces. Various complementary characterisation techniques are applied, including X-ray and neutron diffraction, X-ray absorption spectroscopy, different thermal analysis methods, optical spectroscopy and electron microscopy. For chemical analysis atomic absorption and X-ray fluorescence spectroscopy are used. In addition, various physical properties like electrical and thermal conductivity, heat capacity, dielectric behaviour, magnetic and magnetolectric properties are investigated.



3-3 heterostructure of BaTiO_3 and CoFe_2O_4

Current Projects and Future Goals:

Functional magnetic materials

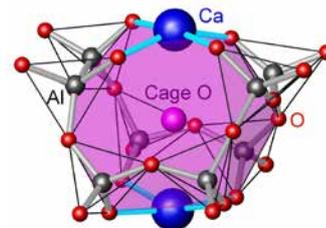
Materials with high and adjustable magnetization or exotic spin structures are interesting e.g. for power generators and spintronics. To investigate the (anisotropic) magnetic properties of oxides and intermetallic phases, high quality single crystals are grown using the floating zone method or flux techniques.



Optical floating zone furnace

Mayenite as universal host material

Due to its unusual cage structure, mayenite shows an excellent oxygen mobility required e.g. for solid oxide fuel cells and oxidising catalysts. Upon reduction, the to date only known temperature and moisture stable electride ($\text{Ca}_{12}\text{Al}_{14}\text{O}_{32} \cdot 2e^-$) is formed. This unique material is studied with the aim to stabilize exotic ionic species.



Cage structure of the oxygen ion conductor $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33.6}$

Anion-substituted perovskites

Oxide ions in perovskites can partially be replaced by N^{3-} , F^- or H^- . Oxynitrides are highly promising photocatalysts, while oxyfluorides are interesting candidates for fluorine-based battery systems and oxyhydrides may serve as hydrogen storage materials. Our goal is to identify new phases using (*in-situ*) X-ray and neutron diffraction and to study their catalytic and physical properties in detail.

Multiferroic heterostructures

Magnetolectric multiferroics are potential candidates for next-generation data storage and sensor systems. We investigate composites consisting of ferroelectrics like BaTiO_3 or $\text{Sr}_{1-x}\text{Ba}_x\text{Nb}_2\text{O}_6$ and ferromagnetic alloys or spinels. The effects of stoichiometry, dimensionality and the properties of the oxide interfaces are studied for 0-3-, 2-2-, and 3-3-heterostructures.

Institute of Chemistry

Photochemistry

Fields of Research:

- › Mechanistic and kinetic photochemistry
- › Laser-flash photolysis
- › NMR spectroscopy

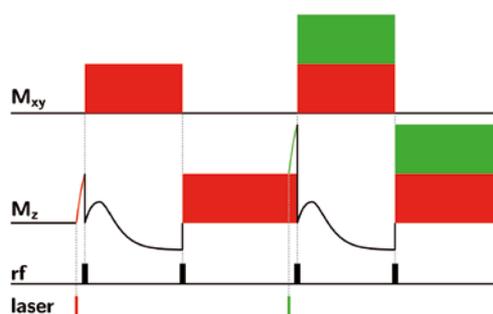
The importance of photochemistry can hardly be overstressed, taking into account the rapidly nearing exhaustion of fossil fuels – which are not only the world's energy sources but also the raw materials for most industrial organic syntheses – and the fact that all these fuels originate from photosynthesis.

We investigate the mechanisms and kinetics of photoreactions, using a variety of spectroscopic techniques. Our specialized expertise is in the areas of two-colour laser-flash photolysis at extremely high excitation intensities, of magnetic field effects, and of photo-CIDNP (photochemically induced dynamic nuclear polarizations). In the two-colour experiments, we use one laser pulse to prepare a short-lived intermediate, and then apply a second pulse to do photochemistry on the latter. This, as well as the high excitation intensities, opens up completely new reaction pathways. By the application of magnetic fields, the product yields can be modified; although a seemingly esoteric phenomenon, this is the underlying mechanism of the orientational system of migratory birds. Photo-CIDNP is basically laser-flash photolysis with NMR detection. This extremely powerful method yields information about all stages of a chemical reaction that is often inaccessible otherwise.

Current Projects and Future Goals:

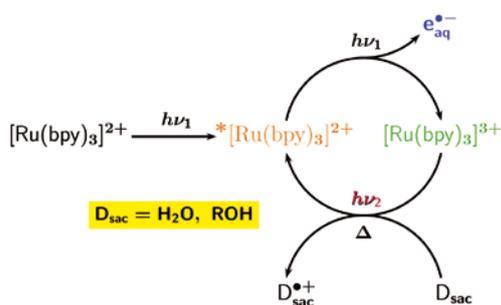
Photo-CIDNP spectroscopy

On one hand, we develop new and improved pulse sequences, on the other hand, we use this spectroscopic technique for in-depth mechanistic and kinetic investigations of organic photoreactions. In collaboration with the group of P. J. Hore at Oxford, we apply CIDNP to biorelevant molecules and their reactions, such as protein folding.



New photoionization mechanisms

We have discovered, and are currently investigating, a variety of mechanisms that yield more than one electron per molecule, e.g., catalytic cycles, where the photoionized intermediate is regenerated by a chemical reaction with a sacrificial electron donor. A related issue is the strong effects that small structural or electronic changes (e.g., the conversion of a triplet into a radical anion) can have on the photoionization efficiency. We aim to understand such changes, and utilize hydrated electrons for green photoredox catalysis.



Magnetic field effects

We use magnetic field effects to elucidate the details of organic photoreactions and diffusional dynamics, especially in microheterogeneous systems (e.g., micelles). A second focus is on the development of new experimental methods for measuring magnetic field effects. This project is part of an ongoing collaboration with the group of C. R. Timmel at Oxford.



Prof. Dr. Martin Goez

1986

PhD in Physical Chemistry (Friedrich-Alexander-Universität Erlangen, Germany)

1986–1988

Research scientist (Philips Research Laboratory Aachen, Germany)

1988–1995

PostDoc and Heisenberg fellow (Universität Carolo-Wilhelmina, Braunschweig, Germany)

1993

Habilitation in Physical Chemistry (Universität Carolo-Wilhelmina, Braunschweig, Germany)

Since 1995

Full Professor (C3) of Organic Chemistry (Martin Luther University Halle-Wittenberg, Germany)

2000–2001, 2004–2005, 2008

Visiting Professor (University of Leeds, University of Oxford) and Visiting Fellow (Magdalen College, Oxford, UK)

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Selected publications:

T. Kohlmann, C. Kerzig, M. Goez. Laser-induced Wurtz-type syntheses with a metal-free photoredox catalytic source of hydrated electrons. *Chem. Eur. J.* 2019, 25, 9991.

R. Naumann, F. Lehmann, M. Goez. Generating hydrated electrons for chemical syntheses by using a green light-emitting diode (LED). *Angew. Chem. Int. Ed.* 2018, 57, 1078.

R. Naumann, M. Goez. First micelle-free photoredox catalytic access to hydrated electrons for syntheses and remediations with a visible LED or even sunlight. *Chem. Eur. J.* 2018, 24, 17557.

M. Goez. Photo-CIDNP spectroscopy. *Annu. Rep. NMR Spectrosc.* 2009, 66, 77–147.

M. Goez et al. Quenching mechanisms and diffusional pathways in micellar systems unraveled by time-resolved magnetic-field effects. *Chem. Eur. J.* 2009, 15, 6058–6064.

K. H. Mok et al. A pre-existing hydrophobic collapse in the unfolded state of an ultrafast folding protein. *Nature* 2007, 447, 106–109.



Prof. Dr. Jörg Kressler

1978–1983

Studies of Chemistry at TU Dresden, Germany

1983–1997

PhD at TU Dresden and several PostDoc stays in Amherst, Tokyo, and Freiburg

1993–1997

Research scientist at Freiburg Materials Research Center

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Habilitation in Physical Chemistry, TU Dresden

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Full Professor (C4) on Physical Chemistry of Polymers, Martin Luther University Halle-Wittenberg

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Selected publications:

S.W.H. Shah, C. Schwieger, J. Kressler, A. Blume. Monolayer behavior of pure F-DPPC and mixed films with DPPC studied by epifluorescence microscopy and infrared reflection absorption spectroscopy. *Chem. and Phys. Lip.* 230, 104918, 2020.

Z.N. Hasan, C. Fuchs, C. Schwieger, K. Busse, O. Dolynchuk, J. Kressler. Crystallization of poly(ϵ -caprolactone) at the air-water interface studied by IRRAS and GI-WAXS. *Polym.* 196, 122468, 2020.

R. Alaneed, T. Hauenschild, K. Mäder, M. Pietzsch, J. Kressler. Conjugation of amine-functionalized polyesters with dimethylcasein using microbial transglutaminase. *J. Pharm. Sci.* 109, 981-991, 2020.

M.H. Samiullah, M. Pulst, Y. Golitsyn, A. Bui, K. Busse, H. Hussain, D. Reichert, J. Kressler. Tailored melting temperatures and crystallinity of poly(ethylene oxide) induced by designed chain defects. *ACS Appl. Polym. Mater.* 1, 3130-3136, 2019.

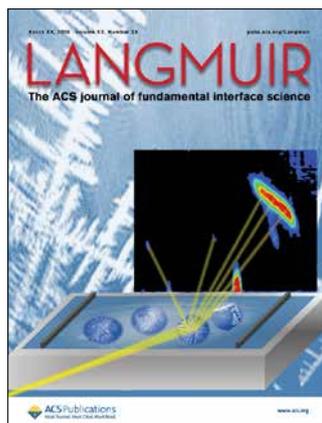
Institute of Chemistry

Physical Chemistry of Polymers

Fields of Research:

- › Physical Chemistry of Polymers
- › Thermodynamics of Polymer Blends, Ion Conductivity, Polymer Crystallisation

We deal with thermodynamic properties of polymers in solution and in bulk. Frequently employed experimental methods are X-ray scattering (see Figure), NMR- and FTIR spectroscopy, and thermo-analytic methods. Furthermore, we study the ion conductivity of polymer electrolytes. In cooperation with the pharmacy department, we develop modern drug release systems.



Crystallization of PEO on the surface of salt solution studied by GI-WAXS.

Current Projects and Future Goals:

■ **Polymer Crystallization on the Water Surface**

The crystallization of PCL on the water surface is studied by various experimental techniques. Especially grazing incidence wide angle X-ray scattering reveals details on the morphology development of PCL crystals which appear during compression of a thin polymer film on a Langmuir trough. Furthermore, the crystallization of PEO on the surface of different salt solutions is investigated with respect to the Hofmeister series.

■ **Modification and Characterization of PEO Networks**

Different PEO network structures have been synthesized by “click” chemistry. The morphology of the networks is investigated by scattering techniques and solid state NMR spectroscopy. Additionally, the Li-ion conductivity for various network structures is studied by impedance spectroscopy.

■ **Biopolyesters for Pharmaceutical Applications**

Aliphatic biopolyesters have been synthesized by enzymatic polycondensation using CAL-B. Thus, functional polyesters with OH-groups at the polymer backbone are obtained. The OH-groups are used for conjugation with drugs or pharmaceutical proteins. A well-defined drug release profile can be achieved.

■ **Modified Hydroxyethyl Starch**

Hydroxyethyl starch is a biodegradable and biocompatible polymer with various applications in pharmacy. It is hydrophilic and water soluble. When OH-groups are partially converted with fatty acids, amphiphilic polymers result. They form different nanostructures in water which are employed for different drug release systems.

Institute of Chemistry

Field Coordination Chemistry and Homogeneous Catalysis

Fields of Research:

- › Preparation and characterization of transition metal complexes and organometallic compounds
- › Synthesis of highly sensitive compounds under inert atmosphere
- › Investigation of reactivity patterns and bond activation processes
- › Homogeneous catalysis involving H_2 : (de)hydrogenation, hydrogen borrowing, hydrogen isotope exchange
- › Catalysis in high pressure autoclaves
- › Quantum Chemical Investigations

Catalytic reactions are used in the production of approx. 80% of the industrially relevant compounds and coordination compounds with tailored properties are commonly used as homogeneous catalysts. The research in our group is focused on basic aspects in coordination chemistry with a special emphasis on the development of new catalysts and potential materials by the utilization of novel ligand-types with tailored properties. This includes the synthesis of new ligands and transition metal complexes under inert atmosphere, as well as the investigation of their reactivity in bond activation processes and catalytic reactions. We focus in our studies on key features of these ligands, such as their donor strength or their cooperative interaction with the central metal atom.

NMR spectroscopy and single crystal X-Ray diffraction are essential methods for our research, which are complemented by quantum chemical investigations in addition to other standard spectroscopic methods in molecular chemistry.

Current Projects and Future Goals:

Novel ligand platforms

Novel ligand platforms for transition metal complexes can lead to new reactivity patterns and trigger unusual bond activation reactions. Ligands based on the element boron were modified in a way that they act as very strong electron-donating ligands in transition metal complexes, which have been used in various catalytic applications so far. By rational modifications of these ligand platforms we intend to increase the activity of catalysts and extend the spectrum of reactions that can be catalyzed.

Catalytic reactions involving hydrogen

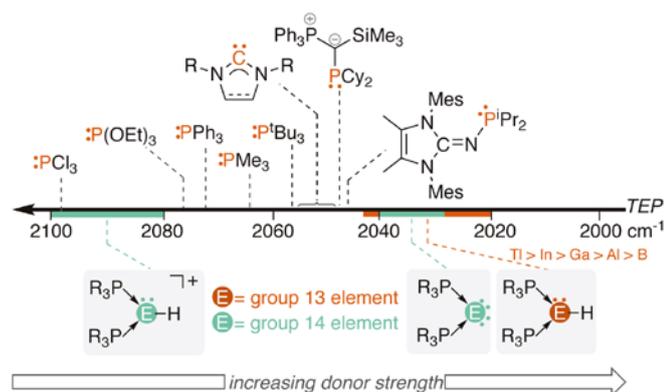
Reactions involving dihydrogen are known to be atom economic and potentially useful for hydrogen storage as well as the preparation of CO_2 -neutral fuels, but they require the presence of a catalyst. Our goal is to develop more environmentally benign catalysts, which are, for instance, based on 3d-metals for these reaction.

Umpolung of Lewis acids Substrates

The reaction of a Lewis acid with a Lewis base usually yields an adduct or a 'frustrated' Lewis pair. This reactivity can be circumvented in the presence of certain dimeric metal complex and a reduced species is formed instead, which subsequently may be transferred to unsaturated substrates. In near future the goal will be to extend this unprecedented reactivity to a large number of Lewis acids and develop new catalytic reactions based on this reactivity.

'Templated' substrate activation

We study unusual S-O, C-N and C-O multiple bond activation schemes triggered by metal-ligand cooperation (MLC) in substrates with nitrile-, imine-, and carbonyl groups, as well as SO_2 and seek to apply the MLC activation sequences in atom-economic coupling reactions (C-C), allowing for waste-free conjugate addition reactions, circumventing classical oxidative addition / reductive elimination processes.



Prof. Dr. Robert Langer

2001–2006

studies in Chemistry at Martin Luther University Halle-Wittenberg and University Karlsruhe (TH), Germany

2009

PhD in Inorganic Chemistry with Prof. Dr. D. Fenske, University Karlsruhe (TH), Germany

2009–2011

Postdoc with Prof. Dr. D. Milstein, Weizmann Institute of Science, Rehovot, Israel

2011–2019

Independent group leader, Philipps-University Marburg, Germany

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Selected publications:

A. Bäcker et al. Redox-active, boron-based ligands in iron complexes with inverted hydride reactivity in dehydrogenation catalysis, *ACS Catalysis* (2019), 9, 7300–7309.

Maser et al. Quantifying the Donor Strength of Ligand-Stabilized Main Group Fragments, *J. Am. Chem. Soc.* (2019), 141, 7596–7604.

Vondung et al. Ambireactive $(R_3P)_2BH_2$ -groups facilitating temperature-switchable bond activation by an iron complex. *Chem. Eur. J.* (2018), 24, 1358–1364.

Grätz et al. Donor ligands based on tricoordinate boron formed by B-H-activation of bis(phosphine)boronium salts. *Chem. Commun* (2017), 53, 7230–7233.

Vondung et al. Phosphine-Stabilized Borylenes as Ligands? Redox Reactivity in Boron-Based Pincer Complexes. *Angew. Chem. Int. Ed.* (2016), 55, 14450–14454.

Schneck et al. Selective Hydrogenation of Amides to Amines and Alcohols Catalyzed by Improved Iron Pincer Complexes. *Organometallics* (2016), 35, 1931–1943.

Donor strength of different ligands in comparison



Jun.-Prof. Dr.
A. Wouter Maijenburg

2014

PhD in Inorganic Materials Science,
University of Twente, Enschede, the
Netherlands

2014–2016

Postdoc, GSI Helmholtz Centre for
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Selected publications:

F. Caddeo et al. Tuning the size and shape of nanoMOFs via templated electrodeposition and subsequent electrochemical oxidation, *ACS Appl. Mater. Interfaces* (2019), 11, 25378–25387.

L. Movsesyan et al. ZnO nanowire networks as photoanode model systems for photoelectrochemical applications, *Nanomaterials* (2018), 8, 693.

H. Zhang et al. Bifunctional heterostructure assembly of NiFe LDH nanosheets on NiCoP nanowires for highly efficient and stable overall water splitting, *Adv. Func. Mater.* (2018), 28, 1706847.

A.W. Maijenburg et al. Insight into the origin of the limited activity and stability of p-Cu₂O films in photoelectrochemical proton reduction, *Electrochimica Acta* (2017), 245, 259–267.

A.W. Maijenburg et al. Preparation and use of photocatalytically active segmented Ag₂ZnO and coaxial TiO₂-Ag nanowires made by templated electrodeposition, *J. Vis. Exp.* (2014), 87, 51547.

A.W. Maijenburg et al. Ni and p-Cu₂O nanocubes with a small size distribution by templated electrodeposition and their characterization by photocurrent measurement, *ACS Appl. Mater. Interfaces* (2013), 5, 10938–10945.

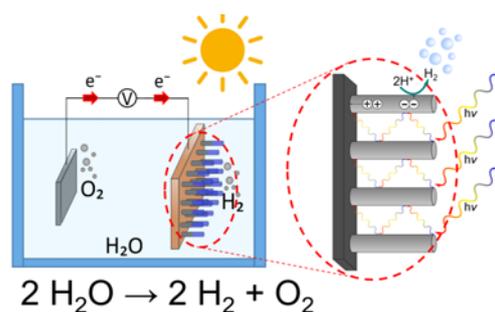
Institute of Chemistry & ZIK SiLi-nano

Inorganic Functional Materials – Light for Hydrogen

Fields of Research:

- › Nanostructure design for solar water splitting
- › Photochemical and photoelectrochemical water splitting
- › H₂ evolution reaction (HER) and O₂ evolution reaction (OER)
- › Soft-chemical nanostructure synthesis via e.g. electrodeposition and electrospinning
- › Photochemical and -physical characterization via e.g. PEC, GC, fs-TAS and PEIS

In our group, we are specialized in the preparation of different kinds of nanostructures like nanowires or nanofibers, and investigate their efficiency for the formation of hydrogen as a renewable and clean energy source via photo(electro)chemical (PEC) water splitting. The unique physical and chemical properties of quasi-one-dimensional nanostructures that arise by their high surface-to-volume ratio make these nanostructures very promising for photo(electro)-chemical applications, but the physical properties of most semiconductors also demand the use of such elongated nanostructures. For instance, the diffusion length of charge carriers (electrons and electron holes) in Cu₂O is only 20–100 nm, while the absorption depth near the bandgap is approximately 10 μm. This means, that if Cu₂O films would be used for photoelectrochemical water splitting, fast charge carrier transport to the semiconductor surface without electron-hole recombination can only be achieved within the top 1% of a Cu₂O film with optimized thickness for maximum light absorption. On the other hand, with the use of one-dimensional nanostructures, an optimum in both the absorption depth and charge carrier diffusion length can be found for efficient H₂ evolution: i.e. a maximum of solar light can be absorbed over the nanowire length, while the nanowire diameter is small enough for efficient electron and hole diffusion (see figure), and therefore high efficiency.

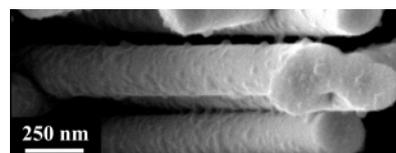


Schematic illustration of optimized photoelectrochemical water splitting using quasi-one-dimensional nanostructures.

Current Projects and Future Goals:

■ Metal-Organic Frameworks

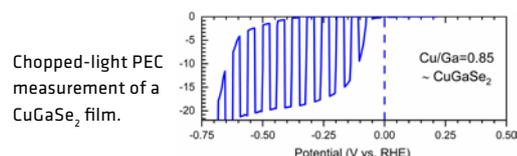
Using controlled electrochemical oxidation, we can convert metal (oxide) nanostructures into a respective Metal-Organic Framework (MOF) and form for instance core-shell Cu₂O@Cu₃(BTC)₂ nanowires (see figure) with new synergistic properties.



Core-shell Cu₂O@Cu₃(BTC)₂ nanowires.

■ Metal oxide nanowires and nanofibers

With soft-chemical methods like templated electrodeposition and electrospinning, we are able to grow metal oxide nanowires and nanofibers in a controlled fashion. Some examples of metal oxides that are highly interesting for photo(electro)chemical applications are CuBi₂O₄, Cu₂O, BiVO₄ and CuFeO₂.



Chopped-light PEC measurement of a CuGaSe₂ film.

■ CuGa_xSe_y films

In collaboration with Roland Scheer, we recently obtained surprisingly high solar-to-hydrogen efficiencies when using CuGaSe₂ and CuGa₃Se₅ films. For CuGaSe₂, we obtained a photocurrent density of -19 mA/cm² (see figure), corresponding to the conversion of 86% of the incident solar light into electrochemical energy.

■ Atomic Layer Deposition

Atomic layer deposition (ALD) is a powerful method for the deposition of high-quality ultrathin films, which can even be used to conformally coat high aspect ratio nanostructures. In collaboration with the MPI of Microstructure Physics, we developed a new ALD recipe for the controlled deposition of CoP, which is a highly interesting HER co-catalyst.

■ Photophysical characterization

To investigate the photophysical processes taking place in our samples, we are for instance using femtosecond Transient Absorption Spectroscopy (fs-TAS) in collaboration with Georg Woltersdorf. Other techniques of interest are Time-Resolved Photoluminescence (TPRL), Surface Photovoltage Spectroscopy (SPS) and PhotoElectrochemical Impedance Spectroscopy (PEIS).

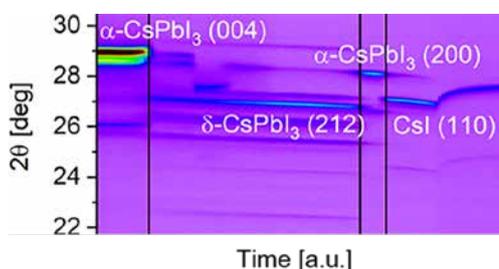
Institute of Physics

Photovoltaics

Fields of Research:

- › Energy converting thin films and complete solar cell devices
- › In-situ growth studies of thin films using real-time X-ray diffraction
- › Electronic device analysis and computer simulation
- › Novel device concepts

Polycrystalline thin film solar cells, also referred to as 2nd generation photovoltaics, are highly complex material systems. Prominent examples are Cu(In,Ga)(Se,S)₂, CdTe, and Halide Perovskites. Cost aspects require their fabrication with low cost but with high performance (high efficiency of solar-to-electrical energy conversion). In order to fulfil these requirements, the solar cells have to be designed based on deep understanding of their functionality and device physics. The strategy of our research group is to tailor their functionality by employing novel schemes for the management of photons and charge carriers, and to analyse their functionality by a combination of electronic experiments and computer simulation. This strategy requires both thin film preparation with the formation of functional devices (complete solar cells) as well as sophisticated analysis techniques. We use a unique thin film growth setup which allows real-time growth control by X-ray methods. And we use sophisticated electronic analysis and simulation techniques in order to study the electronic transport in devices prepared by our group or by research partners from academia and industry.

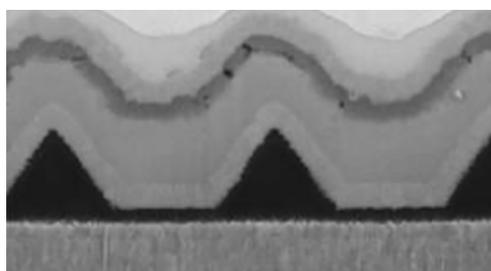


False colour plot of X-ray diffraction intensities during growth and decomposition of perovskite film

Current Projects and Future Goals:

■ Ultrathin solar cells

Ideally, thin film solar cells can be made thinner if light management allows for high absorption and electronic management allows for back contact passivation. We use structured and reflective back contacts for enhanced light absorption in ultrathin devices and we use passivation layers for minimized recombination. For Cu(In,Ga)(Se,S)₂ based solar cells this is done within the framework of the BMWi funded projects MasterPV and EFFCIS.



Cross section of ultrathin structured Cu(In,Ga)(Se,S)₂ solar cell

■ Perovskites for tandems

Mixed halide perovskite solar cells are interesting for tandem devices in combination with Silicon or Cu(In,Ga)(Se,S)₂ bottom cells. However, for this purpose the perovskite thin films need to be prepared by industrially scalable methods. We use co-evaporation in vacuum and study the growth mechanisms by in-situ X-ray diffraction in real-time. The goal is to relate different growth paths with the electronic properties of the resultant thin film devices.

■ Digital twin

In order to optimize the performance of solar cells, a detailed knowledge of their limiting recombination mechanisms is required. In our group, complete 3-dimensional device models are built in the computer which allow to identify the most relevant recombination sites. This work is performed in the frame of BMWi and DFG projects.

■ Novel cell concepts

A completely novel method for photon management could be the combination of 2 photons for one electronic excitation. Thereby much higher efficient solar cells could be built. The trick is to introduce a defect band in the semiconductor. In the framework of a DFG project our group investigates chalcogenide thin films doped with transition metals and analyses their functionality by optical and electronic methods.



Prof. Dr. Roland Scheer

1994

PhD in Solid State Physics, TU Berlin

1994–2010

Staff Scientist at Helmholtz-Centre-Berlin

2002

Research fellow, National Institute for Advanced Industrial Science and Technology, Tsukuba, Japan

2003–2005

Lecturer, Physics Department, University Potsdam, Germany

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Full professorship (W3) for Photovoltaics at the Institute of Physics, Martin Luther University Halle-Wittenberg

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Selected publications:

T Hölscher, S Förster, T Schneider, M Maiberg, W Widdra, R Scheer, Light induced degradation of Cu(In,Ga)Se₂ thin film surfaces, Applied Physics Letters (2017) 111 (1), 011604.

E Jarzembowski, B Fuhrmann, H Leipner, W Fränzel, R Scheer, Ultrathin Cu (In, Ga) Se₂ solar cells with point-like back contact in experiment and simulation, Thin Solid Films (2015) 633, 61–65.

M Maiberg, T Hölscher, S Zahedi-Azad, R Scheer, Theoretical study of time-resolved luminescence in semiconductors. III. Trap states in the band gap, Journal of Applied Physics (2015) 118 (10), 105701.

P Pistor, J Borchert, W Fränzel, R Csuk, R Scheer, Monitoring the phase formation of coevaporated lead halide perovskite thin films by in situ x-ray diffraction, The journal of physical chemistry letters (2014) 5 (19), 3308–3312.

R Scheer, HW Schock, Chalcogenide photovoltaics: physics, technologies, and thin film devices, (2011) John Wiley & Sons.



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PhD in Experimental Physics,
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1999–2003

Group leader, Max Planck Institute
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Habilitation at the Martin Luther
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In conjunction with executive vice
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Selected publications:

X. Liao et al., High strength in combination with high toughness in robust and sustainable polymeric materials, *Science* (2019) 366, 6471, pp. 1376–1379.

Wehrspohn et al., Nanometallurgical Silicon for Energy Production and Storage, *Joule* 3(5) 1172, 2019.

Zhang et al., Bifunctional Heterostructure Assembly of NiFe LDH Nanosheets on NiCoP Nanowires for Highly Efficient and Stable Overall Water Splitting, *Advanced Functional Materials* 28(14):1706847, 2018.

Piechulla et al., Fabrication of Nearly-Hyperuniform Substrates by Tailored Disorder for Photonic Applications, *Adv. Optical Mater.*, 2018, 1701272.

Institute of Physics & Fraunhofer Institute for Microstructure of Materials and Systems**Solid State Physics****Fields of Research:**

- › Silicon electrochemistry
- › Photon management
- › X-ray microscopy for 3D analysis of porous samples

Silicon is the element on which most of the group's work is focused on. We use it to create porous structures via (photo-)electrochemical etching processes or functionalize it by the deposition of various layer via sputtering, chemical deposition or atomic layer deposition. Such Si based materials are tested for new battery concepts like the silicon air battery because of its high specific energy density.

Also more complex structures like transition metal phosphides are used to build electrocatalysts for the efficient direct water splitting. This is part of our contribution to the production of green hydrogen as a future energy carrier.

The second research focus of the group is nanophotonics, i.e. the interaction of light with artificial nanostructures to investigate new ways of light control. A particular emphasis lies on enhancing performance of optoelectronic devices such as solar cells and OLEDs. This also includes the development of scalable fabrication processes to facilitate nanophotonic interfaces on the device level relevant for industrial application.

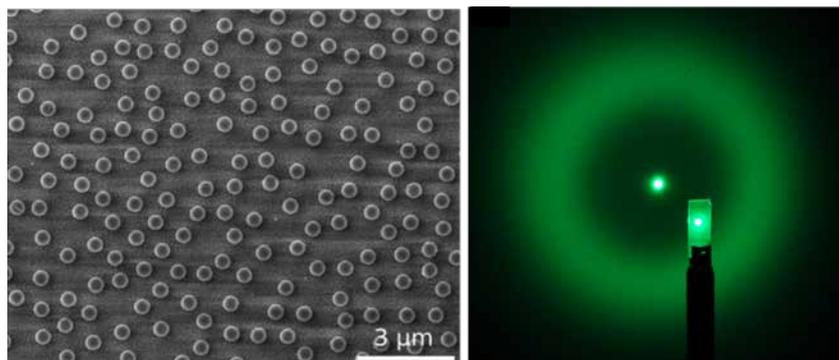
Since November 2017, our chair has been using the X-ray microscope ZEISS Xradia 810 Ultra, financed by the DFG, to study and characterize advanced materials. With our X-ray microscope, we can produce three-dimensional virtual representations of microscopic samples non-destructively, allowing the detailed visualization of internal parts of the sample, their morphological characterization and also the estimation of structural parameters using software analysis.

Current Projects and Future Goals:**X-ray microscopy**

We have used this technique to characterize a few different types of materials in our group, including protein fleeces, porous silicates and drugs. Recently, we characterized sustainable polymeric yarns in a work performed in collaboration with researchers from the University of Bayreuth and other partners in Germany, China, and Switzerland. Our partners have developed a straightforward method to synthesize yarns consisting of nanofibrils of polyacrylonitrile (PAN) aligned in the same direction and interconnected via poly(ethylene glycol) bisazide. The yarns, with high strength in combination with high toughness, have overall properties similar to dragline spider silk. Our characterization using the X-ray microscope was key for the visualization of the orientation of the fibrils. With X-ray imaging, there was no need to cut or destroy the yarns to obtain the three-dimensional of the samples. The images not only enabled the visualization of the yarns non-destructively but also allowed the computational analysis to estimate the high degree of uniform orientation of the fibrils.

Tailored disorder for a tailored optical response

Between the contrary extremes of strictly periodic structures (spectrally well-defined optical response) and purely random structures (broadband response) lies the huge configuration space of correlated disorder, which has just started to being explored. Therein lie configurations of so-called hyperuniform disorder. Hyperuniformity represents exciting new states of disordered -but not at all random- matter, giving rise to unforeseen phenomena not just in the field of optics but for any wave excitations. Our group investigates hyperuniform configurations of optical scatterers to explore novel ways to tailor light scattering on demand.



Disordered hyperuniform configuration of TiO₂ Mie resonators (left) and their scattering spectrum (right) (taken from Piechulla et al., *Adv. Opt. Mater.* 2018, 1701272)

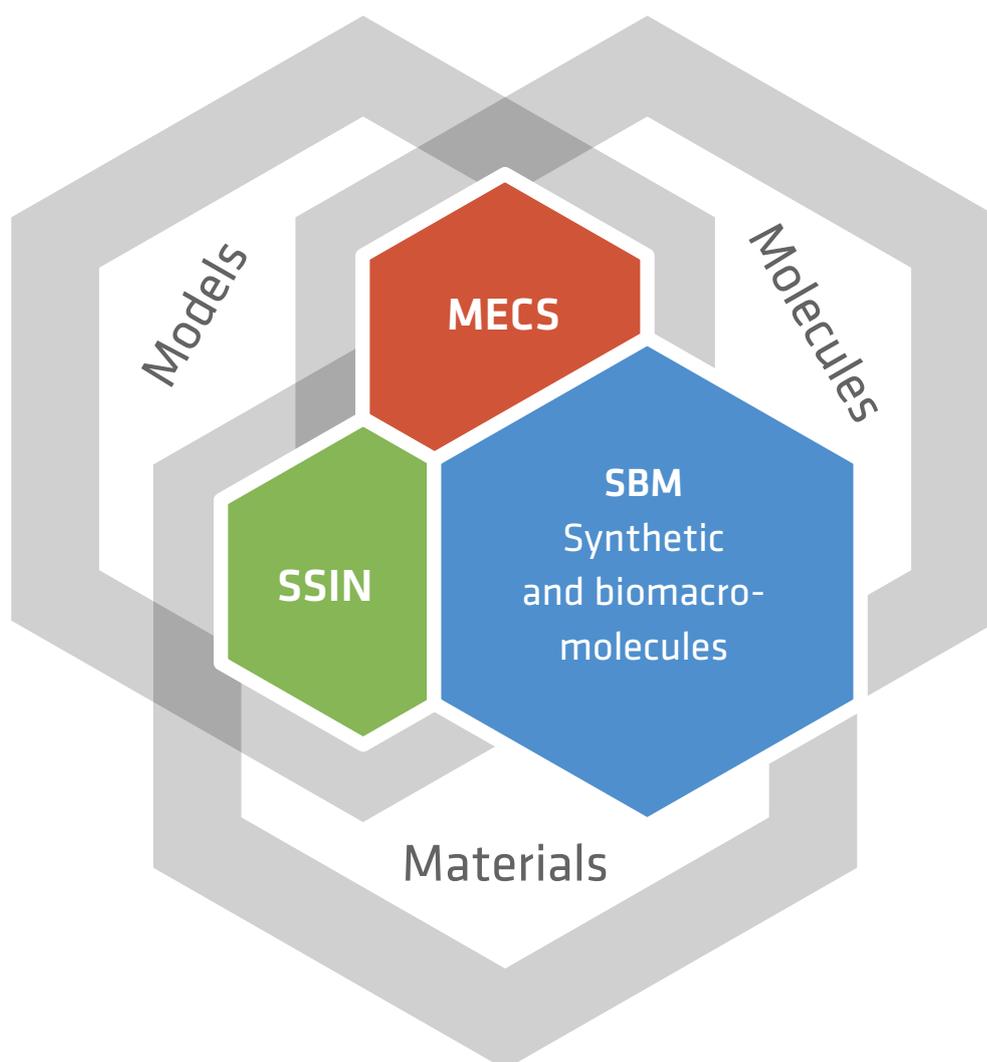


Synthetic and bio- macromolecules

(Bio)-Macromolecules are key molecules, indispensable for modern society. They are not only found in living organisms or used in medicine, but are also needed in modern technology such as in structural materials (aeroplanes, cars) or in modern energy- or information technology. We strive to interface structure, function and dynamics of large (bio)-molecules, aiming to design, prepare and model specific functions of synthetic polymers and (bio)-macromolecules in view of their micro- and nanostructure. The molecular design, synthesis and assembly processes of (bio)-molecules such as lipids, metal-complexes, cellulose, enzymes, synthetic polymers, proteins or carbon-materials are addressed both, theoretically and experimentally.

These activities are supported by several national and international network initiatives such as the SFB TRR 102 (Polymers under Multiple Constraints – Restricted and Controlled Molecular Order and Mobility), the RTG/GRK 2670 (Self-Organization of Soft Matter Via Multiple Noncovalent Interactions), the International Graduate School AGRIPOLY and the Center of Innovation Competence (ZIK) HALOmem.

Being a strongly interdisciplinary oriented research area we address to reach closed material cycles, specifically in the study programs Bachelor and Master in Chemistry/Physics or the special Master program “Polymer Materials Science”.



Institute of Chemistry & BMBF Center HALOmem & Charles Tanford Protein Center

Biophysical Chemistry

Fields of Research:

- › Protein and membrane biochemistry
- › Reconstitutions using model membranes
- › Polyphilic interactions with membranes
- › Structure and dynamics of membrane protein complexes
- › Membrane lateral organization
- › Effects of proteins on membrane morphology and organization
- › Diffusion and binding analysis with fluorescence fluctuation spectroscopy
- › Fluorescence microscopy and cryo-electron microscopy

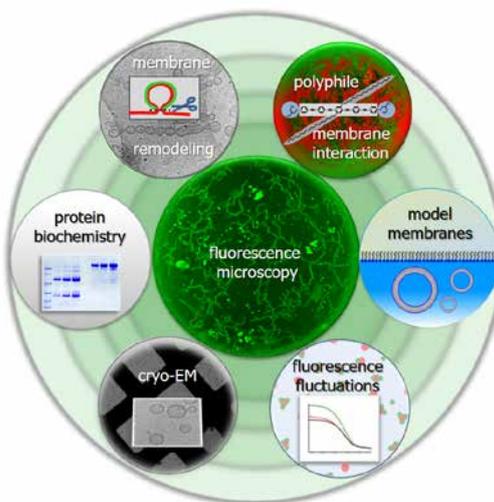
Cellular membranes have crucial roles in many biological functions. We study the interaction between the membrane bilayer and proteins that form an integral part of the membrane or reversibly associate with it. From a life science perspective, we are interested in intracellular trafficking, an essential process that ensures protein and lipid transport between cellular compartments in eukaryotes. We are interested in the spatial and temporal interplay of factors governing transport vesicle formation. In particular, we seek to understand the sculpturing and the separation (fission) of a nascent membrane transport vesicle.

We use a broad range of artificial membrane systems to interrogate dynamic lateral organization, membrane morphology and protein-lipid interactions. Proteins are expressed, purified, fluorescently labeled and studied in combination with various types of model membranes. Biological function is studied using physicochemical and optical approaches alongside with biochemical and molecular biology techniques. Cryo-electron microscopy and confocal fluorescence microscopy allow us to visualize morphological consequences of protein-membrane interactions in reconstituted systems. Fluorescence fluctuation spectroscopy including dual-color Fluorescence Cross-Correlation Spectroscopy is used to obtain quantitative information on binding and dynamics. Model membrane and fluorescence methods are advanced to gain new insights into protein-membrane interactions.

Current Projects and Future Goals:

Fluorescence Correlation Spectroscopy (FCS)

FCS is a powerful, highly selective and highly sensitive optical fluctuation technique that allows to analyze the mobility, coincident motion and interactions of molecules in reconstituted systems and living cells. We have refined dual-color Fluorescence Cross-Correlation Spectroscopy (dcFCCS) to monitor membrane protein reconstitution and to quantitatively analyze protein binding to membranes. We plan to further advance fluorescence fluctuation spectroscopy techniques for a yet more detailed description of protein-membrane binding.



Model membrane systems for research and applications

We develop and apply model membrane techniques to bridge the gap between well-defined, yet simplistic synthetic lipid bilayer models and natural biological complexity. Recently, we have devised a method to generate giant unilamellar vesicles from natural endoplasmic reticulum (ER) membranes, providing an accessible model system for functional *in vitro* studies of the ER. We plan to apply our reconstitution and binding analysis approaches to investigations of further biological systems, such as protein-membrane interactions in plant cells and the uptake of the SARS-CoV-2 virus into human cells.

In vitro reconstitution of intracellular processes

We investigate membrane binding and remodeling activity of the COPII proteins, which are involved in transport vesicle formation at the ER, using dcFCCS, advanced fluorescence microscopy and cryo-electron microscopy in combination with molecular biology. We want to further explore how the hydrolysis of GTP and the membrane remodeling and fission processes are coordinated in space and time.



Prof. Dr. Kirsten Bacia

2001–2007

Graduate student and postdoc (MPI-BPC, Göttingen; MPI-CBG, Dresden; BIOTEC, Dresden, Germany)

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Dr. rer. nat., University of Dresden

2007–2009

Postdoc, UC Berkeley, USA

2009–2015

HALOmem Junior Group Leader, Martin Luther University Halle-Wittenberg

2012–2015

Juniorprofessor (W1), Martin Luther University Halle-Wittenberg

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Professor (W2) of Biophysical Chemistry, Martin Luther University Halle-Wittenberg

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Selected publications:

M. Grimmer, K. Bacia, Giant Endoplasmic Reticulum vesicles (GERVs), a novel model membrane tool. *Sci. Rep.*, 2020, 10(1), 3100.

S. Werner et al., A Quantitative and Reliable Calibration Standard for Dual-Color Fluorescence Cross-Correlation Spectroscopy. *ChemPhysChem*, 2018, 19, 1–10.

D. Krüger et al., Measuring Protein Binding to Lipid Vesicles by Fluorescence Cross-Correlation Spectroscopy. *Biophys. Journal*, 2017, 113(6), 1311–1320.

C. Schwieger et al. Binding of the GTPase Sar1 to a Lipid Membrane Monolayer: Insertion and Orientation studied by Infrared-Reflection-Absorption Spectroscopy. *Polymers*, 2017, 9, 612.

S. Werner et al., Dendritic Domains with Hexagonal Symmetry Formed by X-Shaped Bolapolyphiles in Lipid Membranes. *Chem. Eur. J.*, 2015, 21, 8840–8850.

G. Zanetti et al., The structure of the COPII transport-vesicle coat assembled on membranes. *eLife*, 2013, 2:e00951.



Prof. Dr. Jochen Balbach

1994

PhD in Chemistry, TU München

1994–1996

PostDoc, University of Oxford, UK,
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Senior scientist, Univ. Bayreuth

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Habilitation in Biochemistry,
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Selected publications:

Klamt, A. et al. Hyperbolic pressure-temperature phase diagram of the zinc-finger protein apoKti11 detected by NMR. *J. Phys. Chem.* (2019), 123, 792–801.

Evgrafova, Z., et al. Probing polymer chain conformation and fibril formation of peptide conjugates. *Chem. Phys. Chem.* (2019), 20, 236–240.

Kumar, A. et al. Phosphorylation-induced unfolding regulates p19^{INK4d} during the human cell cycle. *Proc. Natl. Acad. Sci. USA* (2018), 115, 3344–3349.

Kumar, A. et al. Small Molecule Inhibited Parathyroid Hormone Mediated cAMP Response by N-Terminal Peptide Binding. *Scientific Reports* (2016), 6, 22533.

Garvey, M. et al. Molecular architecture of A β fibrils grown in cerebrospinal fluid solution and in a cell culture model of A β plaque formation. *Amyloid* (2016), 23, 76–85.

Dinesh, D.C. et al. Solution structure of the PsIAA4 dimerization domain reveals interaction modes for transcription factors in early auxin response. *Proc. Natl. Acad. Sci. USA* (2015), 112, 6230–6235.

Institute of Physics

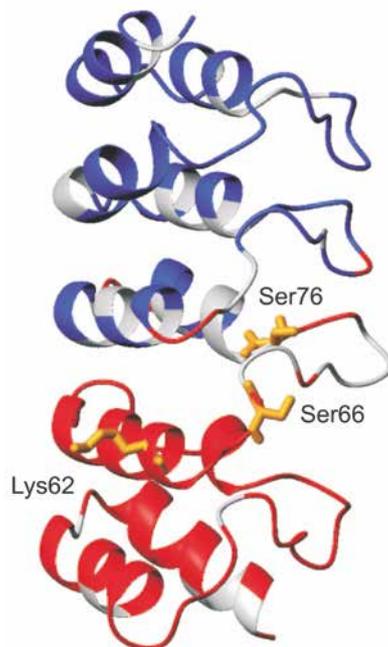
Biophysics

Fields of Research:

- › High-resolution NMR spectroscopy
- › Structural biology of medically relevant proteins
- › Biophysics of protein folding and stability
- › Intrinsically disordered biopolymers
- › Amyloid fibril formation

Proteins and nucleic acids are the biopolymers, which control all processes in living systems. Their function is closely related to their molecular structure. Our group uses high resolution NMR spectroscopy and various biophysical methods (including absorption, fluorescence, CD, calorimetry, and in collaborations crystallography, single-molecule spectroscopy, cryo electron microscopy) to investigate the structure, dynamics, and function of these biomacromolecules as well as functionally relevant interactions with other proteins, nucleic acids, low molecular substrates, metal ions and lipids/membranes.

Our biophysical tools are employed to follow the self-assembly process of the protein chain towards its three dimensional structure, called protein folding. Many protein folding events are closely related to severe diseases and therefore, we investigate aggregation prone and intrinsically disordered proteins and their relation to function and dysfunction. We are interested in the fundamental and polymer physical principles driving protein order and disorder to fulfil their function.



Protein structure of the p19^{INK4d} protein, which regulates the human cell cycle

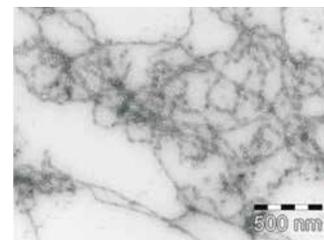
Current Projects and Future Goals:

Protein folding and biophysical methods

The gain of Gibbs free energy (ΔG) drives the protein folding reaction towards the native, biologically active state. Several thermodynamic parameters including the temperature, the chemical potential, or the pressure change ΔG and thus induce un- or refolding. For several proteins, we could disclose the molecular folding mechanism and found a direct link to the respective biological function.

Medically relevant proteins

We investigate the structural biology of several human proteins mainly by NMR spectroscopy including G-protein coupled receptors, hormones, eye lens crystallins, ankyrin repeat proteins, hub proteins and membrane remodelling proteins, which are involved in respective diseases including osteoporosis, cataract, cancer, and muscle dystrophies. We will extend our studies now to different proteoforms of transcription factors of plants, involved in plant pathology and metabolism.



Electron micrograph of functional amyloid fibrils of the human parathyroid hormone

Amyloid fibril forming proteins

Protein folding of soluble, globular proteins is dominated by intramolecular interactions, whereas protein aggregation and fibril formation is dominated by intermolecular interactions between individual peptide and protein chains. The goal is to understand the fundamental, polymer physical principals of fibril formation. Peptides and proteins under current investigations include the Alzheimer peptide A-beta, poly(A) binding proteins, human eye lens crystallins, and the parathyroid hormone. In the future, conjugates between these peptides and synthetic polymers will be studied.

Intrinsically disordered proteins

A fascinating new class are intrinsically disordered proteins. Protein NMR is especially suited to study the conformational remodelling and dynamics of these proteins. We started and continue in future to correlate molecular properties of this protein class to their function by studying the human Gab1/Grb2 protein system, the parathyroid hormone and plant proteins with disordered domains.

Institute of Chemistry

Polymer Reaction Engineering

Fields of Research:

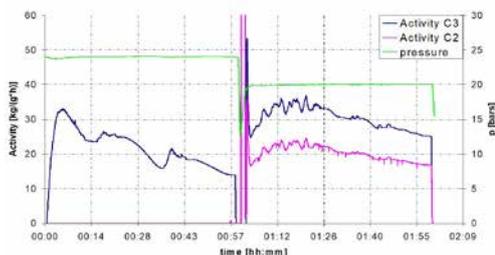
The professorship for Polymer Reaction Engineering is a joined appointment of Martin Luther University Halle-Wittenberg, together with the Fraunhofer Society for Applied Research. Prof. Bartke is also responsible for the Fraunhofer-Polymer Pilot Plant Center PAZ in Schkopau.

Polymers are with a worldwide, annual production of more than 350 Mio. tons an important class of materials. Polyreactions do exhibit various challenges in reaction engineering, e.g. not uniform products, but product distributions are obtained, kinetics of polyreactions are often complex, mass- and heat transfer can play an important role and often there is a significant increase in viscosity during a polyreaction.

Polymer Reaction Engineering deals with the reaction engineering of polyreactions, in particular:

- > analysis, description and optimization of polyreaction kinetics
- > development and design of reactors, reactor configurations and processes

Research focus of our group is in particular measurement and modelling of reaction- and process kinetics of polyreactions.



Kinetic measurements in heco-PP polymerization

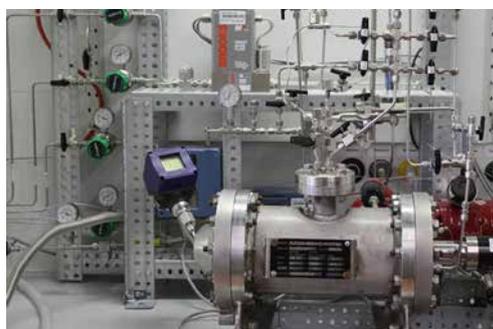
A further focus area is development, optimization and modelling of polymerization processes. A highly specialized lab for coordinative polymerization of olefins is available.

In cooperation with the Fraunhofer Polymer Pilot Plant Center in Schkopau, scale-up of polymerization processes as well as sample synthesis up to the tons scale is possible.

Current Projects and Future Goals:

Kinetic investigations in gas-phase polymerization

In coordinative polymerization, the polymerization kinetics are catalyst dependent. In the frame of an industrially sponsored research project, we investigate the kinetics of industrial catalyst systems in gas-phase polymerization of propene under industrially relevant conditions.



5l gas-phase reactor for polymerization of propene

Reaction Calorimetry

Reaction calorimetry is a method to monitor the reaction rate of exothermic reactions by measuring the chemical heat flow released by the reaction. In our group, we have two different setups for reaction calorimetry. In frame of an industrial co-operation project, reaction calorimetry is applied in order to study kinetics in bulk phase polymerization of propene and to monitor, control and optimize multi-stage polymerization processes, e.g. for the manufacturing of heterophasic polypropylene copolymers.

Scale-up of polyreactions

Scale-up is a critical step during commercialization of new products and processes. In close cooperation with the Fraunhofer Polymer Pilot Plant Center PAZ, which is also headed by Prof. Bartke, scale-up of new processes and products up to the tons scale can be carried out.



Fraunhofer Polymer Pilot Plant Center PAZ, Schkopau



Prof. Dr. Michael Bartke

2002

Dr.-Ing. in Industrial Chemistry, Technical University of Berlin

2001–2005

Senior Scientist, Borealis Polymers Oy, Finland

2005–2006

Research Manager Process Research, Borealis Polymers Oy, Finland

2006–2008

Scientific Director Fraunhofer Polymer Pilot Plant Center (Schkopau, Germany)

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Director Fraunhofer Polymer Pilot Plant Center PAZ, Schkopau

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Selected publications:

Bartke M. Reaktoren für spezielle technisch-chemische Prozesse: Polymerisationsreaktoren. In: Reschetilowski W. (eds) Handbuch Chemische Reaktoren. Springer Reference Naturwissenschaften. Springer Spektrum, Berlin, Heidelberg (2019).

Kröner, T., Bartke, M. Sorption of Olefins in High Impact Polypropylene - Experimental Determination and Mass Transport Modeling. Macromol. React. Eng. (2013), 7, 453–462.

Kröner, T., Lieske, A., Hahn, M., Bartke, M. Modellbasierte Übertragung von satzweisem- auf kontinuierlichen Betrieb am Beispiel einer radikalischen Copolymerisation. Chem. Ing. Tech., (2009), 81, 1837–1843.

Bartke, M. Polymer Particle Growth and Process Engineering Aspects. Kapitel 3 in Severn, J.R., Chadwick, J.C., Tailor-Made Polymers, Wiley-VCH (2008).

Bartke, M., Oksman, M., Mustonen, M., Denifl, P. New Heterogenisation Technique for Single-site Polymerization Catalysts. Macromol. Mater. Eng. (2005), 290, 250–255.



Prof. Dr. Wolfgang H. Binder

1995
PhD in Synthetic Organic Chemistry
(University of Vienna, Austria)

1996-1997
PostDoc (Emory University, USA,
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1997
PostDoc (University of Vienna,
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Since 2007
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Selected publications:

J. Freudenberg and W. H. Binder. Chirality control of screw-sense in Aib-polymers: synthesis and helicity of amino acid functionalized polymers, *ACS Macro Letters* (2020), 9, 686.

S. Chen, S. S. Parkin, W. H. Binder et al. Gating effects of conductive polymeric ionic liquids. *J. Mater. Chem. C* (2018), 6, 8242-8250.

S. Chen, W. H. Binder et al. Opposing Phase-Segregation and Hydrogen-Bonding Forces in Supramolecular Polymers, *Angew. Chem. Int. Ed.* (2017), 56, 13016.

D. Döhler, W. H. Binder et al. CuAAC Based Click Chemistry in Self-Healing Polymers, *Acc. Chem. Res.* (2017), 50, 2610.

P. Michael and W. H. Binder. A Mechanochemically Triggered "Click" Catalyst, *Angew. Chem. Int. Ed.* (2015), 54, 13918.

S. Chen, W. H. Binder et al. Self-Healing Materials from V- and H-Shaped Supramolecular Architectures, *Angew. Chem. Int. Ed.* (2015), 54, 10188.

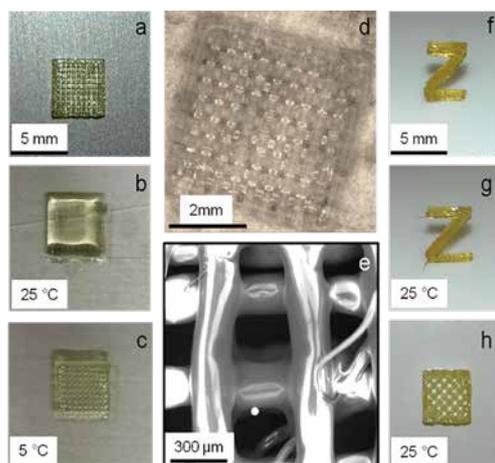
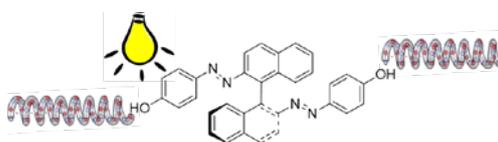
Institute of Chemistry

Polymer Chemistry

Fields of Research:

- › Synthesis and novel analytical methods of macromolecular architectures
- › Biomimetic, renewable and self-healing polymers, 3D-printing
- › Design of nanoscaled medical imaging and drug-delivery systems
- › Develop novel electrolytes for battery and transistor systems
- › Self-healing concepts for thermoplasts, elastomers and electrode-materials
- › Study biological folding, aggregation- and chirality transfer-principles

Macromolecules are key molecules, indispensable for modern society, present as widely known structural materials in e.g. automobiles or aeroplanes, but also in biomedicine, modern energy- or information technology. Research focus in our group is the preparation of *functional polymers* and their application in technology, aiming to design polymers for medicine, as advanced structural materials, or for novel batteries and transistors. Based on the polymer's structural complexity we use all living polymerizations and modern functionalization strategies known from synthetic organic chemistry, including "click"-based methods. Novel polymeric architectures and the site-specific integration of supramolecular interactions (such as hydrogen bonds, ionomers, mechanophores) into tailored macromolecules generate advanced materials in the areas of biomedicine, modern imaging technology, batteries, transistors or for self-healing and 3D-printing technologies.



Current Projects and Future Goals:

Biomimetic, renewable and self-healing polymers

Reuse and life-cycle-enhancement of polymers are among the most pressing societal needs. We address novel concepts for reusing thermoplastics and thermosets based on vitrimers, self-healing materials and reusable rubbers, funded by the graduate school AGRIPOLY, DFG- and EU-projects.

Novel electrolyte-polymers for battery and transistor systems

Improved charge-transport and the compensation of volume-changes is crucial in the technology of modern batteries, fuel-cells and transistors. Several EU/DFG-funded projects (Bat4ever within Horizon-2020, DFG) do address the chemical synthesis of novel self-healing ionomers and ionogels.

Study biological folding-, assembly and chirality transfer-principles

Secondary-structure of proteins and peptides is determining their function in living systems, in its undesired assembly being responsible for e.g. Alzheimer's disease. Projects deal with amyloid-proteins to understand and prevent disease-relevant aggregation via synthetic polymers, able to fold- and unfold during aggregation.

3D-printing of materials

Three dimensional (3D)-printing technology has become societies leading method to form materials for many applications. We use multimode 3D-printing methods to prepare modern materials, with embedded self-healing-, mechanochromic- and pharmaceutical function. Material-focus is placed on novel battery-electrodes, drug-release systems, stress-sensing- and (bio)-degradable soft/hard interfaces.

Design of nanoscaled medical imaging systems and artificial membranes

Imaging technology is among the most important technique for the early detection of diseases in humans, allowing to detect and heal diseases in tissue. We develop novel concepts of ultrascaled nanoparticles for near-infrared (NIR)-detection, able to visualize tissue-morphology via photoacoustic- and (NIR)-techniques. The method is extended towards tissue-specific detection of metabolic profiles.

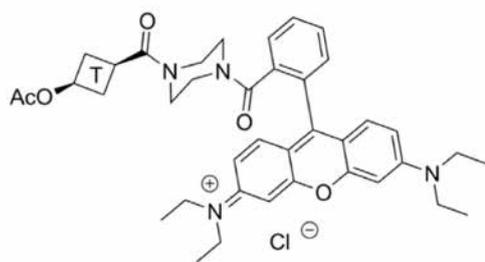
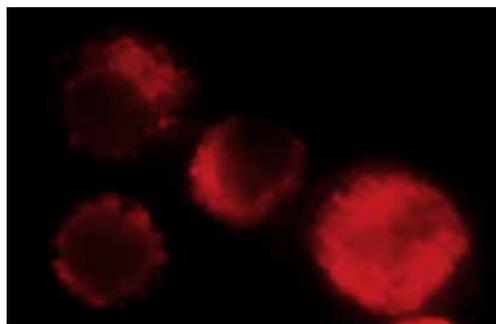
Institute of Chemistry

Organic Chemistry

Fields of Research:

- › Antitumor and antidementia active compounds from natural products
- › Ancient dyes and modern materials for photovoltaics

The evolution of complex life is strictly dependent on mitochondria found in all complex cells. Mitochondria fuel the metabolic reactions that create and maintain all other structures of the cells. Cancer is among the top-most causes of death and one of the most feared diseases. A modern approach to the therapy consists in the triggering of programmed cell death (apoptosis). Mitochondria-targeted drugs may induce apoptosis and overcome problems of drug resistance. Pentacyclic triterpenes and their derivatives are useful candidates to reach these aims. Pentacyclic triterpenes and their structurally simplified derivatives can also be used to make compounds available that might be effective against age-related dementia.



An additional highlight is the synthesis of functionalized (natural) products using biocatalytic reactions as well as advanced catalytic processes to perform reactions with high regio-, enantio- and diastereoselectivity using mild reaction conditions and modern concepts of “green chemistry”. These syntheses are also used to access novel materials for photovoltaics.

A further focus is the analysis of old dyes, colorants and pigments. Thereby, the time span of the examined samples ranges from about 3000 BC to the early industrial age.

Current Projects and Future Goals:

Natural product derived antitumor active compounds

The extraordinary chemical diversity encompassed by natural products continues to be of relevance to drug discovery. Therapy of cancer by inducing programmed cell death (apoptosis) is in the focus of scientific research. Quite often, in cancer cells the sensitivity towards apoptosis is reduced thus ultimately leading to an inappropriate cell survival and malignant progression. These problems can be addressed by developing mitochondria-targeted drugs. Recently we could show that natural product derived conjugates holding an extra rhodamine B moiety attached to the skeleton of the natural product via a suitable spacer exhibit cytotoxicity in a nano-molar range while retaining high tumor cell selectivity. Our future activities will focus on the design and synthesis of molecules that act as “mitocanes” (mitochondrial targeted cytotoxic agents) and at the same time also inhibit other enzymes that are particularly involved in tumor growth. Furthermore, the synthesis of cytotoxic molecules is planned, which are linked to a molecular switch thus allowing biological activity to be turned on and off at will.

Novel materials for OLEDs

The production of reproducible and closed DSSCs (“Dye Sensitized Solar Cells”) was defined as one of the most important goals. The synthesis of proprietary dyes for use in DSSCs and their subsequent evaluation is planned.

This project, which focuses among other things on the synthesis and evaluation of dyes for photovoltaics, is closely related to the development and application of highly sensitive analytical methods. The knowledge gained from these investigations will also be used to carry out dye analysis on historical materials from all over the world.



Prof. Dr. René Csuk

1984

PhD in Organic Chemistry, Graz, University of Technology, Austria

1986–1989

Post-Doc (University Zurich, Switzerland, Prof. A. Vasella)

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Habilitation, University of Heidelberg

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Full Professor (C3), Pharmaceutical Chemistry, University Heidelberg

Since 1995

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Selected publications:

M. Blaess et al., Lysosomes and lysosomotropism in SARS-CoV-2 infection and COVID-19 implicate personal risks and new strategies in prophylaxis and treatment, *Intern. J. Mol. Sci.* (2020), 21, 4953.

B. Brandes et al., Design, synthesis and cytotoxicity of BODIPY FL labelled triterpenoids, *Eur. J. Med. Chem.* (2020), 185, 111858.

M. Garcia-Altare et al., Mapping Natural Product Dyes in Archeological Textiles by Imaging Mass Spectrometry, *Sci. Reports* (2019), 9, 2331.

J. Wiemann et al., An access to a library of novel triterpene derivatives with a promising pharmacological potential by Ugi- and Passerini multicomponent reactions, *Eur. J. Med. Chem.* (2018), 150, 176–194.

S. Sommerwerk et al., Rhodamine B conjugates of triterpenoic acids are cytotoxic mitocanes even at nanomolar concentrations, *Eur. J. Med. Chem.* (2017), 127, 1–9.

K. Miettinen et al., The ancient CYP716 family is a major contributor for the diversification of eudicot triterpenoid biosynthesis, *Nature Commun.* (2017), 8, 14153.



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Marcus A. Glomb

Staatl. gepr. Lebensmittelchemiker

1988–1989

Sandoz AG, Nuremberg, Germany

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PhD in Food Chemistry, University of Stuttgart, Germany

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PostDoc, Case-Western-Reserve-University, Cleveland/Ohio, USA

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Habilitation, Technical University Berlin, Germany

Since 2004

Full Professor (C4) of Food Chemistry, Martin Luther University Halle-Wittenberg

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Selected publications:

T. Baldensperger et al. Comprehensive analysis of posttranslational protein modifications in aging of subcellular compartments, *Sci. Rep.* (2020), DOI: 10.1038/s41598-020-64265-0.

T. Heymann et al. Influence of β -carotene and lycopene on oxidation of ethyl linoleate in one and disperse phased model systems, *J. Agric. Food Chem.* (2020), DOI: 10.1021/acs.jafc.9b07862.

N. Mertens et al. Oxidative fragmentation of aspalathin leads to the formation of dihydrocaffeic acid and the related lysine amide adduct, *J. Agric. Food Chem.* (2020), DOI: 10.1021/acs/jafc.9b07689.

T. Jost et al. Efficient analysis of 2-acetyl-1-pyrroline in foods using a novel derivatization strategy and LC-MS/MS, *J. Agric. Food Chem.* (2019), DOI: 10.1021/acs.jafc.9b00220.

C. Henning et al. Analysis and chemistry of novel protein oxidation markers in vivo, *J. Agric. Food Chem.* (2018), DOI: 10.1021/acs.jafc.8b00558.

M. Smuda and M. A. Glomb. Maillard degradation pathways of vitamin C, *Angew. Chem. Int. Ed.* (2013), DOI: 10.1002/anie.201300399.

Institute of Chemistry

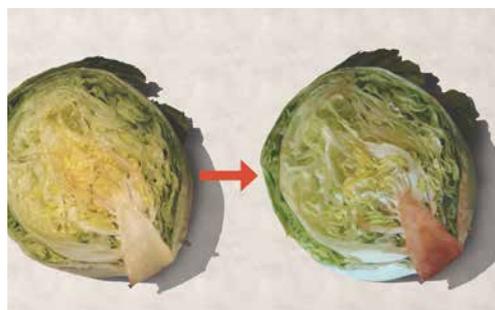
Food Chemistry

Fields of Research:

- › Non-enzymatic browning, Maillard Reaction
- › Enzymatic browning
- › Isolation and characterization of food ingredients
- › Synthesis of target compounds
- › Analytical and preparative chromatography

The term non-enzymatic browning or Maillard reaction describes the amine catalyzed degradation of reducing sugars. Although the reaction in general has been known for a long time, reactive intermediates and major reaction pathways still need to be uncovered. Our group has established all relevant α -dicarbonyl structures within the degradation of major hexoses and disaccharides including ascorbic acid. β -Dicarbonyl and oxidative α -dicarbonyl cleavages were found as the major degradation routes to explain almost all fragmentation products and known end products. In addition, these mechanisms lead to a novel class of Advanced Glycation Endproducts with amide structure, which were established as quantitative important posttranslational protein modifications. In contrast, enzymatic browning involves oxidation of polyphenols and other secondary plant products and follow-up non-enzymatic reactions such as oxidative coupling and polymerization ultimately lead to high-polymeric brown melanins. In this respect the major mechanistic degradation pathways during rooibos tee fermentation were unraveled. Different to the chemistry of black tee the dihydrochalcon aspalathin was identified as the key polyphenolic compound. Rooibos browning mechanisms include single-electron transfer reactions leading to fragmentation and entail protein modification.

As a general approach of our work group target structures are either isolated from food by the complete array of chromatographic methods including counter current setups or are synthesized independently. Authentic materials can then be used in independent model incubations to clarify novel reaction pathways relevant in foods or physiological systems on a molecular basis.



Current Projects and Future Goals:

Controlling Maillard Reaction pathways

Novel mechanistic pathways leading to defined protein modifications can be used to tailor generate foods of specific demands. Ideally this approach only involves traditional preparation techniques without the need for artificial additives or flavorings. It can also be used to generate technical products based on targeted modification of biopolymers from food processing side streams including e.g. gelatin. In vivo this knowledge will help to find cures against late complications of e.g. diabetes and aging. The latter is currently under investigation within a DFG research training group with the focus on the relation of posttranslational protein modifications and aging (ProMoAge – RTG 2155).

Mechanisms of enzymatic browning

The tea related mechanisms were extended to the identification of the major brown chromophores found in cut salad, which is found among other to-days convenient preparations in food markets. In contrast, here enzymatic degradation is based on the modification of bitter components including sesquiterpene lactones rather than that of polyphenols. This opens new insights to alternative reaction pathways based on secondary plant products and to new strategies to prevent unknown browning of vegetables. Thus, secondary plant products are currently screened for their browning potential in addition to physiologically positive effects.

Understanding of fat autoxidation mechanisms

Although general pathways of fat autoxidation are known for decades, most research was conducted in simple one-phased model setups. However, the typical situation in foods is extremely complex and brings major constituents as proteins and carbohydrates as well as minor constituents as secondary plant products in contact to fats typically in multi-phased systems. We have recently established a stable disperse-phased setup to investigate the influences of the various chemical classes on fat oxidation, and as first results were able to differentiate between radical scavenging and physical quenching reactions of selected carotenoids.

Browning of cut iceberg lettuce
(Prof. Dr. M. A. Glomb)

Institute of Chemistry & Helmholtz Center for Environmental Research

Analytical Chemistry of Environmental Processes

Fields of Research:

- › Technical and natural occurring sorbents
- › Environmental fate of organic pollutants
- › Bioaccumulation of organic pollutants
- › Physico-chemical properties of perfluorinated chemicals
- › Predictive methods for equilibrium partitioning

Today a huge number of man-made and naturally occurring chemicals exist that are of environmental concern. This includes organic chemicals, their metabolites and complex mixtures. To protect the environment, we need detailed knowledge about such chemicals – their physical and chemical properties, their fate in the environment, their exposure and toxic effects. A thorough understanding of the environmental fate of organic pollutants has numerous applications: it is required for the registration of chemicals by the authorities, it is a prerequisite for remediation or prevention of environmental contaminations, it helps in the design of environmental monitoring strategies and it allows for the development of optimized analytical methods.

The goal of our group is an improved understanding of all those transport and partition processes that affect the fate of organic chemicals in the environment. We aim for an integrative view that considers the physico-chemical properties of the chemicals just as well as the environmental conditions that can largely vary in space and time. To this end we combine experimental work in the lab with various modelling approaches.

Current Projects and Future Goals:

Bioaccumulation

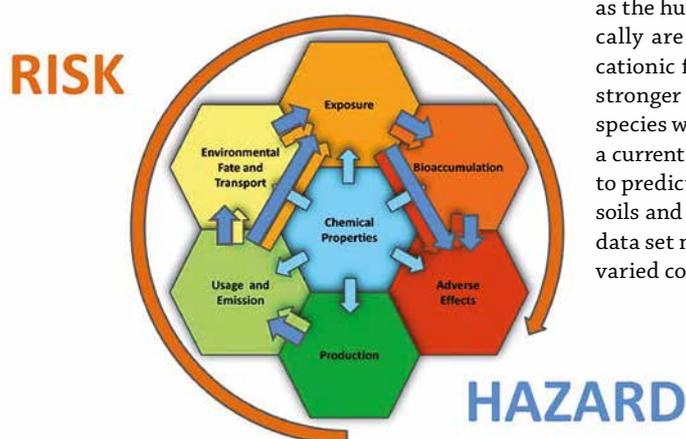
The assessment of the bioaccumulation potential of organic chemicals is part of the chemical legislation in all industrialized countries. Currently, this assessment is based on the assumptions that a) organic chemicals only accumulate in lipids, and b) that the octanol-water partition coefficient can be used to estimate this partitioning to lipids. However, this approach neither applies to terrestrial food chains, nor does it work for compounds that accumulate in proteins. It is also meaningless for ionic compounds. In order to close these gaps we have set out to develop a systematic and comprehensive understanding of the equilibrium partitioning of a broad range of organic chemicals into membrane lipids, storage lipids, structure proteins and serum albumin.

PBPK modelling

The results of our experimental work on biopartitioning of organic chemicals will be also be used in a PBPK (physiologically based pharmacokinetic) modelling approach in order to elucidate the relative importance of different processes (equilibrium partitioning, transport kinetics and metabolism). This modelling will provide us with concentration profiles of the chemicals in all organs and can be used to better analyse epidemiological surveys and toxicological studies. The PBPK modelling results are also useful in assessing the occupational exposure to hazardous chemicals.

Ionic organic chemicals

There are numerous commercial organic chemicals that can carry a negative or positive charge under environmental conditions (e.g. various pharmaceuticals, pesticides and surfactants). This charge has a substantial impact on the sorption behaviour of these compounds. Mineral surfaces as well as the humic material in soils and sediments typically are negatively charged. Consequently, the cationic form of an organic chemical often sorbs stronger in soils and sediments than its neutral species while anionic species sorb less strongly. In a current project we try to develop a general model to predict sorption of ionic organic compounds in soils and sediments based on a large experimental data set measured in the lab under systematically varied conditions.



Prof. Dr. Kai-Uwe Goss

1993

PhD in Environmental Chemistry (University of Bayreuth, Germany)

1994–1995

PostDoc (University of Minnesota, USA, Prof. S. Eisenreich)

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PostDoc/Oberassistent (EAWAG, Switzerland, Prof. R. Schwarzenbach)

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Habilitation (Swiss Federal Institute of Technology Zürich (ETH), Switzerland)

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Privatdozent (Swiss Federal Institute of Technology Zürich (ETH), Switzerland)

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Full Professor (W2) of Analytical Environmental Chemistry (Martin Luther University Halle-Wittenberg)

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Selected publications:

Ebert, A., Goss, K.-U. Predicting uncoupling toxicity of organic acids based on their molecular structure using a biophysical model. *Chem. Res. Toxicol.* 33 (7) (2020), 1835 - 1844.

Ebert, A., Hanneschlaeger, C., Goss, K.-U., Pohl, P. Passive permeability of planar lipid bilayers to organic anions. *Biophys. J.* 115 (10) (2018), 1931 - 1941.

Henneberger, L., Goss, K.-U. Environmental sorption behavior of ionic and ionizable organic chemicals. *Rev. Environ. Contam. Toxicol.* Springer, New York (2019).

Krause, S., Goss, K.-U. In vitro-in vivo extrapolation of hepatic metabolism for different scenarios – a toolbox. *Chem. Res. Toxicol.* 31 (11) (2018), 1195 - 1202.

Krause, S., Ulrich, N., Goss, K.-U. Desorption kinetics of organic chemicals from albumin. *Arch. Toxicol.* 92 (3) (2018), 1065 - 1074.



Prof. Dr. Dariush Hinderberger

2004

PhD Physical Chemistry, Johannes Gutenberg University, Mainz, Germany

2004–2006

PostDoc at the Laboratory of Physical Chemistry at ETH Zurich, Switzerland with Prof. Dr. A. Schweiger

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Staff scientist at the Max Planck Institute for Polymer Research (MPIP) in Mainz

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Junior Faculty of the Max Planck Graduate Center with the Johannes Gutenberg University Mainz (MPGC).

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Selected publications:

J. Hunold, T. Wolf, F. Wurm, D. Hinderberger, Nanoscopic hydrophilic/hydrophilic phase-separation well below the LCST of Polyphosphoesters, *Chem. Commun.*, 55, 3414–3417 (2019).

J. Eisermann, D. Hinderberger, Tuning the shape anisotropy of loosely bound colloid-like ionic clusters in solution, *Phys. Chem. Chem. Phys.*, 21, 1152–1159 (2019).

S. H. Arabi, B. Aghelnejad, C. Schwieger, A. Meister, A. Kerth, D. Hinderberger, Serum Albumin Hydrogels in Broad pH and Temperature Ranges: Characterization of Their Self-Assembled Structures, Nanoscopic and Macroscopic Properties, *Biomater. Sci.*, 6, 478–492 (2018).

D. Kurzbach, T. C. Schwarz, G. Platzer, S. Höfler, D. Hinderberger, R. Konrat, Compensatory Adaptations of Structural Dynamics in an Intrinsically Disordered Protein Complex, *Angew. Chem. Int. Ed.* 53, 3840–3843 (2014).

Institute of Chemistry

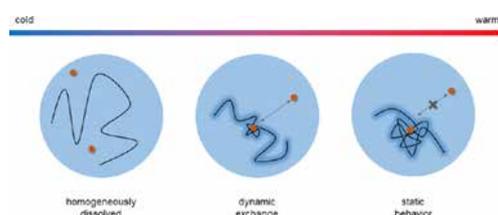
Physical Chemistry – Complex Self-Organizing Systems

Fields of Research:

- › Structure formation in synthetic and biological soft matter by non-covalent interactions
- › Nanoscopic features in hydrogels from synthetic and biological macromolecules
- › Structure formation between small molecules in liquids; solvation
- › Biological and synthetic molecular transporters
- › Intrinsically disordered proteins (IDPs)
- › Stimuli-responsive polymeric materials
- › Method development in electron paramagnetic resonance (EPR/ESR) spectroscopy

Biological and synthetic soft matter has a remarkable ability to self-assemble into larger, complex and even functional structures solely using non-covalent interactions (e.g. electrostatic and hydrophobic forces). Dariush Hinderberger's research group uses electron paramagnetic resonance (EPR) spectroscopy as its main research tool to study soft matter from the underlying fundamental interactions to more applied questions. Research in the group currently has a focus on solvation and self-assembly of small molecules (e.g. in aqueous solutions or ionic liquids), on complex biomedical questions (e.g. abundant transport proteins such as albumin or intrinsically disordered proteins (IDP)), and applications such as understanding interactions and dynamics of transported molecules in thermoresponsive polymers for drug delivery.

EPR spectroscopy is a magnetic resonance method that is sensitive to molecular motions from the pico- to microsecond regime and to distances between 0.1 and ~8 nanometers.



Local, nanoscopic interactions of small molecules and thermoresponsive polymers (J. Hunold et al. *Chem. Commun.*)

EPR is complemented by other methods of physical investigation like NMR and IR spectroscopy, electron microscopy, atomic force microscopy (AFM), and dynamic light scattering (DLS), and by synthetic chemistry, which allows a unique approach to study these classes of complex materials.

Current Projects and Future Goals:

The Nanoscale of Responsive Polymers

With simple continuous wave (CW) EPR spectroscopy on amphiphilic spin probes we have discovered that thermoresponsive polymeric systems show nano-inhomogeneities in structure and reactivity. These nano-inhomogeneities can be static on an EPR timescale (>~1ns), or dynamic (<~1ns) and can basically be found in all kinds of synthetic and biological thermoresponsive polymers.

Serum Albumin Revisited

Human serum albumin (HSA) is a versatile transport protein for various endogenous compounds and drugs in the human blood. It is the major transport protein for fatty acids (FA) in the circulatory system. We have devised a new EPR spectroscopic approach to gain information on the functional solution structure of HSA, which has remarkably been found to have a much more symmetric than expected from the crystal structure, indicating increased surface flexibility and plasticity for HSA in solution. Going beyond fundamental structural studies, our research platform is also excellently suited for general studies of protein-solvent interactions, temperature effects and ligand binding and we have now extended it to study the molecular/nanoscale level of hydrogels made from albumin as well as from synthetic polymers.

Structure & Dynamics of IDPs and Their Complexes

Intrinsically disordered proteins (IDPs) lack defined tertiary and often secondary structure but fulfill essential tasks in eukaryotic life. It is their structural flexibility that allows IDPs to adapt to and to interact with different binding partners, making them suited for functioning as hubs between several interaction partners. However, this dynamic nature makes IDPs difficult to analyze. We tackle the complexity of characterizing a dynamic structural ensemble with EPR spectroscopy, combined with NMR spectroscopy or IR-based techniques and obtain unique insights into a wide variety of IDPs, including membrane-based proteins that we also characterize at the lipid monolayer and in bilayers.

Molecular Self Assembly in Solution

Using our unique approach to soft matter, we ultimately aim at exploring and understanding structuring and dynamic principles that simple molecules in solution show and that constitute initial steps on the way to more complex assemblies like proto-cells or crystals.

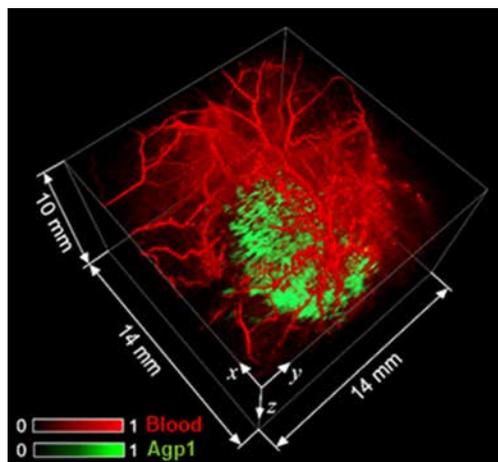
Institute of Physics

Medical Physics

Fields of Research:

- › Biomedical Photoacoustic Imaging and Spectroscopy
- › Development of experimental and computational methods for image acquisition and inversion
- › Technology development (scanners, detectors)
- › Reporter genes and exogenous contrast agents
- › In vivo demonstration and application

Photoacoustic imaging is a hybrid imaging technology that combines the high spectral specificity of optical methods with the high spatial resolution of ultrasound imaging. It relies on the generation of broadband acoustic waves via the absorption of intensity modulated light. The acoustic field is mapped outside the organism using ultrasound detectors. From the measured data, high resolution 3D images of the initial pressure are reconstructed that typically show the vasculature but also optically absorbing contrast agents, such as nanoparticles, dyes or genetically expressed proteins and pigments. Our research activities are focussed on the development of new technologies, experimental and computational methods, and genetic reporters for molecular and functional photoacoustic imaging through a highly interdisciplinary research programme involving physicists, engineers and life scientists.



In vivo image of a subcutaneous tumour expressing photoswitchable phytochrome Agp1 and the vasculature of the surrounding tissue (Märk et al, *Comms Phys* [2019]).

Current Projects and Future Goals:

Electro-optically tuneable Fabry-Pérot ultrasound sensors for high frame rate PA tomography

Camera-based interrogation of electro-optically tuneable Fabry-Pérot polymer film sensors are being developed to enable high speed 3D imaging. This technology may provide, high resolution PA imaging of fast physiological processes, such as neuro-functional and blood flow imaging.

Computational and experimental methods for the quantitative PA tomography

The aim of this project is to develop and experimentally validate experimental and computational methods for the PA inverse problem, i.e. the recovery of absolute chromophore concentrations and physiological parameters, such as blood oxygen saturation, from high resolution multiwavelength 3-D images.

PA imaging of fluorophores using pump-probe excitation

We are developing a PA molecular imaging method for the detection of fluorophores that is based on generating stimulated emission using pump-probe excitation. The images show the location of the fluorophore while the otherwise overwhelming endogenous background signal (blood) is eliminated. Pump-probe excitation provides contrast at fluences below the maximum permissible exposure and is applicable to in vivo deep tissue PA tomography. It also allows the detection of differences in the excited state lifetime.

Development of optically controlled genetic reporters for PA imaging

We are developing genetically expressed reporter proteins and pigments that are tailored to the requirements of PA imaging. For example, we have demonstrated the use of photoswitchable, near-infrared reporter proteins based on phytochromes in vivo. Phytochromes were detected using a dual-wavelength excitation and difference imaging.

PA microscopy of vascularisation

We are developing instrumentation for optical-resolution PA microscopy based on optical ultrasound detection. This technology has the potential to be combined with optical microscopy. A future application is functional PA microscopy of vascular development.



Prof. Dr. Jan Laufer

2000

PhD in Medical Physics, University College London, UK

2001–2002

Bio-Rad Microscience Ltd, Research & Development, Hemel Hempstead, UK

2002–2011

Senior Research Fellow, Department of Medical Physics & Bioengineering, University College London, UK

2012–2016

Research group leader, TU Berlin & Charité Berlin, Germany

Since 2017

Professor of Medical Physics, Institute of Physics, Martin Luther University Halle-Wittenberg

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Selected publications:

J. Buchmann, B. Kaplan, S. Powell, S. Prohaska, J. Laufer. Three-dimensional quantitative photoacoustic tomography using an adjoint radiance Monte Carlo model and gradient descent. *Journal of Biomedical Optics* 24(6), 066001 (2019).

J. Märk, H. Dortay, A. Wagener, E. Zhang, J. Buchmann, C. Grötzinger, T. Friedrich, J. Laufer. Dual-wavelength 3D photoacoustic imaging of mammalian cells using a photoswitchable phytochrome reporter protein. *Communications Physics* 1 (2018).

J. Märk, F.-J. Schmitt, J. Laufer. Photoacoustic imaging of the excited state lifetime of fluorophores. *J. Optics* 18(5), 054009 (2016).

J. Märk, F.-J. Schmitt, C. Theiss, H. Dortay, T. Friedrich, J. Laufer. Photoacoustic imaging of fluorophores using pump-probe excitation. *Biomedical Optics Express* 6(7), 2522–2535 (2015).

A.P. Jathoul, J. Laufer, O. Ogunlade, B. Treeby, B. Cox, E. Zhang, P. Johnson, A.R. Pizzey, B. Philip, T. Marafioti, M.F. Lythgoe, R.B. Pedley, M.A. Pule, P. Beard. Deep in vivo photoacoustic imaging of mammalian tissues using a tyrosinase-based genetic reporter. *Nature Photonics* 9, 239–246 (2015).



Prof. Dr. Miguel Marques

2000

PhD Theoretical Physics (Julius Maximilian University of Würzburg, Germany)

2000-2004

PostDoc at the University of the Basque Country (with Prof. A. Rubio) and at the Free University of Berlin (with Prof. E. K. U. Gross)

2004-2005

Marie-Curie fellow at the University Pierre and Marie Curie – Paris VI (with Prof. F. Mauri)

2005-2007

Invited assistant professor (University of Coimbra, Portugal)

2007-2014

CNRS researcher (University of Lyon, France)

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Habilitation in Theoretical Physics (University of Lyon, France)

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Selected publications:

T.F.T. Cerqueira et al. Density-functional tight-binding study of the collapse of Carbon Nanotubes under hydrostatic pressure. *Carbon* 69, 355-360 (2014).

Ch. Neidel et al. Probing Time-Dependent Molecular Dipoles on the Attosecond Timescale. *Phys. Rev. Lett.* 111, 033001 (2013).

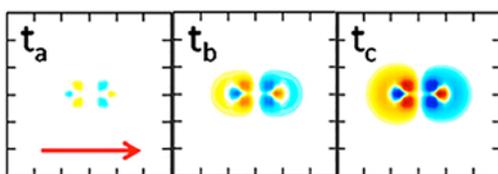
M. Amsler et al. Conducting boron sheets formed by the reconstruction of the α -boron (111) surface. *Phys. Rev. Lett.* 111, 136101 (2013).

S. Botti and M.A.L. Marques. Strong renormalization of the electronic band gap due to lattice polarization in the GW formalism. *Phys. Rev. Lett.* 110, 226404 (2013).

Institute of Physics**Mesoscopic Quantum Dynamics****Fields of Research:**

- › Global structure prediction and materials design
- › Materials for energy applications
- › Fundamentals of (time-dependent) density functional theory and beyond
- › Attosecond dynamics of electrons in strong laser fields
- › Scientific software for high-performance computing

In present days there is a clear shift towards a new way of doing physics, which relies strongly on the use of computational means. Computational Physics, which is expanding with the availability of modern and more powerful computers, has been offering new insights on various natural phenomena, complementing and going beyond more traditional visions based on analytical approaches. The cornerstone in the study of hard matter was the development, in 1965, of density functional theory, certainly one of the most successful theories in Physics for the past 50 years. Nowadays density functional theory allows us to calculate the properties of atoms, molecules, and solids in a computer with a remarkable accuracy and simplicity. We can also perform “in silico” experiments that complement and help to interpret a wealth of experimental data. This is true not only for structural, electronic, and thermodynamic properties, but even for dynamical processes such as the interaction of electrons with fast and strong laser fields.

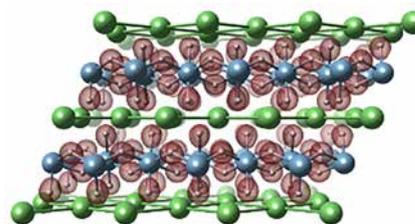


Probing attosecond electronic motion in small molecules

More recently, another major step was given in this field: we can now “design” in the computer new materials with tailored properties for different applications ranging from photovoltaics, to energy storage, to crystals with exotic properties. This is made possible by the combination of techniques stemming from solid-state physics, artificial intelligence, and high-performance computing. This new interdisciplinary field, nowadays called “accelerated discovery of materials” or “materials design”, is still in its infancy and is expected to revolutionize many areas of Materials Science.

Current Projects and Future Goals:**Global structural prediction and materials design**

In the field of (global) structural prediction one tries to obtain the lowest energy crystal structure for a given composition. This is a very difficult problem, as the number of minima (i.e., meta-stable structures) increases exponentially with the number of atoms in the system. It is also an integral part of any strategy to design materials, as it is the only way to assure that the predicted materials are the ground-state in some area of the phase-diagram and that can therefore be experimentally synthesized. We are currently using these techniques to find new materials that have interesting properties for energy production and storage.



A material designed for hydrogen storage

New materials for photovoltaic applications

Transparent conductive oxide (TCO) materials, have attracted a considerable amount of interest, especially due to their applications in displays and in solar cells. In fact, many new solar cells technologies, like the CIS and CIGS thin film solar cells, use TCOs as contacts. Our group works to provide a reliable theoretical understanding of the band structures and absorption spectra of these materials. This understanding is achieved by using state-of-the-art self-consistent GW methods (for the band structures) combined with the solution of the Bethe-Salpeter equation for the evaluation of the absorption.

Development of scientific software

We are active developers of the computer code octopus. This program, which is open source software under the GNU general public license (GPL), simulates the dynamics of electrons and nuclei under the influence of time-dependent fields. The electronic degrees of freedom are treated quantum-mechanically, while the nuclei are considered to behave as classical point particles. In this code, all quantities are discretized in real space using a grid, and the simulations are performed in real time. Over the past years, octopus has evolved into a fairly complex and complete tool, and is now used by more than 150 research groups around the world.

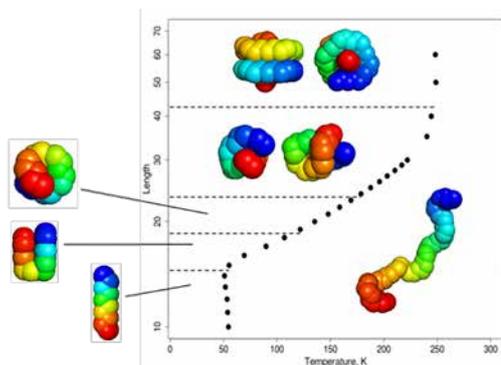
Institute of Chemistry

Theoretical Polymer Physics

Fields of Research:

› Synthetic and Biological Macromolecules

Polymer science is a highly interdisciplinary field with questions ranging from materials science to basic theoretical physics. Rational design of polymer-based materials needs an understanding of structure and dynamics on the molecular scale. Computer simulations of chemically realistic as well as coarse-grained models yield insight into molecular processes and help to interpret experiments. The hierarchy of length scales and time scales inherent in often complex molecular architectures and material morphologies lead to the necessity for a multi-scale modeling approach. This in turn needs model as well as methods development for efficient Molecular Dynamics and Monte Carlo simulations. Already single (bio-) polymers or small aggregates are fascinating objects in themselves which can exhibit phase transition-like phenomena as, e.g., protein folding. The search for a basic statistical physical understanding of these phenomena links polymer theory to biophysics and biology.



Folding transition of short alkane chains from a random coil to a highly structured ground state

The conformations of linear polymers are intimately connected to path integrals or random walk theory. The methods for their analytical description link polymer theory to quantum field theory (statistical field theory) and the theory of stochastic processes. Fundamental questions in quantum theory and a stochastic processes based understanding of quantum mechanics are research interests growing out of these connections.

Current Projects and Future Goals:

■ Phase transitions of synthetic polymers

In experiments, polymer crystallization is a process where thermodynamic forces and kinetic constraints interact in a hardly controllable way, which can, however, be captured by Molecular Dynamics simulations of the crystallization process. Pure thermodynamics is addressable via simulations for single chain phase transitions of alkanes which we will extend to chains at interfaces and under other constraints. Copolymers can undergo phase separation and ordering within a single molecule and variations of chain topology and chemical composition lead to a variety of micro-phase separated structures with always the molecular scale as the resulting length scale of the macroscopic morphology.

■ Conformations and thermodynamics of proteins and their aggregates

Proteins and peptides are able of intra-molecular structure formation and often need to assume specific structures to perform their molecular function. The same interactions (e.g., hydrophobic or hydrogen bonding) generating these structures can, however, also lead to chain aggregation, e.g., amyloid formation, underlying many neurodegenerative diseases. Understanding of the statistical mechanics and the kinetics of these competing structure formation processes can be obtained from advanced Monte Carlo simulations of specifically designed models. At the same time, this yields insight into morphology generation in supramolecular chemistry.

■ Quantum Hamilton equations

We recently derived quantum Hamilton equations of motion from the formulation of quantum mechanics (QM) as a stochastic optimization problem and showed how they can be applied to obtain the complete spectrum of bound states of a quantum system. The numerical treatment of the resulting coupled forward-backward stochastic differential equations needs further improvement concerning efficiency. We will extend the theory to include a treatment of particle spin and interactions between spin and positional degrees of freedom. The stochastic processes based approach to quantum mechanics should also be extendable to relativistic quantum mechanics.



Prof. Dr. Wolfgang Paul

1989

PhD Theoretical Physics, Johannes Gutenberg University, Mainz, Germany

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Selected publications:

- E. Lee, W. Paul, Additional Entanglement Effect Imposed by Small Sized Ring Aggregates in Supramolecular Polymer Melts: Molecular Dynamics Simulation Study, *Macromolecules* 53, 1674 (2020).
- T. Shakirov, W. Paul, Folded alkane chains and the emergence of the lamellar crystal, *J. Chem. Phys.* 150, 084903 (2019).
- J. Köppe et al., W. Paul, Derivation and application of quantum Hamilton equations of motion, *Ann. Phys. (Berlin)* 529, 1600251 (2017).
- W. Janke, W. Paul, Thermodynamics and structure of macromolecules from flat-histogram Monte Carlo simulations, *Soft Matter* 12, 642 (2016).
- M. Solar et al., The dielectric α -relaxation in polymer films: A comparison between experiments and atomistic simulations, *Europhys. Lett.* 104, 66004 (2013).



Prof. Dr. Reinhard Paschke

Since 1993

Head of office of the BioCenter of the Martin Luther University and Head of the Medicinal-Pharmaceutical Chemistry unit.

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Vanchanagiri, Kranthi, Emmerich, Daniel, Bruschke, Monique, Bache, Matthias, Seifert, Franziska, Csuk, Rene, Vordermark, Dirk, and Paschke, Reinhard. Synthesis and biological investigation of new carbonic anhydrase IX (CAIX) inhibitors. *Chem.-Biol.Interact.* 284, 12-23 (2018).

Liebscher, G., Vanchanagiri, K., Mueller, Th, Feige, K., Cavalleri, J.-M. V., and Paschke, R. In vitro anticancer activity of Betulinic acid and derivatives thereof on equine melanoma cell lines from grey horses and in vivo safety assessment of the compound NVX-207 in two horses. *Chem.-Biol.Interact.* 246, 20-29 (2016).

Kommer, Harish, Kaluderovic, Goran N., Kalbitz, Jutta, and Paschke, Reinhard. Lupane Triterpenoids-Betulin and Betulinic acid derivatives induce apoptosis in tumor cells. *Invest.New Drugs* 29[2], 266-272 (2011).

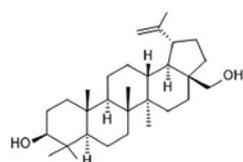
Medicinal-Pharmaceutical Chemistry

Isolation, modification and biological testing of herbal antitumor agents

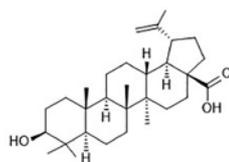
Fields of Research:

- › Plant derived antitumor drugs
- › Chemical modification
- › Biological testing

The preclinical development of bioactive natural products and their analogues as chemotherapeutic agents is a major objective of our research group. Triterpenoids are one of the most important classes of natural products occurring widely in the plant kingdom. The derivatives of triterpenoids have been one of the most interesting areas of research in the past few years vested to their broad range of biological and medicinal properties. Betulinic acid and betulin belong to the class of pentacyclic lupine type triterpenes.



Betulin



Betulinic acid

The plane tree is one of the substantial source for betulinic acid.



Plane Tree

Betulinic acid is one of few such compounds that have been shown to possess several medicinal properties including anticancer, antimalarial, antimicrobial and anti-HIV activities. Betulinic acid was found to cause cancer cell death by induction of apoptosis through changes in the mitochondrial membrane potential, production of reactive oxygen species, and permeability of transition pore openings. These processes lead to the release of mitochondrial apoptogenic factors, activation of caspases, and DNA fragmentation.

Our research group performs both the isolation of the active ingredients and their chemical modification as well as the biological testing of the obtained compounds.

Current Projects and Future Goals:

■ **01 November 2019 to 31 October 2022**

Betulin sulfate conjugates to overcome the hypoxic radiation resistance of breast cancer in vitro and in vivo, DFG

■ **01 October 2020 to 30 June 2023**

Extraction of exopolysaccharides of the red algae porphyridium sp. as an active substance for the treatment of the bee disease Nosemosis; BMEL, Fachagentur Nachwachsende Rohstoffe

■ **01 June 2020 to 30 April 2022**

Antibacterial and antifungal effects of ingredients and extracts from Artemisia for use as antitumor agents and antibiotic alternatives; Land S-A, IB Sachsen-Anhalt

■ **01 October 2019 to 31 January 2022**

CA-InhibiTool Carboanhydrase Inhibitors (CAI) - Development of a diagnostic tool for the rapid and safe determination of carboanhydrase activity of antitumor markers and agents; Land S-A, IB Sachsen-Anhalt

■ **01 April 2017 to 30 September 2020**

TopiDrugHorse Cooperation Project Biocapsule - "TopiDrugHorse", Drug Synthesis and Analytics; ZIM, VDI/VDE Innovation + Technik GmbH

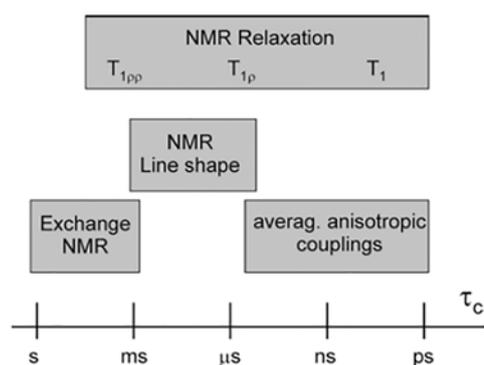
Institute of Physics

Dynamic Solid-State NMR

Fields of Research:

- › Structure and dynamics of solid polymers by NMR
- › Structure-dynamic-property relationship in pharmaceutical compounds, solid polymers, polymer networks and Solid-Polymer Electrolytes
- › Method development in solid-state NMR

Solid materials and in particular polymeric systems exhibit an astonishing variety of segmental motions as well as molecular reorientations which have important effects on mechanical, transport and optical properties of polymers, the activity of proteins, the stability of pharmaceuticals, the transport properties in zeolites, behavior of amorphous materials near the glass transition, ion transport in organic and inorganic ionic conductors, and other structural properties of organic and inorganic systems. Solid-state NMR provides powerful techniques for elucidating details of segmental dynamics and local conformation in solid materials]. These methods allow detailed studies of dynamics occurring over a wide range of frequencies and correlate these information on the microscopic level with structural data as well as on the macroscopic level with application properties.



Time-scales of Dynamic Solid-State NMR methods

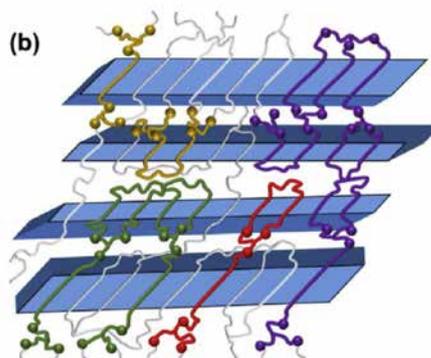
Current Projects and Future Goals:

Dynamics in bulk polymers

A number of factors have influence on the practical applications of the synthetic polymers. For Semi-crystalline polymers one of the most significant mechanical properties is macroscopic drawability. There is evidence that the underlying microscopic process on the microscopic level is lateral chain diffusion in the crystallites and that is can be investigated by solid-state NMR in very detail. In the past, we investigated the helical jumps of the crystalline stems of a number of polyolefins. Now, we turned our attention to biodegradable polymers like poly(lactic acid) and focus in particular on the effect of different crystalline structures.

Structure-dynamics-properties relationship in Solid-Polymer Electrolytes

The aim of these studies is a molecular understanding of chain mobility, polymer crystallization and of the hierarchical structure formation in the polymer networks made of poly(ethylene oxide). Besides new fundamental insides into the crystallization process in networks, these networks might serve as a material for polymer electrolytes. Thus, the interactions of the polymer chains with salts will be a future scope of this project.



Schematic picture of polymer network chains in crystallites. (Y. Golitsyn et al., 2019).



Prof. Dr. Detlef Reichert

1990

PhD Experimental Physics, TU, Merseburg, Germany

1992

PostDoc at Weizmann Institute of Science, Rehovot, Israel, with Z. Luz

Since 1993

Staff scientist at the Institute of Physics of Martin Luther University Halle-Wittenberg (since 2013 as apl. Professor)

2003

Habilitation in Experimental Physics, Martin Luther University Halle-Wittenberg

Since 2013

Extraordinary (apl.) Professor, Martin Luther University Halle-Wittenberg

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<http://www.physik.uni-halle.de/Fachgruppen/nmr/reichert.html>

Selected publications:

Y. Golitsyn et al., Crystallization in PEG networks: The importance of network topology and chain tilt in crystals, *Polymer*, 165, 72–82 (2019).

Y. Golitsyn et al., Molecular Dynamics in the Crystalline Regions of Poly(ethylene oxide) Containing a Well-Defined Point Defect in the Middle of the Polymer Chain, *J. Phys. Chem. B* 121, 4620–4630 (2017).

C. Hackel et al., The trehalose coating effect on the internal protein dynamics, *PCCP* 14, 2727 (2012).

A. Krushelnitsky et al., Direct Observation of Millisecond to Second Motion in Proteins by Dipolar CODEX NMR, *JACS* 131, 12097 (2009).

D. Reichert et al., Slow Dynamics in Glassy Methyl α -L-Rhamnopyranoside Studied by 1D NMR Exchange Experiments *PCCP* 10, 542 (2008).



Prof. Dr. Kay Saalwächter

1991–1997

Studies of Chemistry at the Universities of Mainz, Germany, Freiburg, Germany, and Massachusetts, Amherst, USA

1997–2000

Doctorate at the MPI for Polymer Research, Mainz, Germany with H. W. Spiess, Dr. rer. nat. in Physical Chemistry (U. of Mainz, Germany)

2001–2004

Habilitation at the Institute for Macromolecular Chemistry, U. of Freiburg, Germany, with H. Finkelmann

2004–2005

Lecturer, U. of Freiburg, Germany

Since 2005

Full Professor (W2) of Experimental Physics, Martin Luther University Halle-Wittenberg

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www.physik.uni-halle.de/nmr

Selected publications:

A. Mordvinkin et al., Hierarchical Sticker and Sticky Chain Dynamics in Self-Healing Butyl Rubber Ionomers. *Macromolecules* 2019, 52, 4169.

A. Naumova et al., Microscopic State of Polymer Network Chains upon Swelling and Deformation. *Macromolecules* 2019, 52, 5042.

R. Kurz et al., Intracrystalline Jump Motion in Poly(ethylene oxide) Lamellae of Variable Thickness: A Comparison of NMR Methods. *Macromolecules* 2017, 50, 3890.

M. Roos et al., Coupling and Decoupling of Rotational and Translational Diffusion of Proteins under Crowding Conditions. *J. Am. Chem. Soc.* 2016, 138, 10365.

A. Papon et al., Glass-Transition Temperature Gradient in Nanocomposites: Evidence from Nuclear Magnetic Resonance and Differential Scanning Calorimetry. *Phys. Rev. Lett.* 2012, 108, 065702.

K. Saalwächter., Proton multiple-quantum NMR for the study of chain dynamics and structural constraints in polymeric soft materials. *Progr. Nucl. Magn. Reson. Spectrosc.* 2007, 51, 1.

Institute of Physics

Nuclear Magnetic Resonance Spectroscopy

Fields of Research:

Molecular-level structure and dynamics in soft materials:

- › **Physics of synthetic and biological macromolecules and liquid crystals**
- › **Polymer melts, elastomers and hydrogels**
- › **Dynamics and interface phenomena in (nano)composites**
- › **Polymer crystallization**
- › **Self-organization and dynamics in functional polymers**
- › **Method development in solid-state NMR**

The function and rational design of modern polymeric and other “soft” materials rests on their often self-organized microstructure and the molecular dynamics. Our group focuses on molecular-level probes of structure and dynamics in soft matter, mainly (bio)polymers and liquid crystals, in order to link up molecular processes with structure and function on the meso- and macroscopic scales. This concerns for instance the mechanical behavior of polymer melts and elastomers, their thermodynamic behavior, nanoscale morphologies arising from self-assembly including partial crystallization, or structure-function relationships in transient (self-healing) networks.

Our main method is NMR spectroscopy as one of the most versatile molecular probes of structure and dynamics. Modern multi-dimensional NMR at high as well as low field provides access to diverse observables such as interatomic distances, rotational dynamics covering many decades in time, translational diffusing (using pulsed field gradients) and structure on the nanoscale (employing the spin-diffusion effect). We seek to apply, and newly develop, different NMR experiments, complemented by a variety of other techniques in order to validate and improve our conceptual understanding in soft-matter physics.

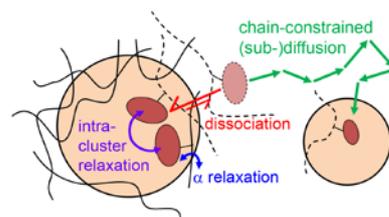


Fig. above: Molecular dynamic processes in a side-chain modified self-healing elastomer (Mordvinkin et al.)

Fig. right: Low-field NMR study of chain stretching in deformed elastomers to (in)validate elasticity models (Naumova et al.)

Current Projects and Future Goals:

New aspects in polymer crystallization

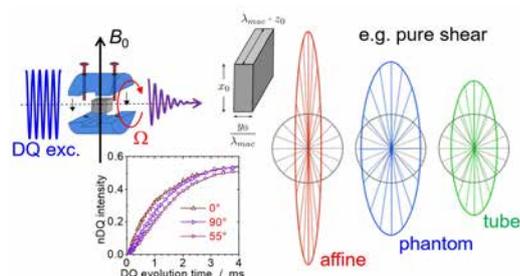
While being a seemingly well-understood phenomenon, the crystallization of polymers has moved into the focus again, thanks to new experimental and theoretical tools. In a collaborative project with the Thurn-Albrecht group, we study the so far underestimated influence of intracrystalline chain dynamics and the accumulation of entanglements in the amorphous phase, both quantified by NMR. These turn out to have a decisive influence on the semicrystalline morphology.

Segmental and chain dynamics in functional polymers and nanocomposites

The fascinating mechanical behavior of long-chain polymer melts, and related materials such as supramolecular elastomers or nanocomposites, rests upon classical concepts such as de Gennes’ “reptation” model, the more general tube model, and variants that take into account additional constraints to the dynamics. We apply advanced proton NMR techniques on inexpensive benchtop spectrometers to probe segmental and chain dynamics, investigating in particular the modifications arising from “sticky” functional groups or confinement due to the presence of interfaces. Our usually collaborative efforts combine NMR spectroscopy with scattering techniques, dielectric and mechanical spectroscopy, and computer simulations.

Molecular-level characterization of elastomers

Tire materials have a unique mechanical property profile arising from entropic elasticity of crosslinked and entangled chains, and from additional synergistic effects related to inorganic fillers. We investigate the relations between internal structure, inhomogeneous molecular dynamics, and the mechanical properties of unfilled and filled elastomers by comparing industrially relevant rubbers with model networks and nanocomposites. Our goal is to identify and validate the most suitable of the many theoretical models that are available. This range of activities is again a showcase of the great potential of inexpensive low-field NMR methodologies.



Institute of Chemistry

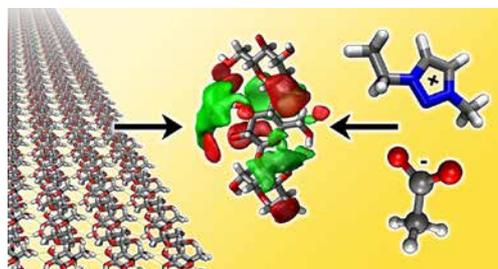
Theoretical Chemistry

Fields of Research:

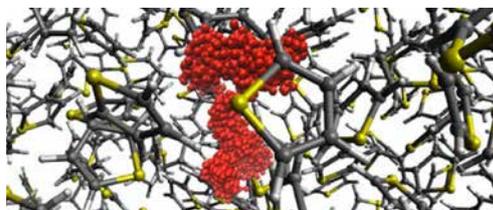
- › Proton and Lithium conduction in solids
- › Novel solvents (ionic liquids) for biopolymers
- › Lithium-Sulfur batteries
- › Theoretical Spectroscopy
- › Ab-initio molecular dynamics simulations

There is a lot of molecular “life” in liquids but also in crystalline and amorphous solids. Small ions such as protons and lithium nuclei are very mobile, which is important for designing high-performance ion conductors (as fuel cell membranes) and batteries. The simulation of molecular dynamics on the basis of Theoretical Chemistry allows the direct modeling of ion mobility in such complex condensed phase systems. Here, the quantum-mechanical orbitals (the “chemical bonds”) are the driving forces behind the atomic motion.

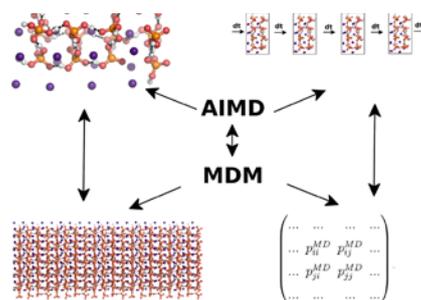
We compute the electronic orbitals on large-scale computers, and subsequently we model the molecular and atomic motion based on these orbitals. This gives access to atomic/ionic mobility properties, spectroscopic parameters as function of local morphologies, as well as the properties of a compound as a solvent for different types of solutes. Several atomic properties determine which types of molecules are dissolved in which other types of molecules (solutes and solvents). The resulting behavior is often categorized via different “philicities” such as hydro-, lipo-, silano- or fluoro-philic characteristics of a compound. Our simulations can predict the philicities of novel molecules with tailored functional groups of several philicity classes. This is of special importance for “difficult” solutes such as cellulose:



No conventional solvent is able to dissolve the hydrogen-bonded biopolymers of this type. However, we have discovered that a novel solvent (triazol/acetate, an ionic liquid) is indeed able to disrupt this highly stable hydrogen bond network and thus dissolve cellulose materials.



The motion of a lithium ion in an amorphous thiophene matrix during a short time (100ps) is shown here as superposition of all visited locations. The direct simulation of this ionic dynamics helps to understand how the (slow) motion of the thiophene molecules controls the (fast) motion of the solvated Li ions. Such thiophene compounds are interesting as diffusion inhibitors for sulfur molecules within Lithium-Sulfur batteries.



The direct simulation of atomic and molecular mobility is powerful but inherently restricted to short timescales, due to the enormous computational effort required for the explicit calculation of all chemical bonds (i.e. all electronic orbitals) of the entire system. Coarse-grained simulations have the potential for simulating longer time intervals at the expense of a reduced detail level. We have developed a multi-scale method for the simulation of ion mobility that combines atomistic resolution with very long simulation timescales. To this end, we combine molecular dynamics simulations of the local atomic structure with a lattice Monte-Carlo simulation of the ion dynamics. This gives access to mobility phenomena with characteristic timescales of up to microseconds. All molecular dynamics simulation can be combined with the quantum chemical calculation of several kinds of spectra, such as infrared-, Raman-, NMR, UV/vis- and VCD spectra within the phase space covered by the molecular dynamics simulation. We have recently computed how weak intermolecular coupling interactions within a molecular crystal determines the shape of the VCD spectrum.



Prof. Dr. Daniel Sebastiani

2001

PhD Theoretical Physics at the Max Planck Institute for Solid State Research, Stuttgart

2001-2009

Project leader at the Max Planck Institute for Polymer Research, Mainz

2002

Visiting Scientist at the ETH Zurich, Rothlisberger Group, Zurich, Switzerland

2004

Visiting Scientist at Princeton University, Car Group, Princeton, USA

2009-2012

Heisenberg Group leader at the Physics Department, Free University Berlin

since 2012

Professor for Theoretical Chemistry, Martin Luther University Halle-Wittenberg

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Selected publications:

Ch. Dreßler, G. Kabbe, M. Brehm, D. Sebastiani, Dynamical matrix propagator scheme for large-scale proton dynamics simulations, *J. Chem. Phys.* 2020, 152, 114114.

M. Brehm, M. Pulst, J. Kressler, D. Sebastiani, Triazolium-Based Ionic Liquids: A Novel Class of Cellulose Solvents, *J. Phys. Chem. B*, 2019, 123, 18, 3994–4003.

P. Partovi-Azar, D. Sebastiani, Mechanism of Lithium Cation Hopping between Tetragonal Thiophene Cages, *Batteries & Supercaps* 2019, 2, 695–700.

M. Ekimova, F. Hoffmann, G. Bekçioğlu-Neff, A. Rafferty, O. Kornilov, E. Nibbering, D. Sebastiani, Ultrafast Proton Transport between a Hydroxy Acid and a Nitrogen Base along Solvent Bridges Governed by the Hydroxide/Methoxide Transfer Mechanism, *J. Am. Chem. Soc.* 2019, 141, 37, 14581–14592.

S. Jähnigen, A. Scherrer, R. Vuilleumier, D. Sebastiani, Chiral Crystal Packing Induces Enhancement of Vibrational Circular Dichroism, *Angewandte Chemie*, 2018, 57, 1–6.



Prof. Dr.
Thomas Thurn-Albrecht

1994

PhD Physics, University of Freiburg, Germany

1995–1998

PostDoc/staff scientist at the Max-Planck-Institute for Polymer Research, Mainz, Germany

1998–1999

PostDoc at the University of Massachusetts, Amherst, US

2000–2003

Staff scientist and lecturer at the Institute for Physics, University of Freiburg, Germany

Since 2003

Full Professor of Experimental Physics, Martin Luther University Halle-Wittenberg

Since 2011

Coordinator of the SFB Tranregio 102 Polymers under multiple constraints: restricted and controlled molecular order and mobility

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www.physik.uni-halle.de/fachgruppen/polymer_physics_group

Selected publications:

Schulz, M., et al. The effect of intracrystalline chain dynamics on melting and reorganization during heating in semicrystalline polymers. *Polymer* 196 (2020): 122441.

Tariq, M., et al. Effect of Substrate Interaction on Thermodynamics of Prefreezing. *Macromolecules* 52(23) (2019): 9140–9148.

Dolynchuk, O., et al. Phenomenological Theory of First-Order Prefreezing. *J Phys Chem Lett* 10 (2019): 1942–1946.

Schulz, M., et al. The Underestimated Effect of Intracrystalline Chain Dynamics on the Morphology and Stability of Semicrystalline Polymers. *Macromolecules* 51(21) (2018): 8377–8385.

Balko, J., et al. Surface induced orientation and vertically layered morphology in thin films of poly(3-hexylthiophene) crystallized from the melt. *Journal of Materials Research* 32(10) (2017): 1957–1968.

Institute of Physics

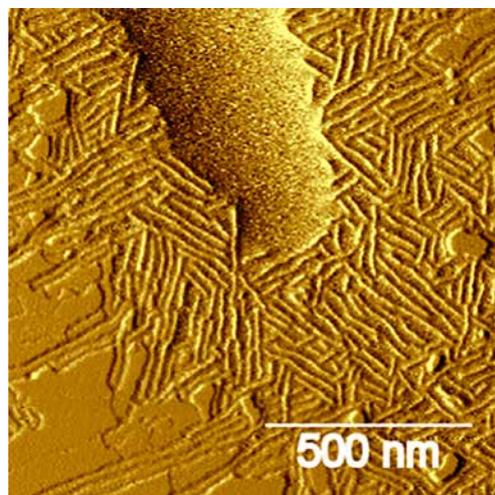
Experimental Polymer Physics

Fields of Research:

- › Crystallization of polymers
- › Structure and mechanical properties of nanostructured polymers
- › Polymers for organic photovoltaics
- › Scattering Methods, Scanning Force Microscopy, Rheology, Calorimetry

Polymers or chain molecules are very versatile materials. Their special mechanical, optical or electrical properties are at the basis of many different applications in which we encounter polymers in daily life. Due to their macromolecular character polymers display a variety of typical and special properties like e.g. viscoelasticity, rubber elasticity or semicrystallinity. Corresponding to their typical size in the nanometre range polymers often form structures on the nanoscale. In our research we investigate the mechanisms of structure formation and self-assembly (e.g. microphase separation or crystallization), develop methods to produce well defined, nanostructured materials, and investigate their properties.

For structural analysis we use a variety of scattering techniques including small and wide angle X-ray scattering. Grazing incidence techniques are used for thin film characterization. Scanning force microscopy serves as a complementary tool to image structures on the nanoscale in real space. The complex mechanical properties of polymers are studied by mechanical spectroscopy or rheology and the thermal behaviour by (fast scanning) calorimetry.



AFM image of a prefrozen film of PCL on MoS₂, partially covered by a liquid droplet. The film is stabilized above the melting temperature by the substrate and in equilibrium with the liquid droplet. Upon cooling it acts as a nucleus and induces fast and oriented crystal growth.

Current Projects and Future Goals:

The overall aim of our research is to understand on a fundamental level, how the morphology of semicrystalline polymers is generated during crystallization and how it determines the mechanical and electrical properties of these important class of materials.

■ Crystallization and Molecular Dynamics of Polymers

Polymers typically crystallize in a semicrystalline structure, consisting of layerlike crystallites with a thickness on the nanoscale separated by disordered amorphous regions. The resulting nanostructure strongly determines the macroscopic mechanical properties. It is therefore important to have a precise understanding of the crystallization process and the accompanying structure formation. We understand polymer crystallization as a complex interplay of the (macro)molecular dynamics in the melt, the growth kinetics of the lamellae, and possible intracrystalline chain dynamics. We use SAXS, DSC, Flash DSC, and rheology for investigation.

■ Interface Induced Crystallization

It is well known that crystallization of liquids most often starts at an interface to a solid. In general, a solid surface can induce crystallization by either heterogeneous nucleation or prefreezing. Our understanding of these processes on a microscopic level is very limited. By combining experimental and theoretical approaches, our aim is to understand the material parameters that affect the thermodynamics of prefreezing and the kinetics of heterogeneous nucleation. We investigate crystallization of thin films and isolated droplets of semicrystalline polymers on solid substrates using in-situ atomic force microscopy (AFM), optical microscopy, and X-ray scattering.

■ Structure Formation in Semiconducting Polymers

We investigate structure formation in semiconducting polymers, which are of interest for organic photovoltaics. A nanostructured morphology is necessary for an efficient charge separation in this class of materials, which we realize by diblock copolymer self-assembly. Since semiconducting polymers usually have an additional crystalline or liquid crystalline order, the structure formation in these materials is complex. We investigate how different influencing factors affect structure formation and ultimately the optoelectronic properties.

Institute of Chemistry

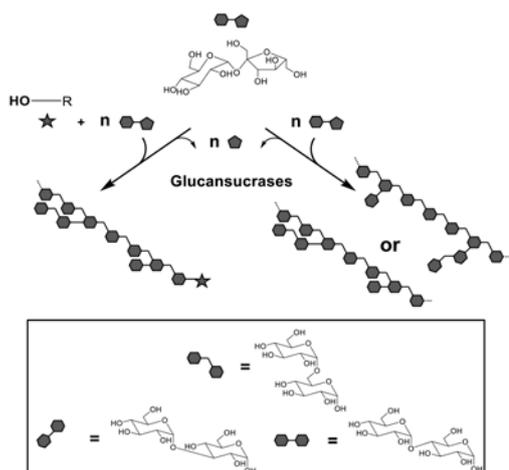
Food Chemistry – Functional Food

Fields of Research:

- › Structural characterization of polysaccharides from bacteria and algae
- › Production, enzymatic synthesis and modification of polysaccharides
- › Development of analytical methods for polysaccharide analysis
- › Synthesis and characterization of carbohydrate conjugates
- › Exploration of carbohydrate-active enzymes

Functional polysaccharides are complex macromolecules which influence the physiological, technological, and biological properties of foods as well as other products. The functionality of these biopolymers is mainly determined by their molecular structure. Therefore, our research is focused on structural characterization of polysaccharides, especially those from bacteria or algae.

To develop a detailed understanding of polysaccharide structures, we apply a wide range of analytical methods such as gas chromatography, ion chromatography, size exclusion / gel permeation chromatography, and nuclear magnetic resonance spectroscopy. We also use these approaches to develop enzyme-based methods for routine structural analysis, which allow a detailed and fast analysis of polysaccharides in model systems or foods. Because the establishment of structure-function relationships requires samples with a defined structure, another focus of our work lies on the synthesis and modification of polysaccharides. For this purpose, we use microorganisms as well as recombinant enzymes which allow for specific polysaccharide hydrolysis and modification as well as the production of tailor-made polysaccharides. Furthermore, we investigate how enzymes or chemical modifications can be used to synthesize novel polysaccharides and polysaccharide conjugates with unique properties.



Current Projects and Future Goals:

Production and advanced structural analysis of dextrans

Dextrans are α -glucans which are enzymatically synthesized from sucrose by various food-born lactic acid bacteria. Depending on source and synthesis conditions, dextrans have a high structural complexity which results in varying functional properties. We aim to improve the understanding of dextran structural architecture and to improve the methods to analyze these polysaccharides. For this purpose, we use recombinant glucansucrases and glucanases for polysaccharide synthesis, modification, and analysis.

Fine structures of insoluble glucans

Some lactic acid bacteria are able to enzymatically synthesize insoluble α -glucans which contain varying portions of α -1,3-linked glucose units. The formation of such polymers is, for example, important for the biofilm formation of cariogenic bacteria. However, less information is available on the detailed structural composition of insoluble glucans from different sources. Therefore, we are using partial enzymatic hydrolysis and several analytical approaches to gain detailed insights into the structures of different insoluble glucans.

Structure-function relationships of carrageenans

Carrageenans are structurally heterogeneous sulfated polysaccharides from red algae which are commonly used as gelling agents. However, some carrageenans have also been shown to inhibit the recrystallization of ice. To investigate which structural elements are responsible for this functionality, we are using different chemical, enzymatic, and analytical approaches to obtain tailor-made and well characterized carrageenans.

Structural characterization of hetero-exopolysaccharides

Lactic acid bacteria but also other microorganisms are able to form highly complex exopolysaccharides. These polymers are promising candidates as functional ingredients or materials. We are investigating the structure of these polymers and work with other groups to correlate structural and functional properties.



Prof. Dr. Daniel Wefers

2016

PhD in Food Chemistry, Karlsruhe Institute of Technology, Germany

2016

PostDoc, University of Illinois Urbana-Champaign, USA, Prof. Isaac Cann

2016–2019

Junior Research Group Leader, Karlsruhe Institute of Technology, Germany

Since 2019

Associate Professor (W2) of Food Chemistry, Martin Luther University Halle-Wittenberg

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Selected publications:

F. Münkel et al. Structural characterization of mixed-linkage α -glucans produced by mutants of *Lactobacillus reuteri* TMW 1.106 dextranase. *Carbohydr. Polym.* (2020), 231, 115697.

T. Klingel et al. Enzymatic synthesis and characterization of mono-, oligo-, and polyglucosylated conjugates of caffeic acid and gallic acid. *J. Agric. Food Chem.* (2019), 67, 13108–13118.

F. Münkel et al. Detailed structural characterization of glucans produced by glucansucrases from *Leuconostoc citreum* TMW 2.1194. *J. Agric. Food Chem.* (2019), 67, 6856–6866.

A. Fischer and D. Wefers. Chromatographic analysis of alginate degradation by five recombinant alginate lyases from *Cellulophaga algicola* DSM 14237. *Food Chem.* (2019), 299, 125142.

R. M. Prechtel et al. Structural characterization of the surface associated heteropolysaccharide of *Lactobacillus plantarum* TMW 1.1478 and genetic analysis of its putative biosynthesis cluster. *Carbohydr. Polym.* (2018), 202, 236–245.

L. Fels et al. Structural characterization of the exopolysaccharides from water kefir. *Carbohydr. Polym.* (2018), 189, 296–303.

Fig.: Reactions catalyzed by glucansucrases from lactic acid bacteria.



Jun.-Prof. Dr.
Martin Weissenborn

2009–2012

Dissertation (funded by Marie-Curie-Fellowship), Manchester Institute of Biotechnology, United Kingdom (Advisor: Prof. Flitsch)

2012–2016

Post-Doc, University Stuttgart, Germany (Advisor: Prof. Hauer)

2016

Post-Doc, ETH Zürich, Switzerland (Advisor: Prof. Hilvert)

Since 2016

Jun.-Prof. Organic Chemistry at the Martin Luther University Halle-Wittenberg and Junior-Research Group Leader at the Leibniz-Institute of Plant Biochemistry, Halle (Saale), Germany

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Selected publications:

Knorrscheidt et al., Identification of novel unspecific peroxygenase chimeras and unusual YfeX axial heme ligand by a versatile high-throughput GC-MS approach *ChemCatChem*, (2020) 10.1002/cctc.202000618.

K. J. Hock et al., Tryptamine synthesis by iron-porphyrin catalysed C–H functionalisation of indole with diazoacetonitrile *Angewandte Chemie* 58, 3630–3634 (2019).

P. Püllmann, C. Ulpinnis et al. (Collab. Koenigs Group), Golden Mutagenesis: An efficient multi-site saturation mutagenesis approach by Golden Gate cloning with automated primer design *Scientific Reports*, 9, (2019).

M. J. Weissenborn, S. A. Lowet et al., Enzyme-Catalysed carbonyl olefination by the *E. coli* protein YfeX in the absence of phosphines, *ChemCatChem*, 8, 1636–1640 (2016).

M. J. Weissenborn, R. Castangia, et al., Oxo-ester mediated native chemical ligation on microarrays: an efficient and chemoselective coupling methodology, *Chem. Commun.* 48, 4444–4446 (2012).

Institute of Chemistry & Leibniz-Institute of Plant Biochemistry

Employing and engineering enzymes for chemically challenging transformations

Fields of Research:

- › Directed evolution in yeast-based systems
- › Enzymatic degradation of polymers and mycotoxins

Despite the growing ‘toolbox’ of commercially available enzymes, which are capable of catalysing functional group interconversions with unparalleled regio- and stereoselectivity, biocatalysts mediating the formation of C—X bonds and those enabling convergent synthesis remain mostly undeveloped. Expansion of the biocatalytic toolbox to incorporate such enzymes, as well as the development of biocatalysts which mediate reactions not seen in nature, would allow us to approach synthetic design in an entirely different way.

Besides the inherent or promiscuous activity of enzymes for chemically challenging reactions, the feasibility of these transformations for specific molecule classes with high turnovers and yields is pivotal. The enzymes, therefore, ought to be engineered to fulfil these properties. The method of choice is here **directed evolution** that allows the design of tailor-made catalysts for specific purposes and was awarded the **Nobel Prize in Chemistry in 2018**.

Current Projects and Future Goals:

Enzymatic Hydroxylations

One of the chemically challenging transformations is the selective functionalisation of C—H bonds to form alcohol products. Fungal unspecific peroxygenases (UPOs) solely rely on hydrogen peroxide as co-substrate and show impressive total turnover numbers (TTN) of up to 300,000 for sp³-carbon hydroxylations. We were able to heterologously express a range of peroxygenases in yeast and are currently engineering them by directed evolution for enantioselective hydroxylation reactions.

Method development for directed evolution

Directed evolution requires the analysis of multiple hundreds of samples a week and hence necessitates a rapid screening system. We have developed a high throughput GC-MS system, which allows the sample injection in 33 s intervals, thereby substantially shortening the analysis time. This method enables us to engineer our enzymes towards any substrate of interest, which can be analysed by GC-MS.

Discovering novel enzymatic reactivities

Since proteins carry inherent promiscuity, each enzyme can perform a multitude of different “new-to-natural” reactions. Therefore, screening thousands of different proteins and protein classes for chemically challenging reactions in one experimental setup with a high-sensitive detection device is a powerful tool. This system is solely discovering protein scaffolds, cofactors or active site architectures, which enhance or catalyse the reaction of interest. The aim is not to discover a hidden, natural protein activity, but protein’s—and nature’s—diversity is harvested to randomly identify novel protein reactions, which will then serve as ‘starting points’ for directed evolution endeavours.

Polymer degrading enzymes

Apart from building molecules, enzymes could prove to be excellent tools for the degradation of polymers. We are engineering enzymes to improve their activity towards the cleavage of polymer chains to recycle them.

Institute of Chemistry & Leibniz Institute of Plant Biochemistry

Natural Products & Bioorganic Chemistry

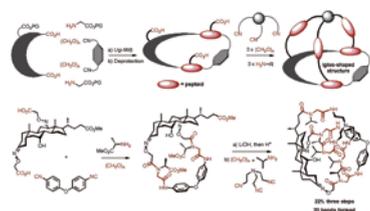
Fields of Research:

- › Biologically active natural products and metabolomic profiling
- › Total synthesis and medicinal chemistry
- › Multi-component reactions, rapid synthesis, and peptoids
- › Biotransformations
- › Chemoinformatics

Our research focuses on the identification and understanding of small molecules and their effects within biological systems, and on the application of such compounds to probe and modify biological systems monitored by bioassays, computational, metabolomic and proteomic techniques.

Three main lines of research are followed to achieve this: (1.) We try to learn from nature's chemistry through both elucidation of natural structures as well as understanding basic principles of nature's application of chemistry in a biological context; (2.) We use total and diversity oriented synthesis of natural products and derivatives, including biotransformations, for applications in biology, medicine, nutrition and agrochemistry; (3.) We try to increase our understanding of molecular interaction and construction processes and develop new tools, probes and recognition compounds to study these.

The analysis, isolation, characterization, and modification of natural products and enzymes from plants and higher fungi is the basis of our efforts to understand the properties of these biomolecules or to disclose their function in nature, and finally to explore their use in chemistry, biology and medicine. Applications are driven by the discovered properties and include such diverse areas as agrochemicals, lead structures in medicinal chemistry or novel food ingredients, biological research tools, or the utilization of enzymes as biocatalysts. This is backed by the development of analytical tools, e.g. for metabolic and affinity based protein profiling, by a synthesis program to increase compound availability and molecular diversity, and by computational methods to aid the understanding and design processes through theoretical models. Advanced projects usually proceed with additional collaboration with external academic or industrial partners.

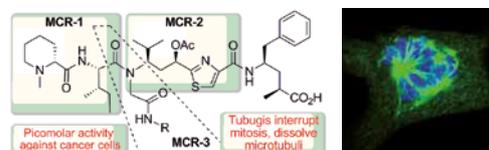


One pot assembly of igloo-type macromulticycles by multiple MCRs

Current Projects and Future Goals:

Isolation and synthesis of bioactive compounds

Plants and fungi are prominent producers of bioactive molecules. We develop new methods for the discovery of active ingredients with a current emphasis on anticancer drugs, fungicides, and taste modulators. This work often is done in close cooperation with international partners in South-East Asia, Arabia, Latin America and Africa, and with industrial partners. Based on the natural lead structures, we develop total synthesis routes to the natural product and its derivatives. In order to optimize the desired properties and to understand the drug-protein interaction, we integrate the chemical research with biochemical or biological assays and computational methods like molecular modelling or bioinformatics. As an example, we recently synthesized and patented new peptides with picomolar cytotoxicity, i.e. they belong to the most active anticancer compounds known to date.



Highly potent anticancer Tubugi-peptide (left), and its effect on a human cancer cell (right). (MCR: multicomponent reaction; green: microtubules; blue: chromosomes)

Enzyme biotechnology

The chemical industry currently undergoes a rapid change that sees a considerable increase in biobased chemical production technology. Biocatalysts play a crucial role in this transformation process as they often allow otherwise difficult or impossible reactions, or give more efficient, environmentally benign or acceptable processes. We focus on the discovery, mechanistic understanding, and application of biocatalysts with a focus on methyl, prenyl, and glycosyl transfer reactions. This will lead to new processes for the production of important plant products of terpenoid or flavonoid origin which are important, e.g. in the fine chemicals and flavor & fragrance industries.

Multiple multicomponent reactions (MCRs)

MCRs are unrivalled for the speedy construction of complex molecules. This is potentiated if multiple or sequential MCRs are applied. The theoretically quite demanding processes are often simple in practice and allow hitherto unknown possibilities for the construction of molecules of a complexity otherwise only found in nature's proteins or polysaccharides.



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Selected publications:

M. G. Ricardo et al. Improved Stability and Tunable Functionalization of Parallel β -Sheets via Multicomponent N-Alkylation of the Turn Moiety. *Angewandte Chemie* (2020) 132: 265-269; *Angew. Chem. Int Ed.* (2020), 59: 259-263.

L. Holzmeyer et al. Evaluation of plant sources for anti-infective lead compound discovery by correlating phylogenetic, spatial, and bioactivity data. *Proc. Nat. Acad. Sci. - PNAS* (2020). 117(22): 12444-12451.

M. Dippe et al. Coenzyme A-conjugated cinnamic acids-enzymatic synthesis of a CoA-ester library and application in biocatalytic cascades to vanillin derivatives. *Adv. Synth. Cat.* (2019), 361: 5346-5350.

B. Michels et al. Memory enhancement by ferulic acid ester across species. *Science Advances* (2018), 4: eaat6994.

M.A. Farag et al. Comparative Metabolomics Approach Detects Stress-Specific Responses during Coral Bleaching in Soft Corals. *J. Proteome Res.* (2018) 17: 2060-2071.



Prof. Dr.
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Selected publications:

B. Westermann et al.
Discovery of potent and selective inhibitors of the *Escherichia coli* M1-aminopeptidase via multicomponent solid-phase synthesis of tetrazole-peptidomimetics
Eur. J. Med. Chem. 2019, 163, 481 – 499.

B. Westermann et al.
Diversity Driven Decoration and Ligation of Fullerene by Ugi and Passerini Multicomponent Reactions
Chem. Eur. J. 2018, 24, 9788 – 9793.

D. Hinderberger, B. Westermann et al.
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B. Westermann et al.
Highly Stereoselective Synthesis of Natural Product-like Hybrids by an Organocatalytic/Multicomponent Reaction Sequence
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B. Westermann et al.
Isolation and Asymmetric Total Synthesis of Fungal Secondary Metabolite Hygrophorone B12
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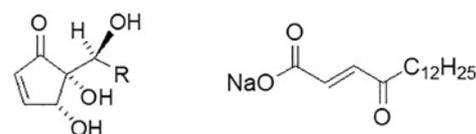
Institute of Chemistry & Leibniz Institute of Plant Biochemistry

Organic Chemistry Biofunctional Synthesis

Fields of Research:

- › Natural product synthesis
- › Diversity oriented synthesis
- › Multi-component reactions
- › Probes for protein profiling

In close collaboration with partners from the Leibniz-Institute of Plant Biochemistry, the MLU and internationally with collaborators mainly from Cuba and Brasil, we want to gain insight into the formation and action of secondary metabolites from plants and fungi. These findings will be applied for plant- as well for human health issues.



Natural products from fungi provide provide interesting synthetic challenges and intriguing biological features (example: natural products from *Hygrophorus*-species provide strong fungicidal compounds).

The biofunctional synthesis of plant- and fungi-derived natural products is necessary for several reasons: i) conformation of relative and absolute stereochemistry, ii) synthesis of derivatives to carry out structure-activity relationships, iii) combination with dyes/spin labels to study cellular uptake and structural features. To allow for an efficient synthesis of these products, we are developing new synthetic methodologies, with multi-component reactions in the focus. These protocols provide access in very low number of synthetic steps and can be carried out in “green” and sustainable fashion.

Current Projects and Future Goals:

Multi-Component Reactions

Multicomponent reactions (reactions of three and more components at the same time) are very efficient due to their high atom- and step economy. Among these, isonitrile-based MCRs (Passerini-, Ugi-, Ugi-Smiles-reaction) are suited best to accomplish the synthesis of natural-like peptoids and depsipeptides. These reactions will be done in the context of approaches to the synthesis of chemical probes, where they provide dual read out probes (fluorescence, EPR-spectroscopy). Parallel monitoring of biological processes will be made possible, such as the localization and the determination of e.g. reactive oxygen species (ROS). Some of these studies are carried iteratively with the biological departments of the IPB.

Ligations, click-chemistry

Studying click-reactions beyond the well-known copper-catalyzed alkyne-azide cycloadditions (CuAACs) as well as strain-promoted (SPAACs) will be developed. These reactions are very useful tools for ligations and bioconjugation. Recently, we have explored a new strategy, which is based on the Sakai reaction generating triazoles in highly chemo- and regioselective manner. We have begun to study this method as bioorthogonal reaction providing modified compounds in vitro and in vivo. Specifically, we want to synthesize with our Cuban colleagues protein adducts amenable for vaccination studies. In addition, we also examine in collaboration with our Brazilian partners photo-chemical reactions for hitherto unknown ligations. The main challenge of all of these reactions is the necessity to run them in aqueous solutions at ambient temperatures.

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...auf eine fruchtbarere praktische Anwendung ...
...scientia naturali seiner Ausübung zum Zweck ...
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...wird ich nicht mehr ...

Research in education and history of science

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Mathematics and the natural sciences are among the topics which, as school subjects, receive much attention when it comes to the questions "How do we learn? What do future teachers in mathematics, physics or chemistry need, how can we equip them to be competent teachers that know about the latest research in education?" The ongoing global challenges make it more and more clear how important it is not only to have basic knowledge in the sciences, in terms of facts, but to learn how to argue logically, to find mistakes and to critically ask about the interpretation of data.

While the subjects have some specifics, e.g. abstract thinking, logical arguments, a mixture of theoretical knowledge and the ability to plan, perform and interpret experiments, there are also some overarching themes that are at the heart of ongoing research projects.

Some examples:

The active process of knowledge construction, planning, testing, evaluating and implementing teaching-learning-arrangements, the role of language proficiency, identity work and educational choices, expectations, orientation and feeling "self-effective". There is also research on methods that prepare teachers for the challenges in the classroom, ongoing reflection and self-evaluation in order to continually monitor their skills.

Institute of Mathematics

Mathematics Education

Fields of Research:

Design Research on teaching and learning geometry

Learning mathematics as an active process of knowledge construction is in the heart of the research field "Design Research on teaching and learning geometry". As part of Design Research Studies, several cycles of specifying and structuring learning goals and contents, developing designs for teaching-learning-arrangements, conducting and analyzing design experiments, and developing local theories on teaching and learning processes are conducted. In this way, research not only leads to theoretical contributions but also to design results such as teaching-learning arrangements (tasks with supplementary materials for teachers) that can be implemented in mathematics classrooms in schools but also in various teacher education settings.



Photo: Pauline Amler

Participation in discourse practices and mathematical learning opportunities

Statistical studies repeatedly show that students with higher language proficiency outperform students with lower language proficiency in terms of mathematical achievement. In this context, our work aims at a better understanding of this connection with a focus on students' participation in classroom interaction and in particular in practices of explaining or negotiating meanings, arguing the validity of claims, or collective reasoning as these practices are interrelated with rich conceptual mathematical learning opportunities. Building on these insights, design principles for designing and enacting instruction that enhance language for mathematics learning can be investigated and prepared for implementation in teacher education and mathematics classrooms. In this way, we contribute to the aim of making mathematics accessible to all students, also those with lower (academic) language proficiency.

Current Projects and Future Goals:

■ **Design Studies**

At the moment two Design Research studies are conducted in the field of geometry. One on teaching and learning trigonometry and one on teaching and learning the mathematical concept similarity. As part of the latter, also possible supports for productive interaction in phases of group work are explored. In the future, the aim is offering a complete series of teaching-learning arrangements in geometry starting in German grade 8 classrooms.

■ **Project MESUT 2**

In the project MESUT 2 (funded by the DFG, in cooperation with Susanne Prediger, TU Dortmund), 3 PhD students work on different aspects of the large intervention study on language responsive teaching. At MLU our work focuses on a better understanding of the discovered differential effects for different groups of students and on transferring the projects' insights and results towards regular mathematics classrooms and teacher education.

■ **Project EsCo**

Starting in 2022 with the EsCo project, an international collaboration on research on and development of school mathematics teaching with linguistically disadvantaged learners is established together with J. Ingram from Oxford and N. Planas from Barcelona. In the next years, we will intensify our collaboration and aim at building a strong network together with other colleagues to promote collective research and development in Europe.

■ **Future Projects**

For the near future, A.-M. Vogler and K. Erath are planning a project on understanding possible obstacles in learning mathematics during the transition from elementary schools to secondary schools with a particular focus on divergent interactional practices. Furthermore, a project is planned aiming at strengthening the implementation of real-life data in learning mathematics using digital tools. In this way, we will explore how to support students in experiencing mathematics as important and inherent for their lives at the moment and in the future.



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PhD in Mathematics Education,
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PostDoc at the Institute for
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Selected publications:

Prediger, S., Erath, K., Weinert, H. & Quabeck, K. (in press). Only for multilingual students at risk? Differential effects of language-responsive mathematics instruction in a cluster-randomized controlled trial on fractions. *Journal for Research in Mathematics Education*.

Erath, K. (2021). Enhancing students' language in collective processes of knowledge construction in group work. The case of enlarging figures. *ZDM Mathematics Education*, 53(2). doi.org/10.1007/s11858-021-01253-2

Erath, K., Ingram, J., Moschkovich, J. & Prediger, S. (2021). Designing and enacting instruction that enhances language for mathematics learning. A review of the state of development and research. *ZDM Mathematics Education*, 53(2). doi.org/10.1007/s11858-020-01213-2

Erath, K. (2019). Explorative study on language means for talking about enlarging figures in group work. In U. T. Jankvist, M. Van den Heuvel-Panhuizen & M. Veldhuis (Hrsg.), *Proceedings of the Eleventh Congress of the European Society for Research in Mathematics Education (S. 1632–1639)*. Utrecht, Die Niederlande: Freudenthal Group & Freudenthal Institute, Utrecht University and ERME.



Prof. Dr. Thorid Rabe

2007

PhD Physics Education, University of Potsdam, Germany

2007-2009

Teacher Preparation Service at a Secondary School

2010-2014

Assistant professor of Physics Education (W1), University of Potsdam, Germany

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Selected publications:

Rabe, T. (2020), Wie viel Fach muss sein? Eine (kritische) Annäherung an die Modellierung professioneller Handlungskompetenz aus physikdidaktischer Perspektive. In U. Hericks, M. Keller-Schneider, W. Meseth, & A. Rauschenberg (Eds.), *Fachliche Bildung und Professionalisierung von Lehrerinnen und Lehrern* (pp. 49-76). Bad Heilbrunn: Klinkhardt.

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Rabe, T., & Krey, O. (2018), Identitätskonstruktionen von Kindern und Jugendlichen in Bezug auf Physik - Das Identitätskonstrukt als Analyseperspektive für die Physikdidaktik? *Zeitschrift für Didaktik der Naturwissenschaften*, 24(1), 201-216.

Institute of Physics

Physics Education

Fields of Research:

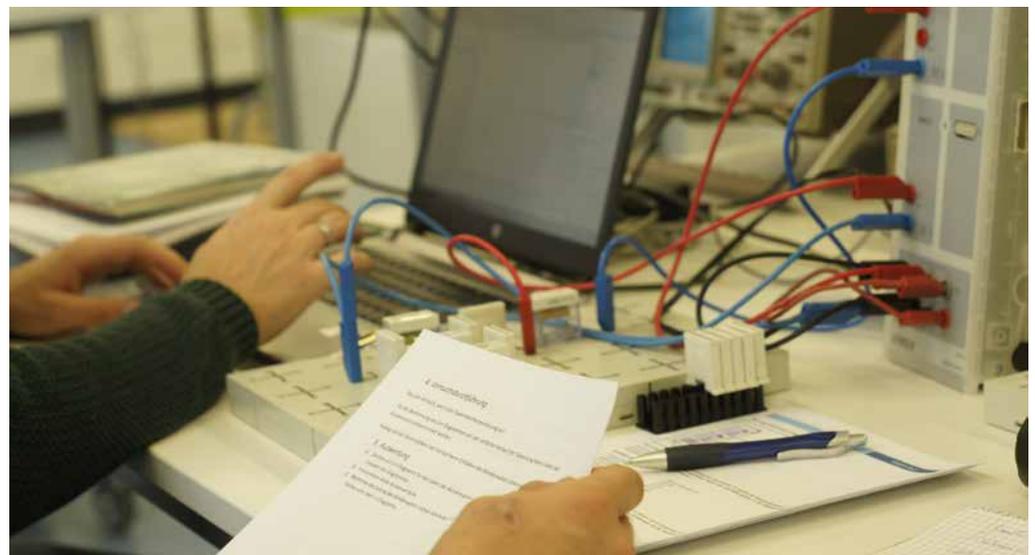
Identity work and educational choices

Decisions on educational pathways are relevant both for individuals and society. The investigation of identity work on physics allows in depth analyses of how adolescents relate themselves to physics and how this is reflected in their educational decisions. Physics identity is defined as the perception by others and the self-perception as well as the (linguistic) behaviour of individuals with regard to physics-related contents, topics and activities. So called "identity work" – the negotiation of one or more identities – takes place in an interplay of individual acting and the influence of social structures.

Teacher education

How to prepare future teachers so that they can plan and conduct their lessons in a professional and reflective way is an important question for physics education. In addition to competencies in the sense of skills, affective aspects such as self-efficacy expectations, orientations on physics and on educational topics are also relevant. Both the development of survey instruments and the investigation of the development of self-efficacy, orientations and identities of teacher students and teachers in the course of their study and career are part of the research interest.

Student teachers plan and carry out school experiments (Photo: Frederik Bub)



Current Projects and Future Goals:

Identity work and educational choices

It can be assumed that attitudes towards physics are formed at an early age and that physics lessons at school play an important role in this. Therefore, the perspectives of the pupils in the first physics lessons in the 6th grade are examined in a qualitative interview study.

A particularly important phase of identity work and educational choices is the transition from school to university or vocational training. In the project 'helpING!' (cf. <https://www.helping.academy>; promoted by the German Ministry of Education) 'orientation academies' are organized addressing young women at the end of their school time. The academies aim at providing orientation about possible career paths into science and technology. A longitudinal interview study with the participating young women will provide a deeper insight into the complexity of educational decisions at the transition from school to further education.

Teacher education

In the field of teacher education, the following three specific issues are examined:

- › Orientations of physics teachers on responsibility and technology in the context of physics teaching.
- › Casuistic teaching in university courses that supplement practical phases with a focus on linguistic aspects of inclusive teaching-learning settings
- › physics teachers' self-efficacy beliefs for teaching physics, specifically in the fields of "experimenting", "dealing with students' conceptions", "analyzing and preparing physics content" and "implementation of physics tasks"



Emeriti

Emeriti

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Undergraduate,
graduate and
postgraduate education

The Faculty of Natural Sciences II is committed to a high-quality scientific education in chemistry, physics, mathematics, and related disciplines, which is reflected in our good positions in national rankings. We combine an in-depth education in the three basic scientific disciplines leading to Bachelor, Master and doctoral degrees with the offer of specific interdisciplinary study programs as well as structured programs on the doctoral level.



Photo: Matthias Ritzmann | MLU

Studying at the Faculty of Natural Sciences II

Chemistry, physics, mathematics

The faculty offers education at undergraduate, masters and postgraduate level in the classical fields of chemistry, physics and mathematics and has an additional focus on related interdisciplinary education with Bachelor and Master programs in Medical Physics, Physics and Digital Technologies, Economathematics, Renewable Energy and Polymer Materials Science. Other programs like the studies in food chemistry and the teacher training in chemistry, physics, astronomy and mathematics prepare students for external final examinations like the German Staatsexamen.

Undergraduate study

The faculty offers exciting course programs and optimal conditions for learning and studying that are very well recognized in national rankings. The major fields of study are chemistry, physics and mathematics and their applications in the natural sciences. Specialized Bachelor programs offer degrees in Medical Physics and Economathematics. In autumn 2019, a new program Physics and Digital Technologies has been launched, which conveys both a general and broad basic physical education and solid knowledge of information technology. End of 2020, the new Bachelor course Physics Plus will start, which allows to study at the interface between science and society. Already on the Bachelor level, students get involved in high-level research performed at the different institutes.

Masters study

Different Master programs are set up to provide a full education in science, paving the path for excellent career opportunities. The consecutive Bachelor and Master programs in Chemistry, Physics, Medical Physics, Mathematics and Economathematics combine the high scientific level of traditional German diploma degrees with the benefits of the common European higher education area according to the Bologna Accords.

The consecutive programs are accompanied by an internationally oriented Master program in Polymer Materials Science taught in English language. The program attracts international as well as German students who enjoy an interdisciplinary topic and a multi-cultural learning environment and atmosphere. The Master program in Renewable Energies will provide a sound basis of chemical and physical knowledge and skills on this very timely topic.

Based on a flexible curriculum, all Master programs provide structured, graduate-level education in advanced research methods. The graduate students get in close contact with research groups in one of the institutes or in other local research institutions.



Photo: Maike Glöckner | MLU

Postgraduate Research

Postgraduate research and qualification

Postgraduate research at the Faculty of Natural Sciences II is typically performed in the framework of a research project in one of the groups at the Institutes of Chemistry, Physics, Mathematics, or at the different local research institutions. Postgraduate students are commonly employed as regular temporary half- to full-time staff members and have furthermore access to the postgraduate qualification program of the International Graduate Academy (InGrA) at Martin Luther University.

International Graduate Academy (InGrA)

InGrA is the “roof” for all structured doctoral programmes at Martin Luther University. It supports graduate students in all phases of their studies up to a successful start of a professional carrier and aims at gender equality and an increasing number of international graduate students.

Doctoral degrees

The Faculty of Natural Sciences II offers doctoral degrees in Natural Sciences (Dr. rer. nat., Dr.-Ing. or Dr. paed., all equivalent to a PhD) in the fields of Chemistry, Physics, Mathematics, or a related discipline after submission of a suitable doctoral thesis (dissertation) and a doctoral examination (defence).

Doctoral studies

Doctoral studies at Martin Luther University, like at most German universities, do not involve the strict course work that accompanies “PhD programs” in the Anglo-Saxon system. In the classical German system, admission to the doctoral student level requires a Diploma or an equivalent Master degree. Applicants on the Bachelor level need to pass one of our Master programs before entering the postgraduate stage.

Structured doctoral programmes

Depending on their research topic, the postgraduate students may, in addition to the thesis-related research work, get the opportunity to join a “Graduate School” (e.g., within a Research Training Group or a Collaborative Research Center of the DFG), and thus to participate in a dedicated doctoral training programme, for which a separate certificate is issued along with the degree.

As one example, in a joint initiative of the Max Planck Institute of Microstructure Physics, the Institute of Physics at Martin Luther University Halle-Wittenberg and the Fraunhofer Institute for Materials Mechanics, the International Max Planck Research School for Science and Technology of Nanostructures (Nano-IMPRS) was established to support excellent young scientists on their way to a doctorate or PhD degree in this specific area.

Other programmes can be found on our web pages:
<http://www.natfak2.uni-halle.de/promotion>

Impressum

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Portrait Photos:

Michael Deutsch, MLU / Jens Schluete, MLU / privat

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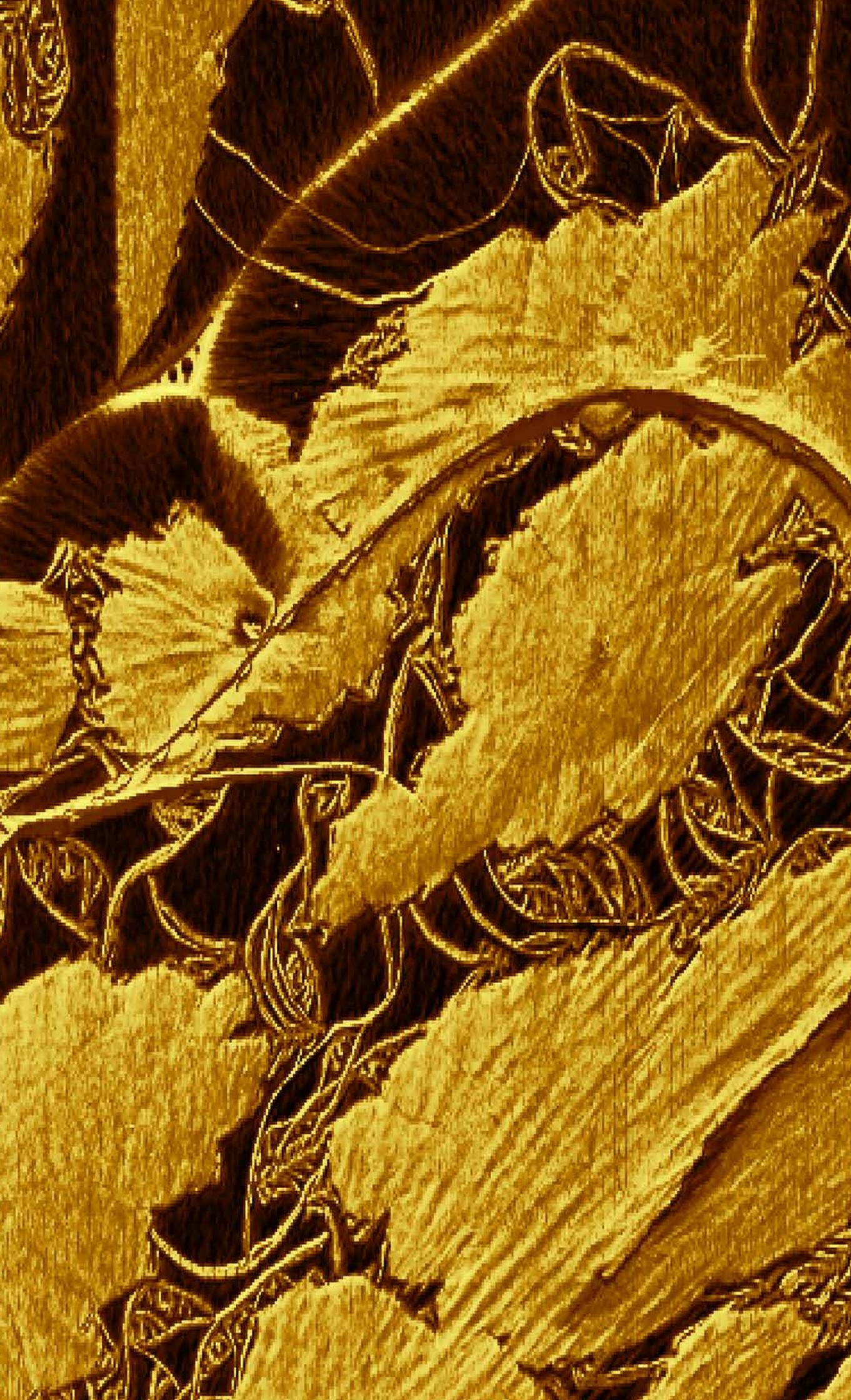


Figure: AFM image showing semicrystalline Poly-ε-caprolactone (PCL) with 2D spherulitic structure on silicon substrate.
Photo: Martha Schulz | MLU