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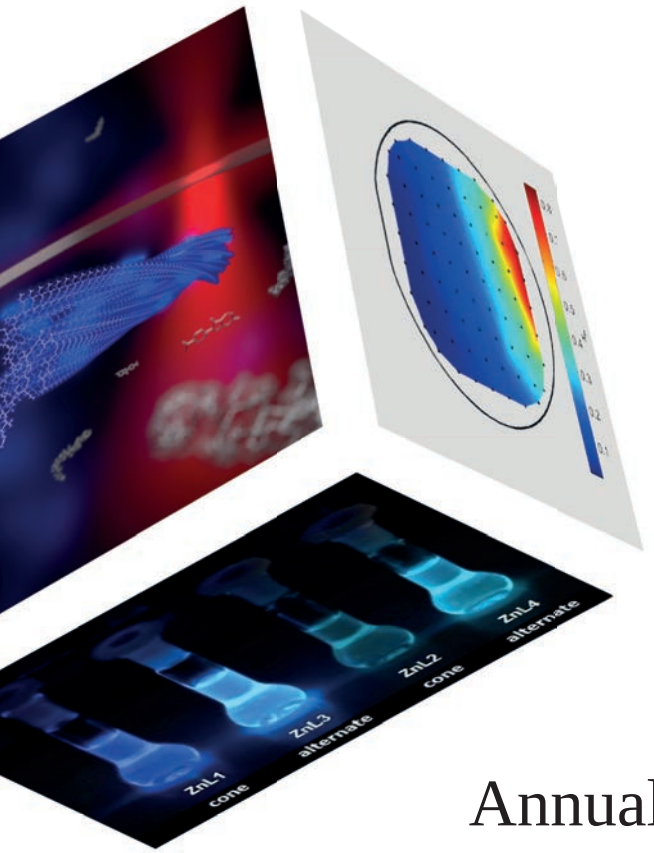
BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2018

Cover image:
⇒ *Left:* Illustration of a growing amyloid fibril in the thermophoretic trap including laser.
⇒ *Right:* False color representation of the indium content *x* of a $(In_xGa_{1-x})_2O_3$ thin film grown on a 2 inch diameter c-plane sapphire substrate.
⇒ *Bottom:* Variation of fluorescence properties of Zn^{2+} ions supported by a macrocyclic calix[4] arene ligand.

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Annual Report 2018

Founded as DFG Graduate School 185 in 2007

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Leipzig School of Natural Sciences – the eleventh year of building with molecules and nano-objects

Preface
Prof. Dr. Marius Grundmann
Speaker of the Graduate School
Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Vice-Speaker of the Graduate School

For already more than ten years, the Leipzig School of Natural Sciences – Building with Molecules and Nano-objects (BuildMoNa) has supported interdisciplinary doctoral studies of young scientists. Excellent research conditions, scientific modules for broadening the horizon, and soft skills training as well as support for various activities such as stays abroad and conference contributions provide a stimulating environment for the doctoral researchers.

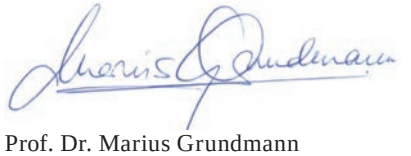
Our materials research concept is based on a “bottom-up” approach. Progressive building blocks, such as nano-objects, smart molecules, polymeric scaffolds, peptides and active proteins, are combined – preferentially by self-organisation – for the creation of fundamentally new classes of materials that are inspired by active, adaptive living matter, and which are environmentally friendly, highly efficient, low-cost devices serving multifunctional purposes for a steadily more diversified modern society. The paradigm shift from uniform bulk materials towards nanostructured multifunctional materials that emerge from combinations of smart molecules, proteins and nano-objects is essential for future knowledge transfer from fundamental to applied sciences. Since the establishment of the Graduate School in 2007, 150 young scientists have finished their doctoral studies with a certificate of the Graduate School. In 2018, 59 doctoral researchers have been enrolled as members of BuildMoNa. Most of them are employed through third-party funded research projects and we are grateful for 5 DAAD-GSSP and 12 other scholarships.

The Graduate School provides a well-structured training program including multi-disciplinary scientific training and a transferable skills program in cooperation with the Research Academy Leipzig. The scientific training program consists of introductory modules to bridge interdisciplinary gaps, thematic modules and advanced modules linked to ongoing research and technological applications.

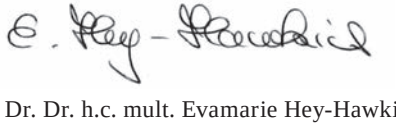
Each year, one of the advanced modules is organised as an international symposium. In 2018, the symposium “Physics of Cancer” was organised by Prof. Josef A. Käs and brought together researchers from pioneering groups worldwide that are investigating the mechanisms underlying cancer progression. The symposium focussed on how physics, chemistry, biochemistry, molecular and materials science can provide a new perspective on oncology as well as the state of the art in diagnostics and therapeutics to identify the current needs. The symposium was also supported by the Deutsche Forschungsgemeinschaft.

Science-related events included the sixth Annual BuildMoNa Conference in March, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School. External speakers, selected and invited by the doctoral researchers of BuildMoNa, covered topics of spectroscopic techniques, organic electrochemistry, multicatalytic transformations, genetically encoded chemical tools and single-molecule sensing in engaging presentations.

After funding by the Deutsche Forschungsgemeinschaft within the German Excellence Initiative until October 2014, BuildMoNa was financially supported as a class at the Research Academy Leipzig until October 2017 through funds of the Research Profile Area “Complex Matter”. From November 2017 on, BuildMoNa has been permanently established as “Graduate School” (Graduiertenschule) within the Research Academy Leipzig and is funded through an agreement (Zielvereinbarung) between BuildMoNa, the rectorate of Universität Leipzig and the three main faculties involved in BuildMoNa. The sustained path established for BuildMoNa will allow us to develop further, widen our reach, flourish in our activities and to continue to supply excellent support and research conditions for our doctoral researchers.

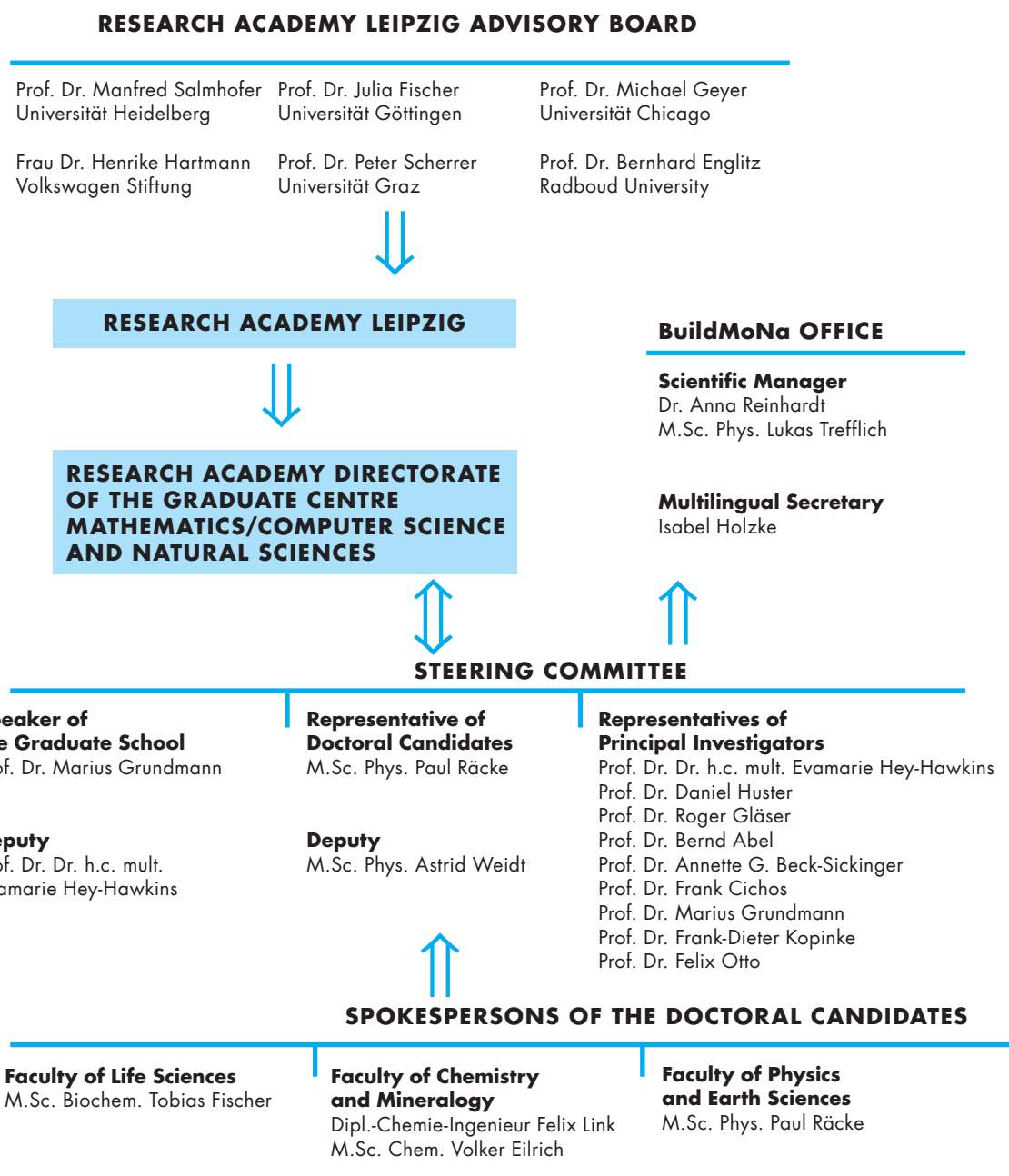


Prof. Dr. Marius Grundmann



Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins

Organisation and management



The Graduate School BuildMoNa is a class of the *Research Academy Leipzig* within the Graduate Centre for Mathematics, Computer Science and Natural Sciences, its director being Prof. Dr. M. Droste. BuildMoNa is represented within the Research Academy by Prof. Dr. M. Grundmann as Research Academy Board member and by Paul Räcke as representative of the doctoral candidates.

The Research Academy Leipzig Advisory Board evaluates the scientific activities of the graduate school by accepting the annual report and providing recommendations for further development.

BuildMoNa's Steering Committee's major tasks are: coordination of activities including advertising, marketing and recruiting in collaboration with the Graduate Centre, management of the recruiting process, establishment and organisation of the training programme, identifying and monitoring whether the programme's deliverables and milestones are achieved, management of the collaboration with other involved scientific institutions and industrial partners, management of funds, and reporting.

The Speaker of the graduate school is head of the Steering Committee as well as the external representative of BuildMoNa.

The spokespersons of the doctoral candidates are responsible for communication between different faculties considering doctoral candidate's issues. They elect one spokesperson, who represents the doctoral candidates within the Steering Committee.

The BuildMoNa Office consists of a professional scientific manager (half-time position) and a multilingual secretary (half-time position), who support the Steering Committee. They coordinate the doctoral training activities and ensure information/communication between participating scientists, doctoral candidates, visiting researchers, and collaboration partners (non-university and industrial). The Office has regular business hours, especially for requests from applicants or doctoral candidates.

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Angela Aleksovska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Photoactive metal-organic-frame-works - synthesis and applications*
M.Sc. Saral Baweja	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis and characterisation of heterobimetallic bifunctional Pd/Ir and Pd/Ru complexes as catalysts for tandem reactions*
M.Sc. Phys. Sascha Becker	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*Photoelectrically detected magnetic resonance of nitrogen vacancy centres in diamond*
M.Sc. Phys. Henrik Christiansen	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Nonequilibrium investigation of (bio-)physical systems*
M.Sc. Chem. Peter Coburger	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*1,2-Dicarba-closo-dodeca-borane(12) as scaffold for the development of new ligands with application in homogeneous catalysis*
M.Sc. Chem. Reike Clauß	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Heterobimetallic complexes in homogeneous and heterogeneous catalysis*
M.Sc. Chem. Jan Dirks	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. B. Abel	*Immobilisation and applications of CyP450 proteins on surfaces*
M.Sc. Chem. Volker Eilrich	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis and applications of phosphorus-rich transition-metal phosphides*
M.Sc. Phys. Alexander Fischer	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Feedback controlled active particle assemblies*
M.Sc. Chem Jan-Patrick Fischer	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Chemical modification and characterisation of therapeuticaly relevant peptide hormones*
M.Sc. Biochem. Tobias Fischer	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe	*Identification of chemerin function*
M.Sc. Chem. Christina Fraunhofer	Prof. Dr. O. Oeckler / Prof. Dr. H. Krautscheid	*Structure and thermoelectric properties of mixed valent chalco-genides*
M.Sc. Phys. Martin Fränzl	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Thermoelectric effects at the nanoscale*
M.Sc. Chem. Marta Gozzi	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Nido-carbaborate complexes as cytoxic agents*
M.Sc. Chem. Peter Hahn	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Calix[4]arenes for binding f-elements, synthesis, characterisation and complex formation*
M.Sc. Phys. Anna Hassa	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Deep UV photodetector arrays based on large bandgap oxides*
M.Sc. Chem. Florian Harth	Prof. Dr. R. Gläser / Prof. Dr. A. Schmid	*Valorisation of glycolate by heterogeneous catalysis in aqueous phase*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Principles of mechanosensitivity and durotaxis in mammatian cells*
M.Sc. Phys. Oliver Herrfurth	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Femtosecond-time-resolved spectroscopic ellipsometry and its application to ZnO-based structures*
M.Sc. Phys. Constantin Huster	Prof. Dr. K. Kroy / Prof. Dr. T. Pompe	*Bottom-up inelastic cell mechanics*
M.Sc. Phys. Patrick Irmisch	Prof. Dr. R. Seidel / Prof. Dr. K. Kroy	*Target recognition by CRISPR-Cas enzymes*
Dipl.-Math. Roger John	Prof. Dr. J. Meijer / Prof. Dr. B. Rosenow	*Coupling ^{13}C-superlattices to single nitrogen vacancy centres in diamond*
M.Sc. Chem. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Heterogeneously catalysed liquid phase oxidation of hydrocarbons over metal-organic frameworks*
M.Sc. Phys. Max Kneiß	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Optical properties and lateral transport in $Mg_xZn_{(1-x)}O$ quantum well nanostructures: A new approach for diluted magnetic semiconductors*
M.Sc. Chem. Kevin Kretschmer	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. I. Coin	*Investigation of protein-protein interactions for the development of therapeutic peptides*
M.Sc. Chem. David Langer	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Application of dendritic catalysts in tandem catalysis*
M.Sc. Phys. Susann Liedtke	Prof. Dr. Dr. h.c. B. Rauschenbach / Prof. Dr. J. Meijer	*Sculptered metal films*
Dipl.-Chem.Ing. Felix Link	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Diesel exhaust catalyst deactivation by biofuel-originated poisons and hydrothermal treatment*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Georgia Mhanna	Prof. Dr. R. Gläser/ Prof. Dr. A. G. Beck-Sickinger	*Hexagonal mesoporous silicates for immobilisation of multi-enzyme conjugates*
M.Sc. Phys. Erik Morawetz	Prof. Dr. J. Käs / Prof. Dr. S. Mayer	*Optical deformability and tumour aggressiveness*
M.Sc. Chem. John Popp	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Redox-switchable catalysis with P-stereogenic dendritic ferrocenyl phosphine complexes*
M.Sc. Chem. Rafaella Precker	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. D. Huster	*MOFs as drug carriers for cancer therapy*
M.Sc. Phys. Paul Räcke	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*High precision fabrication of quantum sensor arrays via ion implantation*
M.Sc. Chem. David Rettke	Prof. Dr. T. Pompe / Prof. Dr. A. G. Beck-Sickinger	*Soft colloidal probe-based biosensors*
M.Sc. Phys. Stefanie Riedel	Prof. Dr. S. G.Mayr / Prof. Dr. J. Käs	*Radiation assisted modification of gelatin and collagen for biomedical applications*
M.Sc. Biotech. Chiara Ruggirello	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Targeted tumour therapy by cell specific receptor internalisation*
M. Sc. Phys. Florian Scheffler	Prof. Dr. R. Seidel / Prof. Dr. F. Cichos	*Layer-by-Layer - DNA origami hybrid systems*
M. Sc. Phys. Clemens Scheuner	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*Microwave detector arrays based on diamond NV centers*
M.Sc. Chem. Jan Schulz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Carborane-based frustrated Lewis pairs for homogeneous catalysis*
M.Sc. Chem. Benedikt Schwarze	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Metal carborate complexes with bioactive ligands as organometallic anticancer agents*
M.Sc. Chem. Axel Straube	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Multi-ferrocene-based phosphorus ligands for homogeneous catalysis*
M.Sc. Phys. Lukas Trefflich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Fabrication and characterisation of carbon-nanodot-based planar microcavities*
M.Sc. Phys. Astrid Weidt	Prof. Dr. S. G. Mayr / Prof. Dr. A. Anders	*Interactions of cells and proteins with titanium dioxide (TiO_2) nanotube scaffolds to develop a novel implant material*

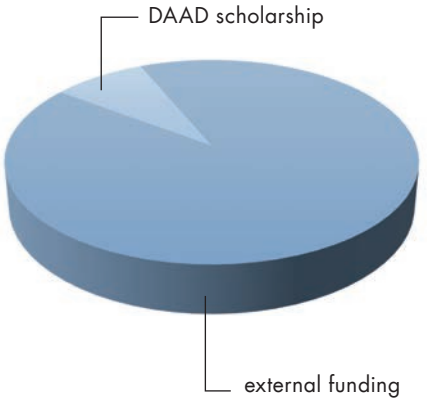
Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Antonia Welk	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Fabrication and characterisation of amorphous zinc magnesium oxynitrides (a-ZnMgON) for thin-film transistor applications*
M.Sc. Chem. Nils Wilharm	Prof. Dr. M. Zink / Prof. Dr. S. G. Mayr	*Electron induced crosslinking of biomimetric hydrogels as a model for the investigation of tumour spreading*
M.Sc. Biochem. Philipp Wolf	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe	*Selective drug uptake via peptide-mediated internalisation of the endothelin system*
M.Sc. Nanoscience Muhammad Ayman Zaheer	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Studying of diffusion in reacting catalytic systems by means of NMR spectroscopic methods*
Dipl.-Math. Heinrich-Gregor Zirnstein	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Topological aspects of Dirac fermions in condensed matter systems*

Alumni 2018

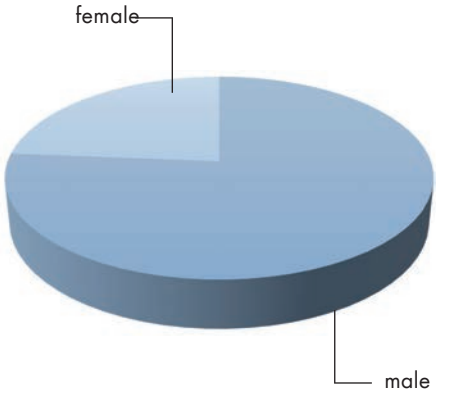
Title and Name	First / Second Supervisor	Title of doctoral thesis
M.Sc. Chem. Antonio Buzharevski	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Synthesis of Carboranyl Analogues of Nonsteroidal Anti-inflammatory Drugs (NSAIDs)*
M.Sc. Chem. Toni Grell	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*New aspects on the coordination chemistry of hexa-tert-butyl-octaphosphine*
M.Sc. Chem. Yuting Guo	Prof. Dr. H. Harms / Prof. Dr. F.-D. Kopinke	*Heterogenic responses of bacteria towards silver nanoparticles*
M.Sc. Phys. Robert Karsthof	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Transparent photovoltaic cells*
Dipl.-Phys. Fritz Lehnert	Prof. Dr. S. G. Mayr / Prof. Dr. Dr. hc. B. Rauschenbach	*Ion-aided synthesis and investigation of nanoporous materials*
M.Sc. Phys. Marcus Purfürst	Prof. Dr. R. Gläser / Prof. Dr. M. Grundmann	*Influence of Soot on the Transport Mechanisms inside the Filter Wall of SCR-Coated Diesel Particulate Filters*
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Optically anisotropic planar microcavities*
M.Sc. Chem. Stefan Saretz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Carbarborane derivates for medical use*
M.Sc. Phys. Peter Schlupp	Prof. Dr. M. Grundmann / Prof. Dr. S. G. Mayr	*Growth and optimisation of amorphous p- and n-type oxide semiconductors for electronic device applications*
M.Sc. Phys. Marcel Wille	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Whispering gallery modes: influence of resonator shape on lasing properties*
M.Sc. Biochem. Dennis Worm	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Targeting of peptide receptors on cancer cells for imaging and advanced cancer therapy*

Statistics

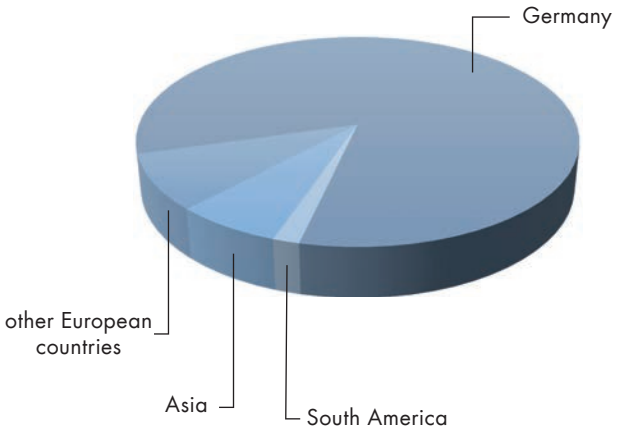
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:

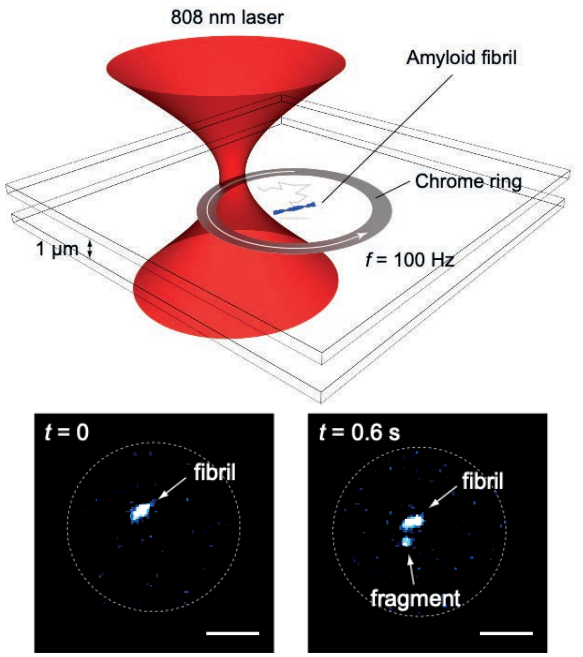


Thermophoretic trap for single amyloid fibrils

Prof. Dr. Frank Cichos
M.Sc. Phys. Alexander Fischer, M.Sc. Phys. Martin Fränzl

The self-organization of individual molecular units into functional or pathological structures is fundamental for life. The aggregation of proteins into fibrillar structures, though, may also yield toxic assemblies which are connected to neurodegenerative disorders. This process is intensively studied on the ensemble level. A major difficulty in the investigation of protein aggregation and other macromolecular nucleation and growth processes is the heterogeneity of the ensemble studied. Ensembles contain aggregates of different sizes which grow in an unsynchronized way. Therefore, single fibril optical microscopy studies aim to disentangle the heterogeneous ensemble, but none of those experiments has been able to follow the growth of a freely suspended fibril without the perturbing immobilization at a solid interface. Secondary processes like fibril branching or fracture have been proposed, but never observed directly.

The Molecular Nanophotonics Group has investigated over the past couple of years the manipulation and trapping of single nano-objects with the help of dynamic temperature fields. The local temperature in a liquid film is increased due to the optical absorption of tiny metal structures at the interface between a substrate and the liquid. The generated temperature gradients can be dynamically changed and cause a thermophoretic drift of the nano-objects in the liquid towards colder regions. With structures as depicted in the figure, the group has managed to capture single Amyloid $A\beta_{40}$ fibrils to observe their growth. This has become possible by observing the rotational diffusion of the fibrils in the trap with high time-resolution for an overall time period up to hours. The fibril growth can be studied under different buffer conditions. The long observation times have also enabled the detection of fibril fracture events, which have previously never been observed directly.



⇐ top) Schematics of the protein trapping setup. An 808 nm laser is rotating along a chrome ring to create a temperature minimum in the solution in the middle of the trapping structure. bottom) Fracture event of a single $A\beta_{40}$ fibril observed in the thermophoretic trap.

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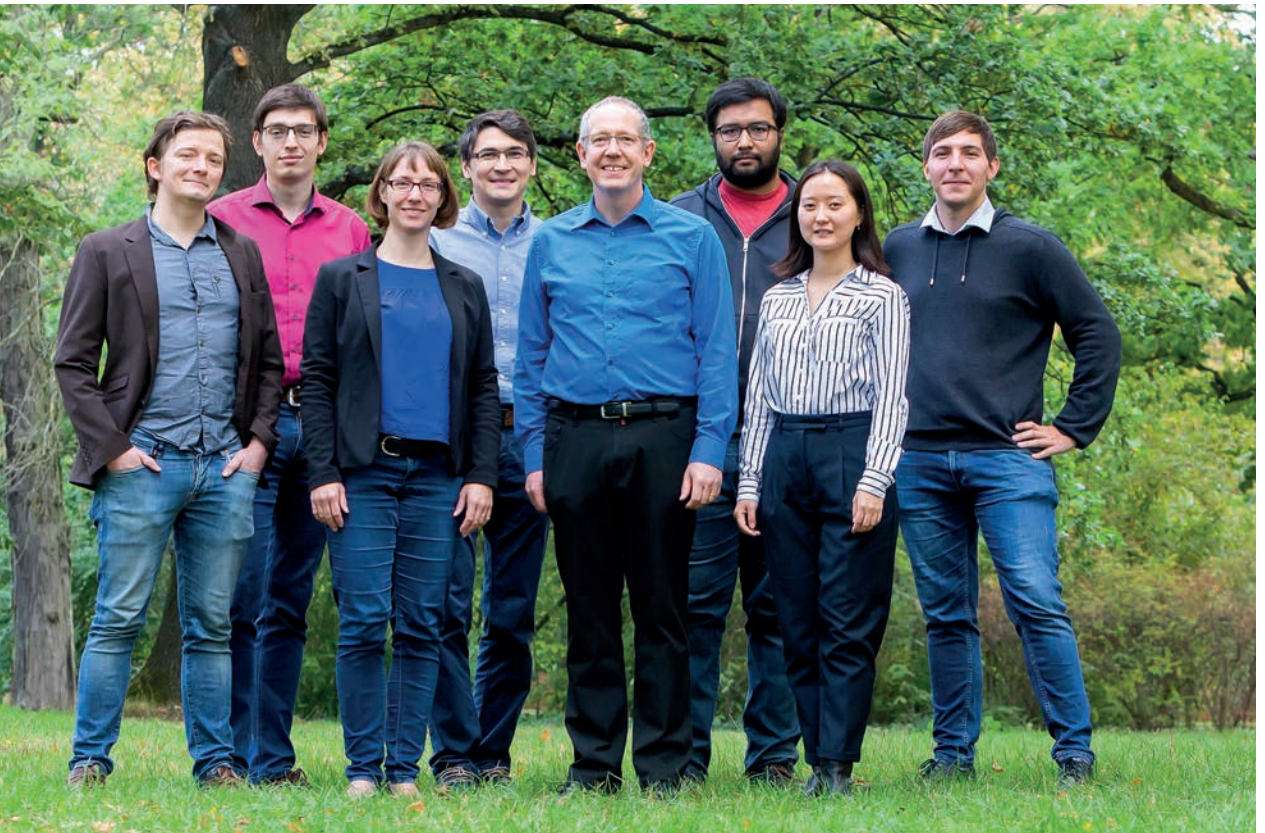
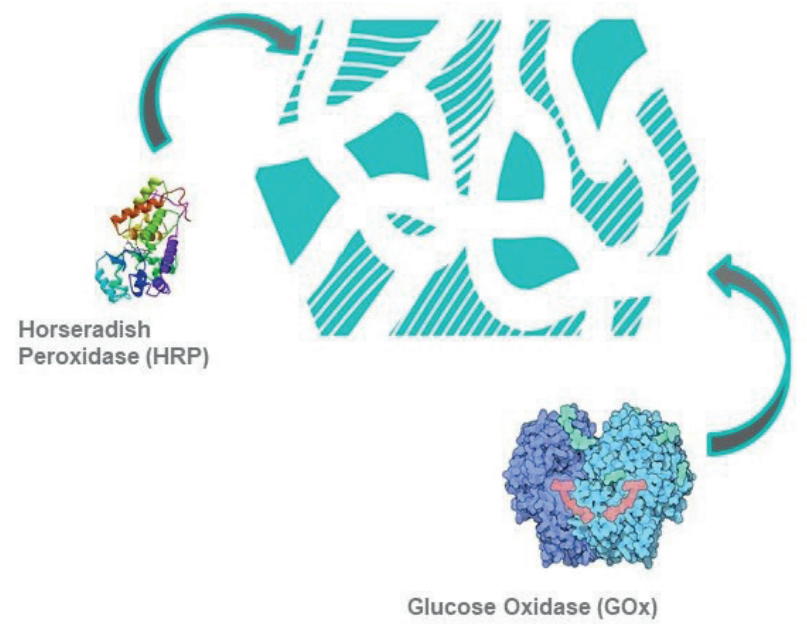
Novel catalytic systems by nano-scale design

Prof. Dr. Roger Gläser
M.Sc. Chem. Ulrike Junghans, M.Sc. Chem. Florian Harth, Dipl.-Chem. Ing. Felix Link, M.Sc. Chem. Georgia Mhanna, M.Sc. Phys. Marcus Purfürst, M.Sc. Nanoscience Muhammad Ayman Zaheer

Nanostructured catalysts with defined porosity on the nanometer scale and tunable active components continue to play a key role for the solution of current challenges in heterogeneous catalysis. An improved mass transfer and stability of the catalysts enables their use in applications. Following the principle approaches of BuildMoNa, the research in our group is focused on the nano-scale design of materials and their use as catalysts and catalyst supports. Solid catalysts for heterogeneously catalyzed hydrogenation reactions often consist of metal nanoparticles, which are finely dispersed on nanoporous support materials. Specifically, we study the influence of catalyst properties, e.g., metal particle size, metal-support interactions as well as the interaction of different metals on the hydrogenation of glycolic acid to ethylene glycol in the aqueous phase.



The goal is to design active, selective and stable catalysts for the upgrading of glycolic acid which can be formed from sunlight and CO_2 by algae. For the selective immobilization of multi-enzyme conjugates, support materials with interconnected hierarchical mesopore systems are studied. This is crucial for the active sites of the co-immobilized enzymes to be accessible, and, to achieve high catalytic activity. In the transesterification of oils, we use post-synthetic treatment to introduce larger pores into the framework of titanosilicate-based catalysts. The rates of molecular diffusion and the progress of the reaction within the catalyst pores are investigated in-situ by Xenon gas as an atomic nano-sensor, along with multinuclear NMR spectroscopy.



⇑ Schematic representation of the co-immobilization of the multi-enzyme conjugate comprising horseradish peroxidase (HRP) and glucose oxidase (GOx) in the pores of a hierarchical large-pore mesoporous silicate.

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Building material gradients laterally and vertically - combinatorial acceleration of material research and new device perspectives

Prof. Dr. Marius Grundmann
M.Sc. Phys. Anna Hassa, M.Sc. Phys. Oliver Herrfurth, M.Sc. Phys. Roberst Karsthof, M.Sc. Phys. Max Kneiß, M.Sc. Phys. Steffen Richter, M.Sc. Phys. Peter Schlupp, M.Sc. Phys. Lukas Trefflich, M.Sc. Phys. Antonia Welk, M.Sc. Phys. Marcel Wille

At the very core of semiconductor technology lies the possibility to combine different materials into so-called heterostructures. This concept, often termed 'bandgap engineering' is the basis for modern electronic and photonic devices such as high-electron-mobility transistors and light-emitting diodes and lasers. Over the last decades various BuildMoNa doctoral students in the Semiconductor Physics Group of Felix Bloch Institute for Solid State Physics have worked on material alloy systems such as (Mg,Cd,Zn)O and $(In,Ga,Al)_2O_3$ with various cation ratios. Additional to the change of bandgap with chemical composition, the change of crystal phase and lattice constant must be considered. In particular for the sesquioxides, a rich field for material physics challenges and design/optimization opportunities opens since the binary materials exhibit different phases (In_2O_3: cubic, Ga_2O_3: monoclinic, Al_2O_3: rhombohedral) and other phases, such as the orthorhombic κ-phase can be stabilized [R1]. The latter has the potential advantage of high polarization and thus is promising for creating high density two-dimensional carrier gases at interfaces.

Using the previously developed technique for pulsed laser deposition (PLD) of lateral material gradients using a radially segmented target, the κ-$(In_xGa_{1-x})_2O_3$ alloy system was investigated [R2]. As can be seen in Fig. 1a, the indium concentration x, as determined by EDX (energy-dispersive X-ray analysis in the scanning electron microscope), varies (non-linearly) over the 2 inch wafer. The correlation of the locally measured X-ray diffraction scans with the indium concentration (Fig. 1b) reveals the continuous shift of the lattice constant and the discontinuity when a different phase develops (at about x=0.35 and x=0.50). This way a complete alloy system can be investigated with one or just a few samples.

A novel technique for PLD has been developed in order to create vertical composition gradients (VCCS-PLD), i.e. gradients along the growth direction. These can be step-wise, as often used for heterostructures, or continuous [R3]. The method is based on an elliptically segmented target as visualized in Fig. 2. The position of the ablation laser beam determines how much of the inner or outer material is ablated and thus the composition of the eventual thin film. Using this concept, quantum

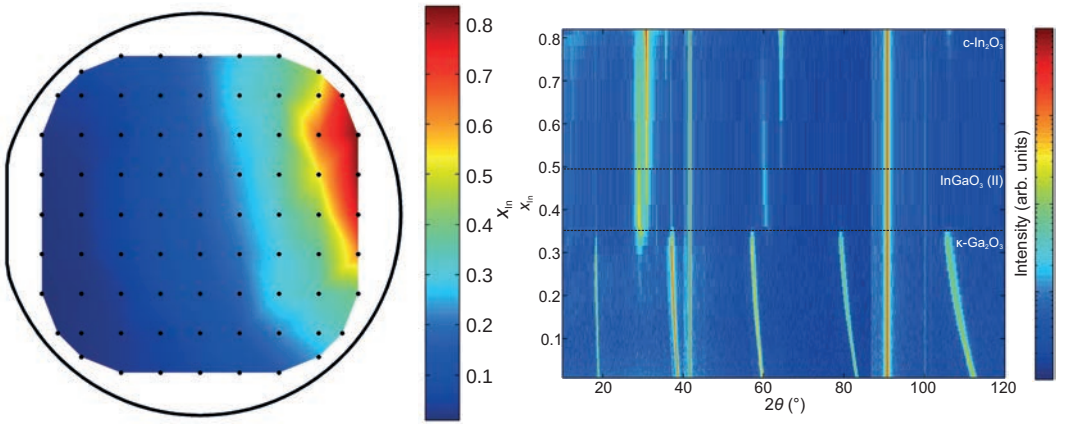
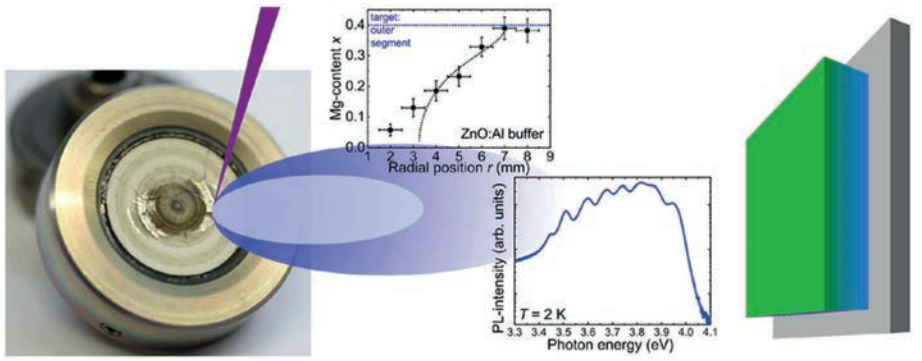


Fig. 1: (a) False color representation of the indium content x of a $(In_0Ga_{1-x})_2O_3$ thin film grown on a 2-inch diameter c-plane sapphire substrate. The black dots indicate measurement spots, data in between was interpolated. The solid black line indicates the gradient direction. (b) False color plot of 55 XRD 2θ-ω measurements acquired along the gradient direction.

well heterostructures with different barrier height can be fabricated from a single target. The VCCS-PLD method opens new possibilities for strain-engineering of heterostructures, e.g. for tuning of the critical thickness and piezoelectric polarization effects.



⇑ Fig. 2: Elliptically segmented target and cartoon of the ablation laser and the resulting plasma plume. The plots show (top, left) the thin film composition as a function of radial laser focus position on the target and (bottom, right) the photoluminescence spectrum of a (Mg,Zn)O thin film with eight stepwise constant concentration values.

Recently, device perspectives for novel photodetectors have been conceptualized for lateral [R4] and vertical [R5] continuous material gradients that will be pursued experimentally in the future.

For his work on κ-phase sesquioxides [R1], Max Kneiß has received the BuildMoNa Award (First Prize) 2019 and the Best Poster Award of the 61st Electronic Materials Conference (EMC 2019), Ann Arbor, MI.

⇒ [R1] *Tin-Assisted Heteroepitaxial PLD-growth of κ-Ga_2O_3 Thin Films with High Crystalline Quality*
M. Kneiß, A. Werner, D. Splith, C. Sturm, H. von Wenckstern, T. Schultz, N. Koch, M. Grundmann / APL Mater. (2019) **7** 022516:1-11

⇒ [R2] *Structural, Optical and Electrical Properties of Orthorhombic κ-$(In_xGa_{1-x})_2O_3$:Sn Thin Films*
A. Hassa, H. von Wenckstern, D. Splith, C. Sturm, M. Kneiß, V. Prozheeva, M. Grundmann / APL Mater. (2019) **7** 022525:1-9

⇒ [R3] *Combinatorial Material Science and Strain Engineering Enabled by Pulsed Laser Deposition Using Radially Segmented Targets*
M. Kneiß, P. Storm, G. Benndorf, M. Grundmann, H. von Wenckstern / ACS Comb. Sci. (2018) **20** 643-652

⇒ [R4] *Monolithic Waveguide-based Linear Photodetector Array for Use as Ultra-Compact Spectrometer*
M. Grundmann / IEEE Transact. Electr. Dev. (2019) **66** 470-477

⇒ [R5] *Monolithic Forward-looking Photodetector for Use as Ultra-Compact Wavemeter with Wide Spectral Range*, M. Grundmann / phys. stat. sol. (a) (2018) **215** 1800651:1-5

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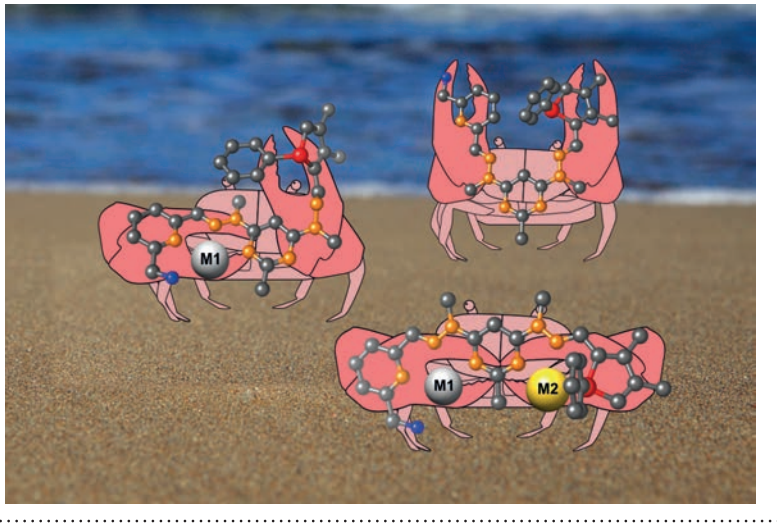
Smart phosphorus- or carborane-containing molecules and transition metal complexes as building blocks in catalysis, materials science and medicinal chemistry

Prof. Dr. Evamarie Hey-Hawkins
M.Sc. Chem. Angela Aleksovska, M.Sc. Chem Saral Baweja, Dr. Antonio Buzharevski, M.Sc. Chem. Reike Clauß, M.Sc. Chem. Peter Coburger, M.Sc. Chem. Volker Eilrich, M.Sc. Chem. Marta Gozzi, Dr. Toni Grell, M.Sc Chem. David Langer, M.Sc. Chem. John Popp, M.Sc. Mater. Sci. Eng. Rafaella Lima de Meneses Precker, Dr. Stefan Saretz, M.Sc. Chem. Jan Schulz, M.Sc. Chem. Benedikt Schwarze, M.Sc. Chem. Axel Straube

The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carborane clusters and antitumour drugs).

Smart Catalysts

Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups (ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the



⇑ Fig. 1: Supramolecular self-assembly of heterobimetallic complexes: a new N,P-based, selective heteroditopic ligand.

pH, etc.) and to develop in this way ”switchable“ phosphines for catalytic applications (J. Popp). A new approach includes C_3-symmetric (A. Straube) and carborane-based (P. Coburger) phosphine ligands.
Furthermore, complexes containing two different catalytic metal centres can offer exciting chemical and physical properties which can be used in catalysis. The key to designing these “heterobimetallic” complexes is the synthesis of a ligand with distinct coordination sites able to bind suitable metal ions. With such a ligand, and the wide range of metal ions available, the construction of different heterobimetallic complexes is limited only by one’s imagination (D. Langer, R. Clauß (Fig. 1), S. Baweja).

⇐ Fig. 2. Exploiting the ring strain of diphosphetanes.

From Molecules to Novel Materials

Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of *functionalised building blocks* for organometallic or phosphorus-based polymers are: strained phosphorus-based rings (T. Grell, P. Coburger (Fig. 2), V. Eilrich) or (planar-chiral) ferrocene derivatives (A. Straube) and bis-, tri- and tetrakis-carboxylates of conjugated aromatic systems as ligands in optically active coordination polymers or MOFs (A. Aleksovska).
Molecular precursors: Binary metal phosphides MP_x often exhibit interesting optical, electronic and magnetic properties and thus have a wide range of applications, such as corrosion resistors, catalysts, semiconductors, electrode materials in lithium-ion batteries, etc. We have developed an approach to this class of compounds starting with volatile phosphorus-rich metal complexes (T. Grell, V. Eilrich) as molecular precursors.

Inorganic Building Blocks in Medicinal Chemistry

Carboranes are highly hydrophobic and extremely stable icosahedral carbon-containing boron clusters. The cage framework of these clusters can easily be modified with a variety of substituents, both at the carbon and at the boron atoms and can either be used as pharmacophoric entities in cyclooxygenase (COX) (S. Saretz, A. Buzharevski) or for boron neutron capture therapy (BNCT) as conjugates with tumour-targeting entities, such as a Y_1-receptor-selective neuropeptide Y (NPY) derivative (S. Saretz).
Chemotherapy using platinum-based anti-tumour agents, such as cisplatin, is often associated with strong side effects and is further limited by resistance of tumour cells. Therefore, specific MOFs with large cavities are being studied for targeted drug delivery (R. Precker). Furthermore, to increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. tamoxifen (B. Schwarze)). A new approach utilises the *nido* cluster (carbollide, $[C_2B_9H_{11}]^{2-}$ (which is isolobal to cyclopentadienide) as ligand in metal complexes that exhibit anticancer properties (M. Gozzi, B. Schwarze, Fig. 3).

⇐ Fig. 3. Boron-based compounds potential and emerging applications in medicine.

⇒ *Supramolecular Self-assembly of Heterobimetallic Complexes: A New N,P-Based, Selective Heteroditopic Ligand*
D. J. Hutchinson, R. Clauss, M. Sárosi, E. Hey-Hawkins / Dalton Trans. (2018) **47** 1053-1061

⇒ *Composites Based on Heparin and MIL-101(Fe): The Drug Releasing Depot for Anticoagulant Therapy and Advanced Medical Nanofabrication*
V.V. Vinogradov, A.S. Drozdov, L.R. Mingabudinova, E.M. Shabanova, N.O. Kolchina, E.I. Anastasova, A.A. Markova, A.A. Shtil, V.A. Milichko, G.L. Starova, R.L.M. Precker, A.V. Vinogradov, E. Hey-Hawkins, E.A. Pidko / J. Mater. Chem. B (2018) **6** 2450-2459

⇒ *Versatile Coordination Modes of Triphospha-1,4-pentadiene-2,4-diamine*
A.K. Adhikari, T. Grell, M.B. Sárosi, P. Lönnecke, E. Hey-Hawkins / Inorg. Chem. (2018) **57** 3297-3304

⇒ *12-Vertex Zwitterionic Bis-phosphonium-nido-carborates via Ring-opening Reaction of 1,2-Diphosphetanes*
J. Schulz, A. Kreienbrink, P. Coburger, B. Schwarze, T. Grell, P. Lönnecke, E. Hey-Hawkins / Chem. Eur. J. (2018) **24** 6208-6216

⇒ *Half- and Mixed-sandwich Metallacarboranes in Catalysis*
M. Gozzi, B. Schwarze, E. Hey-Hawkins / invited contribution, in: Boron Chemistry in Organometallics, Catalysis, Materials and Medicine, eds. N. S. Hosmane and R. Eagling, ISBN ISBN: 978-1-78634-441-0, Imperial College Press/World Scientific Publishing (UK) Ltd., Ch. 2, Vol. 2, pp. 27-80 (2018)

⇒ *Half- and Mixed-sandwich Transition Metal Dicarbollides and nido-Carboranes(–1) for Medicinal Applications*
B. Schwarze, M. Gozzi, E. Hey-Hawkins / invited contribution, in: Boron-Based Compounds: Potential and Emerging Applications in Medicine, chapter 1.4, ed. E. Hey-Hawkins and C. Viñas Teixidor, ISBN 9781119275558, Wiley, pp. 60-108, 2018

⇒ *A Stable meta-Carborane Enables the Generation of Boron-rich Peptide Agonists Targeting the Ghrelin Receptor*
D.J. Worm, S. Els-Heindl, M. Kellert, R. Kuhnert, S. Saretz, J. Koebberling, B. Riedl, E. Hey-Hawkins, A. G. Beck-Sickinger / J. Pep. Sci. (2018) **24** e3119

⇒ *Exploiting the Ring Strain of Diphosphetanes: A Synthetic and Computational Approach towards 1,2,5-Selenadiphospholanes*
P. Coburger, R. Aures, P. Schulz, E. Hey-Hawkins / ChemPlusChem (2018) **83** 1057-1064

⇒ *Selective Formation of a Two-dimensional Coordination Polymer Based on a Tridentate Phospholane Ligand and Gold(I)*
R. Hoy, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2018) **47** 14515-14520

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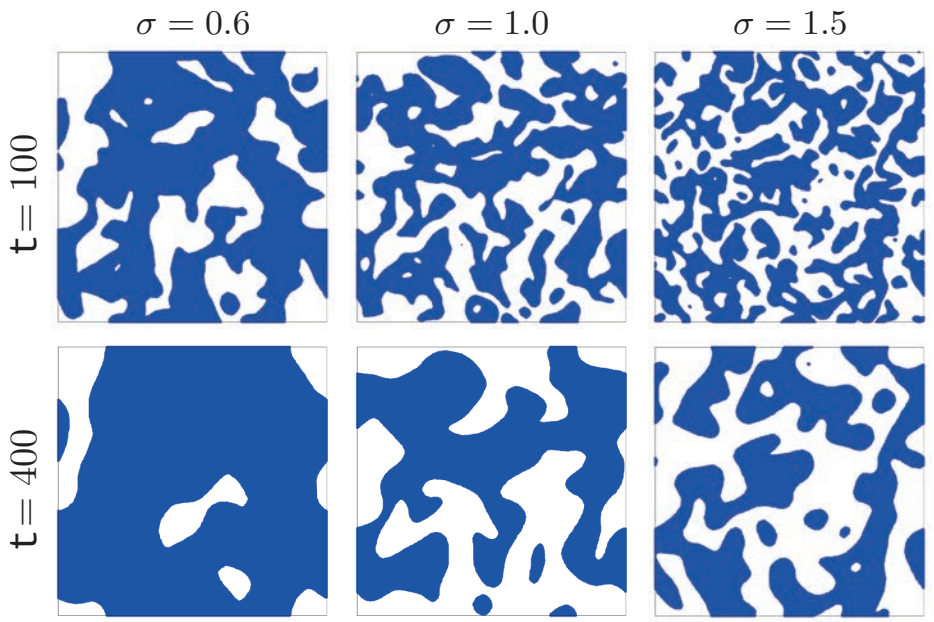
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
M.Sc. Henrik Christiansen

The BuildMoNa related research activities of the computationally oriented theoretical physics group (CQT) focus on several interrelated projects. In most of them, the employed methodology relies mainly on sophisticated Monte Carlo (MC) computer simulations based on generalized ensemble methods such as multicanonical and parallel-tempering (sometimes also called replica-exchange) techniques, chain-growth algorithms with population control, (thermostated) molecular dynamics (MD) methods, and exact enumeration techniques. These methods are adapted and tailored by us to the problems at hand and will be constantly further improved in order to cope with the complexity of the considered problems:

(i) Martin Marenz develops with the help of a few of his fellow PhD students a tool box ("framework") for multi-scale MC computer simulations of mesoscopic and atomistic models of polymers in confined geometries such as a spherical cage or in interaction with a solid substrate. By generalizing our previous studies of a generic bead-stick model of flexible polymers to the case of semiflexible polymers governed by bending stiffness, he discovered with a combination of parallel-tempering and multicanonical simulations for the unconstrained bulk system novel thermodynamically stable phases of knotted polymers of different topologies. In further studies he investigates structure formation processes under spherical confinement and the adsorption propensity to solid substrates.

(ii) Johannes Bock focuses on the intriguing properties of semiflexible polymers and proteins in quenched, disordered environments ("crowded cell problem") and thereby continues the work of a previous BuildMoNa PhD student (Sebastian Schoebl) by extending it from the hitherto considered two-dimensional to the three-dimensional case, subject to additional confinement constraints. One main objective is to investigate by means of a "breadth-first" chain-growth algorithm to what extent the disorder can be effectively described by a "renormalized" bending stiffness of the macromolecules.



⇑ Evolution snapshots at different times *t*, demonstrating the ferromagnetic ordering in the long-range Ising model on a square lattice of size 1024 x 1024 when quenched to a low temperature T = 0.1 T_c for different power-law decay exponents σ. Only the up spins (+) are marked.

(iii) Henrik Christiansen studies coarsening and aging phenomena with MC methods by drawing analogies between different systems. For polymers, using a random-coil conformation as the starting point and then suddenly quenching the temperature below the collapse transition, the temporal evolution and the emerging coarsening of the polymer morphology are recorded. The aging behavior can be investigated by analysing related two-time correlation functions. For an Ising spin model with long-range power-law interactions, he has recently verified for the first time a theoretical conjecture for the growth law of the ordered structures. The main goal of such studies is to elucidate the dynamic scaling laws governing the kinetics of complex physical systems.

⇒ *Efficiencies of Joint Non-Local Update Moves in Monte Carlo Simulations of Coarse-Grained Polymers*
K.S. Austin, M. Marenz, W. Janke / Computer Physics Communication (2018) **224** 222-229

⇒ *Scaling Laws During Collapse of a Homopolymer: Lattice Versus Off-Lattice*
S. Majumder, H. Christiansen, W. Janke / Journal of Physics: Conference Series (2018) **955** 012008-1-6

⇒ *Generalized Ensemble Computer Simulations of Macromolecules*
W. Janke / invited Ising Lecture Notes 2016, in: Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory, Vol. 5, ed. Y. Holovatch (World Scientific, Singapore, 2018), pp. 173-225

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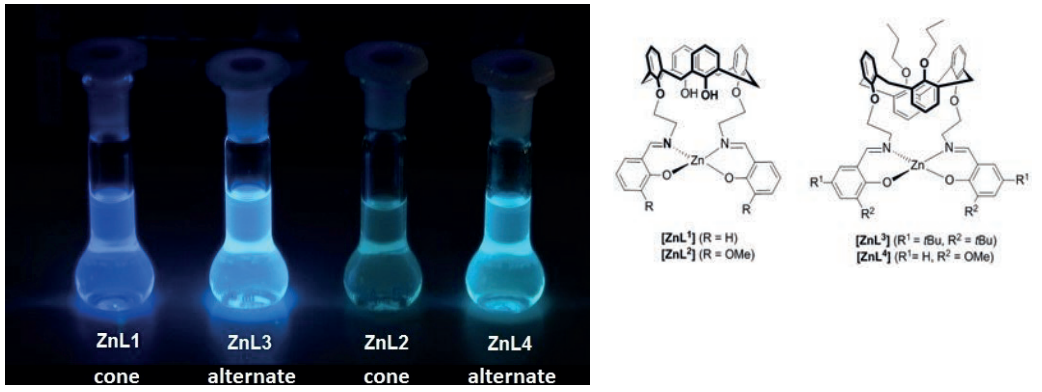
Coordination compounds in supramolecular chemistry and materials chemistry

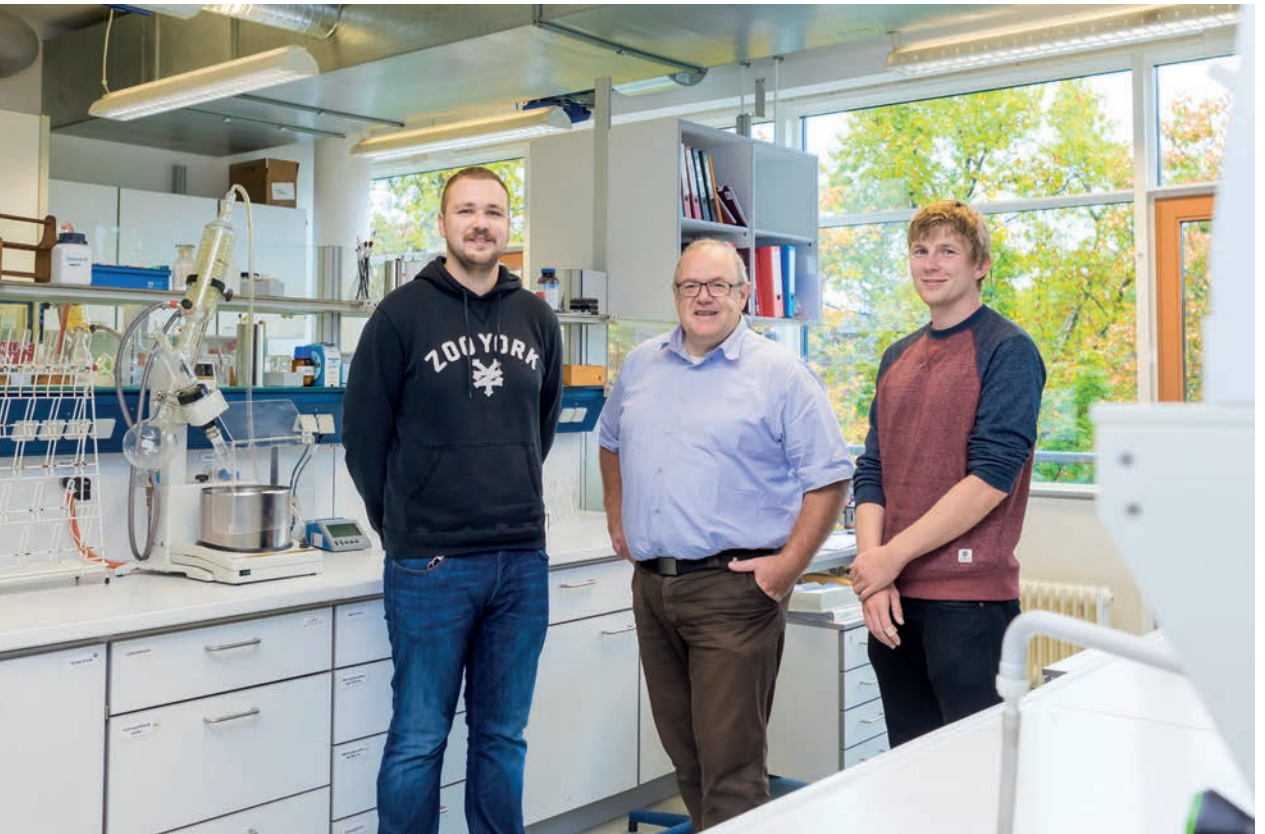
Prof. Dr. Berthold Kersting
M.Sc. Peter Hahn

Our research focuses on the coordination chemistry of macrocyclic ligands based on calixarene and thiophenolate units capable of coordinating to a range of d- and f-block metals. The optical and magnetic properties of the corresponding complexes are studied by luminescence spectroscopy, SQUID magnetometry and X-ray crystallography. These properties can be altered in a targeted fashion by appropriate variation of ligand substituents and metal ions. The compounds are then deposited on surfaces for sensing and signaling applications.

Thus, the synthesis of four new hybrid salicylaldiminato-calix[4]arene ligands and their corresponding zinc(II) complexes have been described recently. The zinc complexes show blue fluorescence, both in solution as well as in the solid state, with λ_{em}, Φ_f, and τ ranging from 472-504 nm, 0.11-0.60, and 2-9 ns, respectively. Complexation reactions were investigated by ESI-MS, IR, NMR, UV-vis absorption and steady-state and time-resolved fluorescence spectroscopy, and X-ray crystallography. The nature of the substituents on the salicylaldiminato fragments was found to be the main parameter that influences the photophysical properties of the zinc complexes. Insights into the electronic nature of the UV-vis transitions were also obtained with time dependent density functional theory (TD-DFT) calculations.

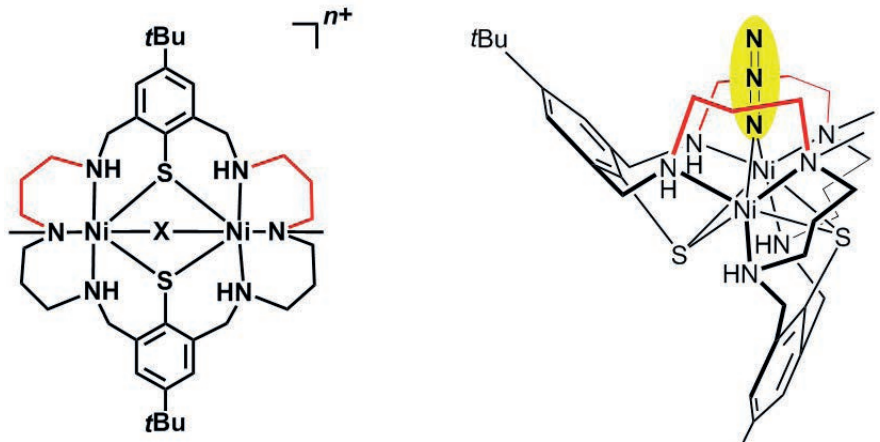


⇑ Variation of fluorescence properties of Zn^{2+} ions supported by a macrocyclic calix[4]arene ligand.



The ability of the dinickel complex $[Ni_2L]^{2+}$ supported by the binucleating hexaazadithiophenolate macrocycle $(L)^{2-}$ to bind linear (OCN^-, SCN^-) and bent triatomic anions (NO_2^-) has been examined (Fig. 2). The complexes $[Ni^{II}_2(L)(\mu_{1,1}\text{-NCO})]BPh_4$ (**3**) and $[Ni^{II}_2(L)(\mu_{1,1}\text{-NCS})]BPh_4$ (**4**) have been synthesized by addition of KOCN or KSCN to $[Ni^{II}_2L](ClO_4)_2$ (**1**) and characterized by IR, ESI-MS, UV-vis, SQUID magnetometry, X-ray crystallography and computational studies. Complex **1** binds cyanate and thiocyanate ions specifically *end-on* via their N atoms yielding face-sharing bis(octahedral) $N_3Ni(\mu\text{-}S_2)(\mu_{1,1}\text{-X})NiN_3$ core structures (X = NCO or NCS), while no reactions occurs with NO_2^-.

The X-ray structure of **3** and accompanying DFT calculations imply that the selective binding of the pseudohalide ions is governed by repulsive host-guest CH···(anion) π interactions. **3** and **4** exhibit an S = 2 ground state that is attained by competing antiferromagnetic and ferromagnetic exchange interactions via the thiolato and cyanato (or thiocyanato) bridges, respectively, with a value for the magnetic exchange coupling constant J of 12.6 and 9.8 cm^{-1} (**H** = $-2JS_1S_2$). The affinity of **1** for cyanate determined by absorption spectrometry in MeCN/MeOH (1/1 v/v) at I = 0.01 M is ca two orders of magnitude higher than for thiocyanate (log K_{11} = 3.92(1) (**3**), 2.16(1) (**4**)). The value for **3** was found to compare favorably well with the equilibrium constant derived by isothermal titration calorimetry.



1 $[Ni_2L][ClO_4]_2$ (no X, n=2)

2 $[Ni_2L(\mu_{1,1}\text{-}N_3)][Y]$ (X = N_3^-, Y = ClO_4^-, BPh_4^-, n=1)

⇑ Complexes **1** and **2** supported by the macrocycle $(L^2)^{2-}$ and side view of the 3D structure of the azido-bridged complex **2**. Complexes **3** and **4** are isostructural with **2**.

⇒ *Photoluminescence Properties of Tetrahedral Zinc(II) Complexes Supported by Calix[4]arene-based Salicylialdiminato Ligands*
S. Ullmann, R. Schnorr, C. Laube, B. Abel, B. Kersting / Dalton Trans. (2018) **47** 5801-5811

⇒ *Selective Coordination of Cyanate and Thiocyanate in the End-On Mode. Synthesis, Structures and Properties of $[Ni_2L(u_{1,1}\text{-}NCO)]^+$ and $[Ni_2L(u_{1,1}\text{-}NCS)]^+$ (L = Macrocyclic Ligand)*
A. Jeremies, S. Gruschinski, S. Schmorl, T. Severin, B. Kersting / New. J. Chem. (2018) **42** 7630-7639

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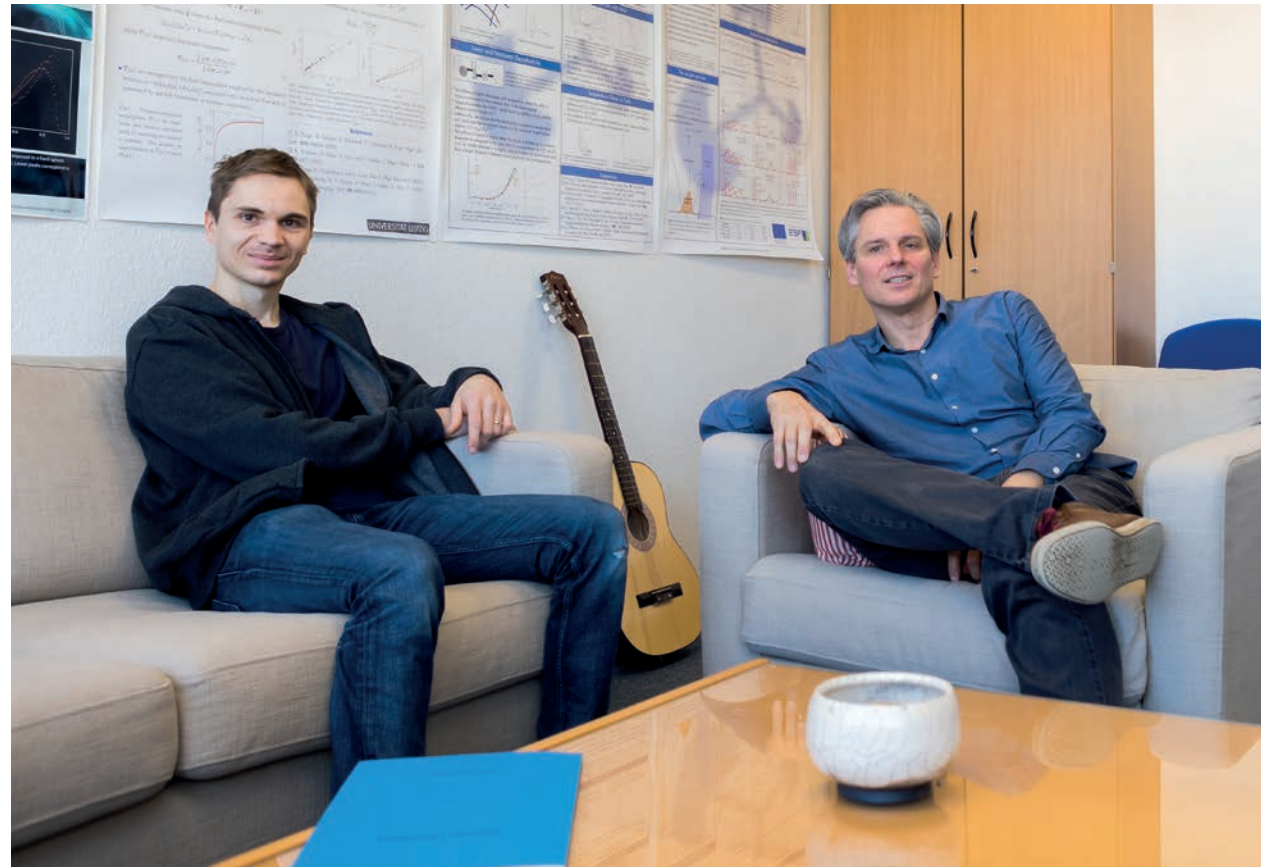
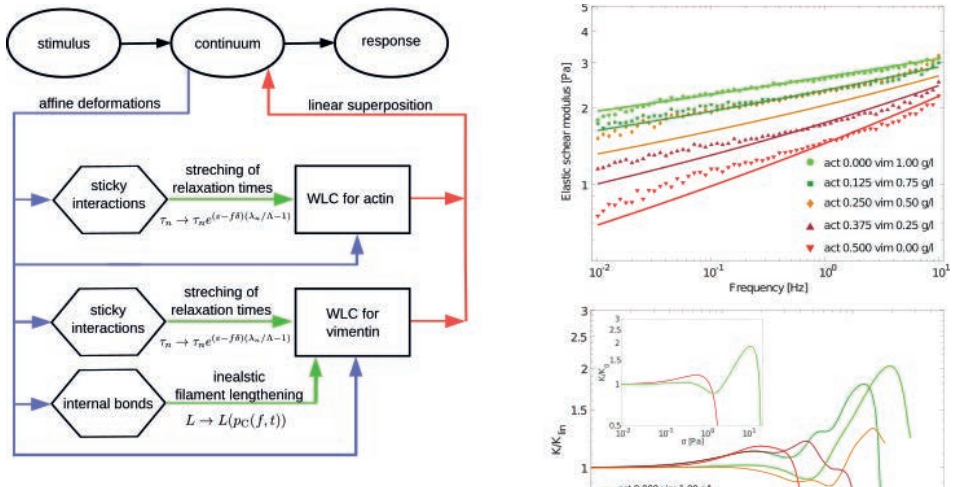
Bottom-up inelastic mechanics of cytoskeletal networks

Prof. Dr. Klaus Kroy
M.Sc. Phys. Constantin Huster

In our modelling approach to the mechanics of cytoskeletal networks we combine two important concepts in bio-mechanics. First, the bottom-up approach to biomechanics that traces back the mechanical response of living matter to its macromolecular constituents. And secondly, the idea that the mechanics of biological systems transcends the viscoelastic dynamics of semiflexible polymers (at least) by one very essential ingredient, namely the slow (un-) binding dynamics of weak reversible crosslinkers. A general framework for inelastic biomechnics is developed which can be used for interpreting existing inelastic models as well as for the construction of new models. Further, the results of experiments using different techniques and probing different systems ranging from single biopolymers, over polymer networks to cells and cellular aggregates can be analyzed and compared.



We thereby aim at a coherent minimalistic description of the universal rheological properties of biomaterials in the liner and non-linear range. In the framework simple models for semiflexible polymers and weak reversible bonds can be combined systematically using interaction rules. A description on the level of the mesoscopic building blocks can then be related to a model on the continuum level employing integration and distribution rules. The developed models are currently used to interpret experimental data measured in various biophysics labs.



⇑ **Left:** Schematic illustration of a model constructed by the inelastic bottom-up framework for cell mechanics to describe the linear and non-linear rheological properties of composite networks of semiflexible polymers, based on the glassy worm-like chain model (GWLC). For the description of actin networks a GWLC is used, while for the vimentin networks the lengthening of single vimentin filaments due the opening of intrafilamental bonds is employed as an additional inelastic mechanism. **Right top:** Power-law rheology in the linear regime. Comparison of data (symbols) and model (solid lines) for the elastic shear modulus G' of networks of different compositions. **Right bottom:** Stiffening and softening in the non-linear regime. The experimental strain dependent differential shear modulus K rescaled by its linear value K_{lin} obtained is shown for networks of different compositions. The inset shows a qualitative description of the phenomenology by the model for actin (red) and vimentin (green) networks. Figure adapted from [1].

⇒ *Glassy dynamics in composite biopolymer networks*
T. Golde, C. Huster, M. Glaser, T. Händler, H. Herrmann, J. A. Käs and J. Schnauß / Soft Matter (2018) **14** 7970-7978

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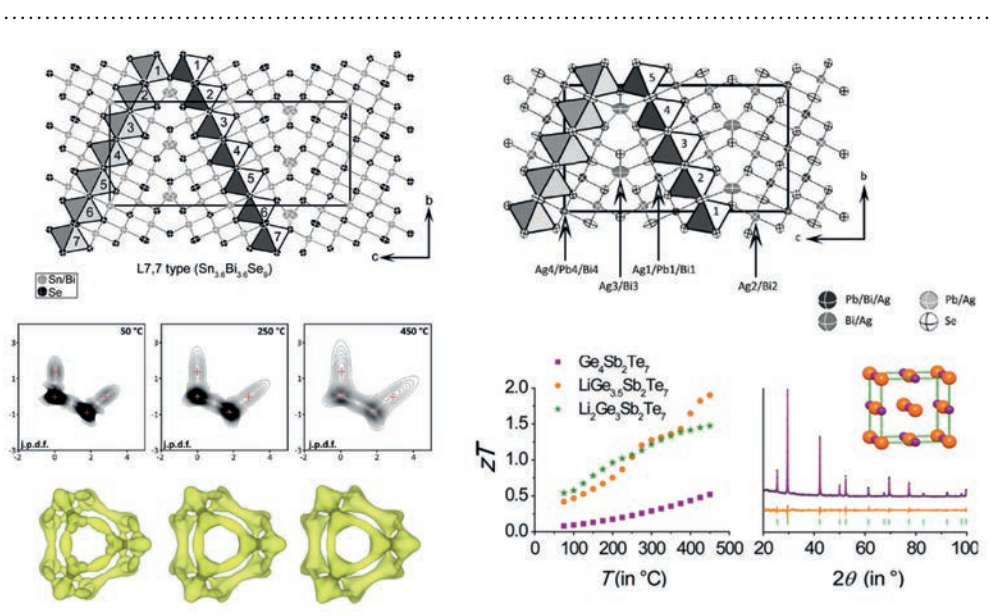
Crystal structures and thermoelectric properties of various multinary chalcogenides

Prof. Dr. Oliver Oeckler
M.Sc. Chem. Christina Fraunhofer

Thermoelectric materials that can directly convert thermal energy into electrical energy are intriguing the growing energy demand of the world, but also very interesting regarding niche applications. Copper-containing chalcogenides have attracted much attention as thermoelectric materials that are much less toxic than classical materials such as PbTe. In addition, they contain only abundant elements. Within BuildMoNa, we have investigated the syntheses, crystal structures and thermoelectric properties of materials with mobile Cu atoms such as substitution variants of $Cu_{5-y}FeS_{4-x}Se_x$ and sulfosalt-like $Cu_{1.7}Bi_{4.7}Se_8$ doped with Mn, Fe or Ag. This is especially interesting in conjunction with the oxidation states of the cations. Mößbauer spectra of

$Cu_{5-y}FeS_{4-x}Se_x$ ($0 \leq y \leq 0.5$ and $0 \leq x \leq 1.6$) reveal Fe^{III} and electron spin resonance spectra of $Cu_{1.5}Mn_{0.4}Bi_{4.5}Se_8$ indicate Mn^{II}. Accurate structure analysis needs to be carried out by resonant X-ray diffraction using synchrotron radiation because of the low scattering contrast between Mn/Fe and Cu. In addition, this technique is useful in the case of mixed site occupancies in combination with cation vacancies as shown in compounds $(SnSe)_xBi_2Se_3$ with $0.8 \leq x \leq 3$. There, lillianite-type structures built up from distorted NaCl-type slabs with significant amounts of cation vacancies are characteristic, but layered structures and disordered rocksalt-type materials could also be characterized.

The mobility of Cu atoms at elevated temperatures has also been observed in related studies focusing at argyrodite-type $Cu_8GeSe_{4.25}Te_{1.75}$, where the dynamical disorder of Cu atoms increases with temperature. The same is true for Ag ions in sulfosalt-like ^{5,5}L-$AgPb_3Bi_7Se_{14}$ or for Li ions in $LiGe_{3.5}Sb_2Te_7$. In the latter case, the mobility results in enhanced thermoelectric properties with thermoelectric figures of merig ZT_{max} up to 1.9 at 450 °C compared to unsubstituted Ge4Sb2Te7 with $ZT_{max} = 0.5$ at 450 °C.



⇑ Projections of the crystal structures of ^{7,7}L-$Sn_{3.6}Bi_{3.6}Se_9$ along [100] (top left) and of ^{5,5}L-$AgPb_3Bi_7Se_{14}$ along [100] (top right); joint probability density function maps and isosurfaces for Cu atoms of the first coordination sphere around Te in argyrodite-type $Cu_8GeSe_{4.25}Te_{1.75}$ at 50 °C, 250 °C and 450 °C (bottom left), and thermoelectric properties and structure refinenent (Rietveld methode) of Li-substituted germanium antimony tellurides (bottom right).

⇒ *Cornucopia of structures in the pseudobinary system $(SnSe)_xBi_2Se_3$: A crystal-chemical copycat*
F. Heinke, P. Urban, A. Werwein, C. Fraunhofer, T. Rosenthal, S. Schwarzmüller, D. Souchay, F. Fahrnbauer, V. Dyadkin, G. Wagner, O. Oeckler / Inorg. Chem. (2018) **57** 4427

⇒ *IArgyrodite-type $Cu_8GeSe_{6-x}Tex$ ($0 \leq x \leq 2$): Temperature-dependent crystal structure and thermoelectric properties*
S. Schwarzmüller, D. Souchay, D. Günther, A. Gocke, I. Dovgaliuk, S. A. Miller, G. J. Snyder, O. Oeckler / Z. Anorg. Allg. Chem. (2018) **644** 1915

⇒ *Structure and thermoelectric properties of the silver lead bismuth selenides $Ag_5Pb_9Bi_{19}Se_{40}$ and $AgPb_3Bi_7Se_{14}$*
F. Heinke, F. Nietschke, C. Fraunhofer, I. Dovgaliuk, J. Schiller, O. Oeckler / Dalton Trans. (2018) **47** 12431

⇒ *Tuning the vacancy concentration in lithium germanium antimony tellurides — Influence on phase transitions, lithium mobility, and thermoelectric properties*
S. Schwarzmüller, M. Jakob, M. Nentwig, T. Schröder, A. Kuhn, A. Düvel, P. Heitjans, O. Oeckler / Chem. Mater. (2018) **30** 7970

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Microwave detection with NV centres

Prof. Dr. Jan Meijer
M.Sc. Phys. Sascha Becker, Dipl.-Math. Roger John, M.Sc. Phys. Paul Räcke, M.Sc. Phys. Clemens Scheuner

The aim of the joint EU project "Microsens" is to develop and optimize broadband microwave detectors based on quantum devices (Fig. 1). Broadband microwave detectors in one frequency range are used in many areas of technology: from distance sensors in the automotive industry to complex radar technologies. The quantum sensors projected here have three major advantages over conventional detectors:

- they are self-calibrating, since the sensor only uses fundamental natural constants and color centers, similar to atoms, which always have the same properties.
- quantum sensors have an extremely high sensitivity up to single photons.
- it is possible to detect and monitor a large frequency space simultaneously.

In this project, broadband and highly sensitive microwave detectors are produced using NV centers in diamond. Our task is to process the materials in such a way that NV centers are optimally placed and generated. Furthermore, the microwaves should be coupled effectively to the NV centers. The various implantation facilities in Leipzig are used for this purpose. In the context of this project, this procedure was optimized, so it is now possible to structure the samples by means of a shadow mask without lithography steps. This makes it possible to implant different ion types or energies in a short time. It was shown that phosphorus implantation can be used to optimize both NV generation and charge stability. Furthermore, it was discovered that the coupling to the NV centers can be achieved by means of ITO on diamond, since the near field of the microwave is coupled to the NV center. The results are arranged according to the work packages.

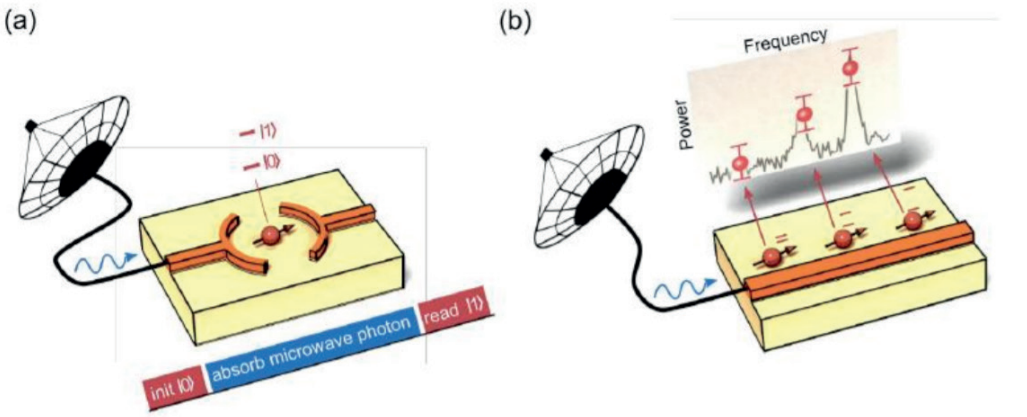

Fig. 1. Expected objectives of the project: a) A highly sensitive microwave detector based on a photon resonator, b) A spectrometer based on a divergent magnetic field. In both cases the detection of the microwaves is performed by implanted NV centers in diamond.

The NV centers act quasi as lasers and amplify the signal; if a transition from m=0 to m=1 is achieved by the tuned microwave frequency at a position in the field gradient, the amplification can no longer take place. The aim is to achieve a high contrast. The creation of a cavity by means of thin diamond layers was achieved by high-dose hydrogen implantation. The graphite layers can then be removed in an oxygen atmosphere at approx. 550° C. However, the removal of the diamond layer proved to be a challenge. Normal etching processes employing acids or plasma were unsuccessful. The BuildMoNa student Clemens Scheuner developed a technique to burn the graphite layer and indeed this method provided a useful result (Fig. 2). Surprisingly, the layer roughness remained within a few nm. This is of great importance for the use as an optical resonator. The next step is to apply a metal mirror and a Bragg mirror to this

diamond layer to create a cavity. The NV centers in the layer also need to be characterized. First investigations unfortunately showed that the NV density was reduced. We suspect that this effect is due to hydrogen implantation. Hydrogen is mobile in diamond and forms NVH. In order to solve this problem, in the next experiments the generation of diamond layers by means of He or oxygen implantations will be carried out. Corresponding experiments are in preparation.

The BuildMoNa student Roger John investigates methods to implant nitrogen ions with subsequent annealing, which could allow precise placement of NV centres. A major problem with this method is the ratio of NV centres per implanted nitrogen ions, also known as creation yield. Especially shallow NV centres which are most useful for surface sensing suffer from a very low creation yield below 1 %. To investigate further on this, a diamond that was subjected to nitrogen molecule implantation with very low energies (1 keV – 2.5 keV) and subsequent overgrow has been measured using optical detected magnetic resonance (ODMR). As the implanted nitrogen molecules should experience straggling below 2 nm, negatively charged NVs created by them should show an observable spin-spin coupling to either a second NV, a substitutional nitrogen (P1), or a negatively charged nitrogen vacancy hydrogen complex (NVH-). First results using double electron electron resonance (DEER) and other pulsed techniques lack evidence of these partners in their listed charge states, which might be explained by the band structure of diamond (Fig. 3).

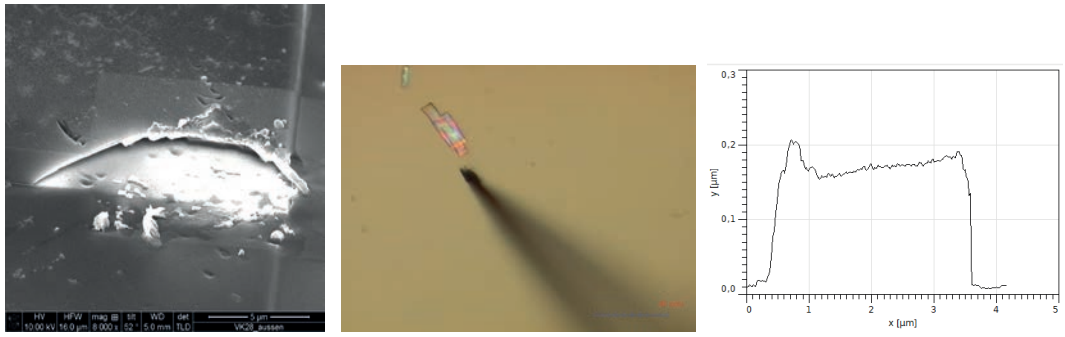

Fig. 2. (a) SEM side view of a diamond membrane created by 30 keV H implantation, (b) diamond layers with a thickness of 180nm. (c) AFM image of the diamond layer. The roughness is below 3 nm (C. Scheuner et al. pub. in preparation).

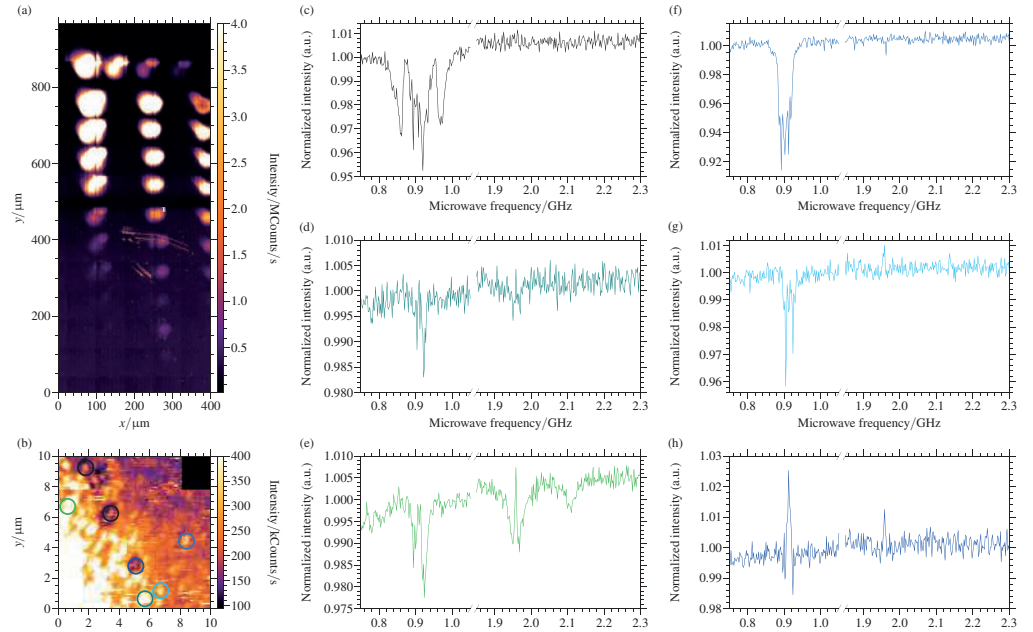

Fig 3. (a) Overview of the implanted area with 5 keV 15N, 5 keV $^{15}N^{+2}$ and 3 keV ^{15}N from left to right with doses decreasing in half decades starting with 1013/cm² from the second row at the top. The marked area is shown in (b) where the circled NVs are connected by colour to their displayed measurements. (c) DEER measurement of the dashed representative showing a similiar splitting to the one in sample 2 (e); both candidates show ^{13}C splitting (single and twofold) in their pulsed spectrum. (d) and (e) show a twofold splitted main resonance together with a feature attributed to spin-1/2. In (e) this feature is clearly split (maybe NVH−?) and accompanied by another peak that does not match any previously described candidates. The centres shown in (f) - (h) also unambiguously show a coupling to a spin-1/2 defect, but as it is not split the most obvious explanation considering the sample to be hpht is V−, although the main splitting differs for all.

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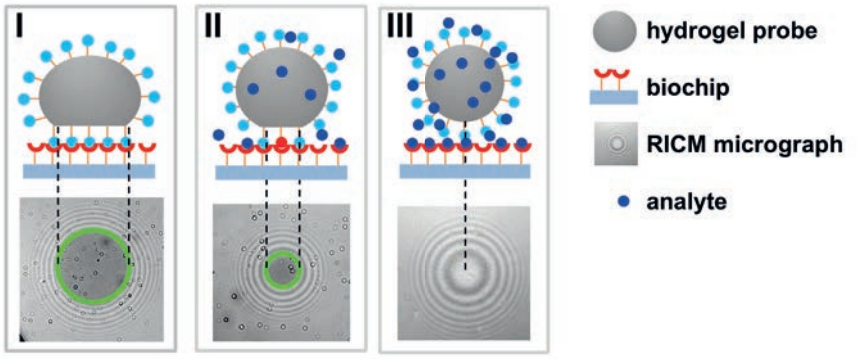
Soft colloidal probes as biomimetic sensors of low molecular weight analytes in aqueous solutions

Prof. Dr. Tilo Pompe
M.Sc. David Rettke

In one research area our group uses synthetic and naturally derived polymer matrices to analyze and control cell fate decisions in dependence on microenvironmental cues. A second research topic deals with the application of bio-/polymer materials to develop biosensors for the detection of anthropogenic analytes in aqueous environments based on functionalized hydrogel microparticles and nanoparticles.

D. Rettke specifically investigates biosensors to detect low molecular weight analytes in aqueous environments i.e. anthropogenic molecules like pesticides, antibiotics and hormones. The biomimetic sensing system utilizes the elastic deformation of hydrogel microparticles (soft colloidal probe - SCP) as a result of the interfacial interaction with an underlying chip surface. The associated contact area of SCP and chip surface can be directly related to the adhesion energy, which is read out using optical microscopy based on reflection interference contrast patterns or other techniques. By functionalization of SCP with biospecific ligands they are capable of interacting with capture binding sites presented on a chip surface. This binding is controlled in a concentration dependent manner by the analytes present in the aqueous solution, which specifically block free capture molecules at the chip surface. Using this biosensing principle highly specific, quantitative read outs in a pM range can be developed. One new technological option to detect the controversially discussed herbicide glyphosate was already applied for patent. Other detection options are currently developed to establish a platform technology.



⇑ Schematic illustration of the assay principle. (I) A functionalized hydrogel microparticle probe adheres strongly to the presented chip-surface in the absence of analytes (e.g. glyphosate), thereby forming a characteristic contact profile at the interface, visualized by reflection interference contrast microscopy (RICM). (II, III) Analytes within sample solutions in turn specifically modulate the strength of probe-biochip interaction. The sensitive response of the sensor, i.e. the reduced contact area between probe and chip, enables precise quantification of the corresponding small molecule analyte.

⇒ *Verfahren zur Detektion von Analyten auf Basis immobilisierter Proteine*
T. Pompe, D. Rettke, S. Martin, K. Ostermann, J. Döring, C. Dahmann, G. Rödel / Inorg. Chem. (2018) **57** 4427 / Patent

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Non-Hermitian topological phases: Bulk-boundary correspondence via Greens functions

Prof. Dr. Bernd Rosenow
Dipl.-Math. Heinrich-Gregor Zirnstein

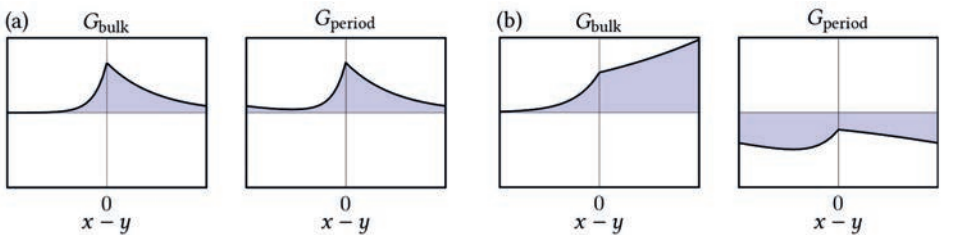
Research in the group focuses on mesoscopic systems. These physical systems are so small that the quantum nature of individual particles in the system becomes relevant, but still large enough such that statistical averaging is possible. One exciting example where both the quantum nature and the collective motion of particles play a fundamental role are the so-called topological quantum phases. These are novel phases of matter which seem ordinary when looking only at a small part of the system (locally), but which, due to quantum effects, are decidedly non-trivial when looking at the system as a whole (globally).

Topological insulators are an example of a topological quantum phase. There, the non-triviality manifests in the following way: A sample of such a material is insulating in the bulk, but due to quantum effects, perfectly conducting surface states emerge at the sample boundary. Moreover, these surface states are robust against small perturbations like disorder. This phenomenon is called the bulk-boundary correspondence. Concrete examples of such systems are two-dimensional electron gases in a magnetic field and HgTe quantum wells.

In recent years, it has been realized that the concept of topological phases can be extended to classical systems, because its main ingredient, the wave-like nature of quantum particles, can be found in any system that supports waves. For example, light in a photonic crystal or microcavity may form a non-trivial topological phase. Again, the main prediction is that such wave systems exhibit robust surface states. For light, this would imply the existence of robust guided modes at the boundary of the medium.

However, the main difference between electrons in a crystal and light in a medium is that the former is a closed (“Hermitian”) system, since electrons rarely escape, while the latter is an open (“non-Hermitian”) system, because radiation loss is common. Moreover, light can even be amplified coherently by lasing (gain). The possibility of gain and loss gives rise to additional topological phases for light that have no counterpart for electrons. Surprisingly, however, the extent of the bulk-boundary correspondence has come into question.

In this project, we have clarified the bulk-boundary correspondence for non-Hermitian systems in one dimension, where the non-Hermitian winding number identifies topological phases that are unique to open systems. We have focused on response (Greens) functions, which describe experimental observables, and found that the bulk-boundary correspondence breaks down once this non-Hermitian winding number takes a non-trivial value: When the winding number changes from zero, the bulk response starts exhibiting exponential growth in space. Since topological bulk quantities are calculated for periodic boundary conditions, and since periodic systems cannot accommodate this spatial growth, they do not reflect the properties of systems with open boundaries.



⇑ Breakdown of the bulk-boundary correspondence. (a) If the bulk Green function decays spatially, then both bulk and periodic Green function agree. (b) If the bulk Green function grows spatially, then the periodic Green function has to change drastically in order to accommodate periodic boundary conditions.

To establish these results, we have put forward a decomposition of the response (Greens) function for an open system into a bulk part, which describes the response deep in the bulk, and a boundary part, which describes modifications due to the boundary. Then, we obtain boundary eigenstates from the pole expansion of the boundary Greens function, thus avoiding pitfalls, like the so-called non-Hermitian skin effect, that arise when trying to distinguish bulk and boundary states by their spatial shape. For a continuum model of Dirac fermions, an analytical solution shows that the presence or absence of boundary eigenstates has little relation to topological quantities computed for periodic boundary conditions. Also, we observe that the bulk response grows in space when the non-Hermitian winding number is nonzero for this model. The latter number counts how often the complex number $\det(H(k))$, the determinant of the Bloch Hamiltonian $H(k)$, winds around the origin of the complex plane as the Bloch momentum k traverses the Brillouin zone. Now, the bulk response can be expressed as a sum of exponentials $\exp(ik_S x)$ where the complex momentum k_S is a zero of the determinant, and we can argue for very general systems that the winding number changes precisely when one of the zeros crosses the real axis, which means that the exponential changes from spatial decay to spatial growth. We were able to extend this argument into a full mathematical justification for generic lattice systems.

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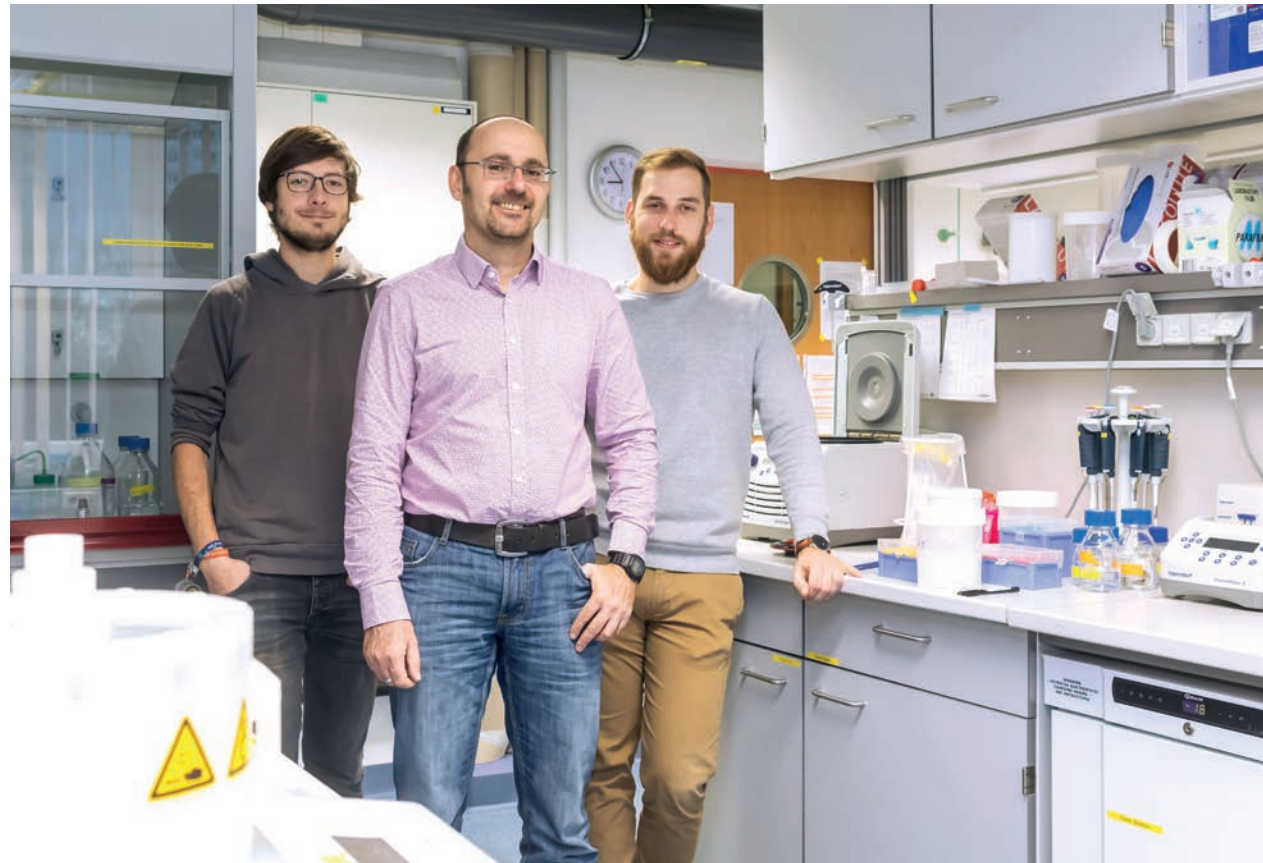
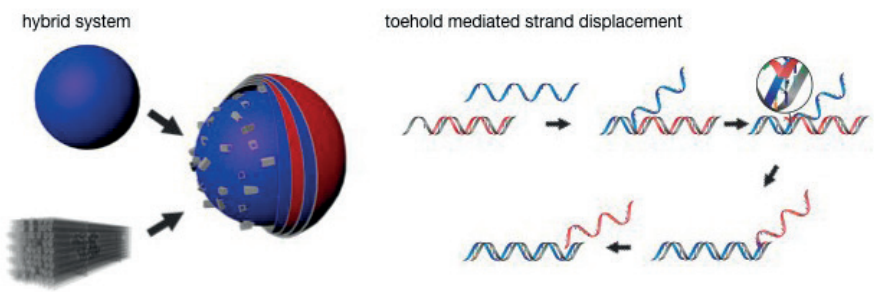
A DNA origami and LbL hybrid carrier for drug delivery

Prof. Dr. Ralf Seidel, PD Dr. Uta Reibetanz
M.Sc. Phys. Florian Scheffler, M.Sc. Phys. Patrick Irmisch

The programmability and responsitivity to external stimuli makes complex three-dimensional DNA nanostructure highly promising candidates for advanced drug delivery sytsems. However, these structures are naturally unstable under physiological and intracellular conditions. Our research focuses on integrating DNA nano cages into the polymeric multilayer of Layer-by-Layer (LbL) micro carriers to achieve a protection against harsh pH conditions and enzymatic degradation throughout the intracellular delivery pathway. We could shown that the integration into the super-ordinated LbL system increases the stability of the DNA nano cages drastically and does not disturb the functionalization capacity of the LbL surface, e.g. by a supported lipid bilayer. Further, we demonstrated an improved intracellular processing of the DNA origami on the carriers compared to unprotected DNA cages. [1]



Next steps towards a smart drug delivery system will include the release of an incorporated model drug (BSA). For this purpose, the initially open DNA structures are closed by addition of DNA lids resulting in a sealed transporter. Aiming for the cytosol, the opening mechanism of the resulting origami trimers is given by toehold mediated DNA strand displacement. During this process an invader strand replaces another strand of a duplex DNA via branch migration after initial binding to a short single stranded overhang on the complementary strand. The required invader strand will be transported within the multishell of the LbL microcarrier and should be released after step-wise degradation of the polymeric multishell. First experiments showed a tuneable reaction time of the replacement reaction and a potential migration of the invader strand through the walls of the DNA trimer and subsequent replacement of the incorporated cargo which is bound by the toehold duplex.
Overall our investigations provide versatile and programmable drug delivery systems that promise enhanced transport of sensitive cargo into the cytosol of different cell lines.



⇑ Hybrid carrier system design and toehold mediated strand displacement. Left: BSA-loaded DNA Origami trimers are integrated as a negative layer in a polyelectrolyte multishell on 2.76 µm SiO_2 particles. Application of additional four polyelectrolyte layers leads to a protection of against environmental factors. Right: The invader strand (blue) is added to a formed duplex of incumbent (red) and the target (black) holding a single stranded „toehold" overhang. Via branch migration the invader replaces the incumbent after initial binding to the toehold region until the incumbent dissociates from the three-strand intermediate.

⇒ [1] *A Hybrid Carrier System Based on Origami Nanostrucutures and Layer-by-Layer Microparticles* F. Scheffler, M. Brueckner, J. Ye, R. Seidel, U. Reibetanz / Ade. Funct. Mater. (2019) **29**(8) 1808116

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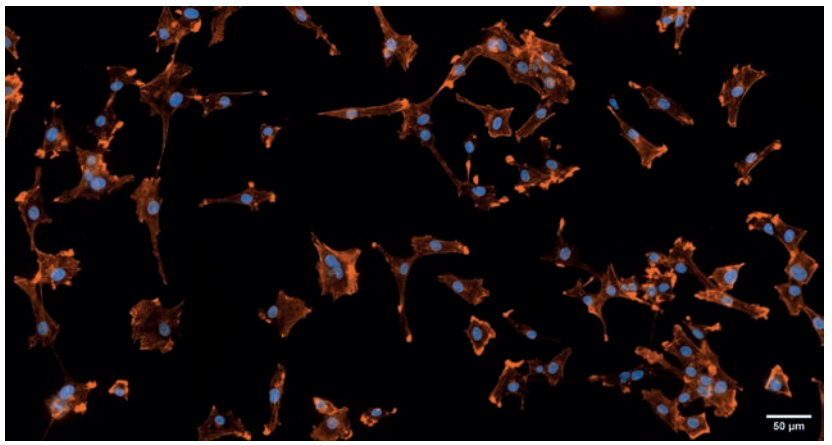
Cellular adhesion, proliferation and migration on artificial biomaterials

Prof. Dr. Mareike Zink
M.Sc. Chem. Nils Wilharm

Cellular adhesion, proliferation and migration on artificial biomaterials – ranging from 2D substrates to 3D matrices – are the aim of your investigations. In collaboration with Prof. Andrea Robitzki, one PhD project focuses on the interaction of human neuronal cells with gold and indium tin oxide substrates, as well as nanostructured titanium nitride surfaces for multielectrode array applications. We study the neuronal cells' adhesion dynamics with an atomic force microscope as well as network formation in order to employ how different surfaces influence neuronal and glial cell behavior important e.g. for brain implants.
Within a second project collagen-elastin hydrogels as model systems for the extracellular matrix are employed in close collaboration with Prof. Stefan Mayr. Elastin is the second most abundant protein of connective tissue besides collagen and it

mainly influences tissue elasticity e.g. of blood vessels. In our study, the two biopolymers are fused by electron irradiation which is also used to control and tune the hydrogel stiffness – important for many biomedical applications. By varying the elastin content and the irradiation dose, the crosslinks and therefore the material properties can easily be adapted to in vivo conditions to mimic mammalian tissues.mainly influences tissue elasticity e.g. of blood vessels. In our study, the two biopolymers are fused by electron irradiation which is also used to control and tune the hydrogel stiffness – important for many biomedical applications. By varying the elastin content and the irradiation dose, the crosslinks and therefore the material properties can easily be adapted to in vivo conditions to mimic mammalian tissues.



⇑ Fluorescent image of glial U87-MG cells on an indium tin oxide (ITO) substrate (orange: actin cytoskeleton, blue: cell nuclei).

⇒ *Early Adhesion of Cells to Ferromagnetic Shape Memory Alloys Functionalized with Plasma Assembled Biomolecules - A Single Cell Force Spectroscopy Study*
M. V. Cakir, U. Allenstein, M. Zink, S. G. Mayr / Materials & Design (2018) **158** 19

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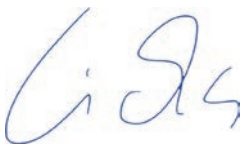
Experiences

BuildMoNa's eleventh year – a principal investigator's view

Prof. Dr. Frank Cichos

What makes a graduate school like BuildMoNa a graduate school? What is a graduate school teaching doctoral candidates? Why go to a school again after you have passed so many exams in school and during your studies?
That might be the questions students and doctoral candidates would ask you if they have never heard of graduate schools before. But that are also the questions I ask myself repeatedly to find the motivation for my doctoral candidates and me.
When I joined BuildMoNa, the graduate school was funded by the DFG, well equipped with grants for doctoral candidates, money for consumables and travelling, symposia and other teaching activities. Together with other technical benefits and the stamp of excellence, BuildMoNa has attracted more than 100 doctoral candidates and their principle investigators to form a strong interdisciplinary community. It has given doctoral candidates and PIs the occasion to meet, to exchange and to work together and not only during the Annual BuildMoNa Conference. Already at that time, it was anticipated that the funding will change at some point in the future. Such a change in funding naturally goes along with a change in the benefits PIs and doctoral candidates draw from the graduate school and thus puts the formed community to the test.
If I look back at the last year or even the years before, I feel as if we are still in that testing phase. The outcome of the target agreement (Zielvereinbarung) with the university administration has set a new frame for BuildMoNa and has changed the weights of importance for its benefits to all of us. What resides, however, is the understanding that communities enable. Being a nerdy scientist, that reminds me of nucleation, where you first have to invest energy to take benefit from a new collective state. Most of us have experienced this new collective state, with excellent talks of doctoral candidates and full lecture halls during the ABC, excellent speakers and a large variety of topics covered. As a result, we were able to award a graduation certificate to doctoral candidates, which have a wider view on the topics in natural sciences, a broader skill set for their future professional career and the ability to communicate those critically to an audience. For me personally, this is what a graduate school like BuildMoNa is made for – to make doctoral candidates better in a community than they already are as an individual.
Of course, that needs still the continuous investment to cross that barrier and that investment has to come from the PIs, the doctoral candidates and finally also from the university as there is no continuous success without investment.



Prof. Dr. Frank Cichos

BuildMoNa's eleventh year – a doctoral candidate's view

M.Sc. Phys. Astrid Weidt

After the sometimes relaxing, sometimes challenging Master Studies, the PhD life seems to be a more complex situation. You are not only responsible for managing your own project, you might also supervise Bachelor or Master students, you have to be creative and do innovative work. Simultaneously, your social or environmental commitment might demand higher personal resources, while your time is limited.
Fortunately, structured doctoral programs as BuildMoNa aim to provide help. Courses, conferences and discussions with principal investigators facilitate the entry into the scientific community. As BuildMoNa is an optimal synergy of the research disciplines biochemisty, biology, chemistry and physics, doctoral candidates gain new perspectives and approaches from their interdisciplinary and international colleagues. This stimulates scientific discussions and broadens the own field of knowledge. At the same instant, valuable contacts are formed that might end up in scientific collaborations.

The scientific courses offered by BuildMoNa aim to provide insights into the basic concepts of biochemisty, biology, chemistry and physics. Furthermore, distinct symposia and conferences round off the BuildMoNa portfolio. More general courses, like „good scientific practice“ or „grant writing“ offered by the Research Academy Leipzig (RAL) complete the extensive program. By granting travel allowances, doctoral candidates are encouraged to give a talk or present a poster at international conferences or summer schools. Additionally, the BuildMoNa principal investigators, the BuildMoNa office and the doctoral candidates representatives always help with problems. In this way, an excellent and integrated personal scientific development of all PhD students is ensured. Finally, the BuildMoNa certificate summarizes these educational efforts, as scientific courses, soft skills, the participation in international conferences and the overall interdisciplinary approach.
In retrospective, 2018 was the year of reorganization. Within BuildMoNa, nearly all positions changed: the speaker and vice-speaker, scientific manager, secretary and also the doctoral candidates representatives. Furthermore, the famous „Zielvereinbarung“ (agreement of objectives) between the rectorate of University Leipzig and BuildMoNa was debated. This rather unstable situation sometimes shifted the focus of BuildMoNa to the organizational architecture. Thus, only four scientific modules were offered. Hopefully, this represents only a local minimum of BuildMoNa's eigenfunction.
The upcoming „Zielvereinbarung“ between the rectorate of University Leipzig and BuildMoNa will surely provide a safe long-term financing of the graduate school. This gives new possibilities to shape the graduate school and to create new formats for the doctoral candidates.
In this manner, we all hope to see BuildMoNa growing and prospering.

M.Sc. Phys. Astrid Weidt

Training

The research training programme consists of the research work and a well-structured training programme in accordance with the guidelines of the Research Academy Leipzig at Universität Leipzig and the faculties' graduation rules.

The training programme organised by the graduate school has a modular structure (see table), from which doctoral candidates may choose, based on their individual skills and time management, within three years of their graduation studies, provided that 20 credit points (10 graded, 10 non-graded) have been obtained.

In addition to the graduate school's training programme, doctoral candidates can participate in events of the Research Academy and HIGRADE (at the Helmholtz Centre for Environmental Research) including transferable skills and scientific activities.

TRAINING CONCEPT

Training activity	Type	Min. CP	Month (March to February)											
			M	A	M	J	J	A	S	O	N	D	J	F
			summer term							**winter term**				
Research work	R	–												
Scientific and methods modules	R/E	10	M	M	M	M	M			M	M	M	M	M
Workshop for doctoral candidates	R								W					
Scientific symposium	R/E		SY											
Literature seminars	R/E			S		S		S		S		S		S
Guest lectures/colloquia	E	5	L	L	L	L	L	L	L	L	L	L	L	L
Tutoring	R/E			T	T	T	T			T	T	T	T	
Research stays abroad	E		flexible during the whole year (1 week up to a few months)											
Summer/winter schools	E													
Industrial training	E													
Active participation in conferences/workshops	R/E		flexible during the whole year (1 up to a few days)											
Transferable (generic) skills	R/E	5		S	S	S	S			S	S	S	S	
					M		M				M		M	

BuildMoNa training programme: M, W, SY, M: two-day blocks,
S: 1–2 hours, L, T: 2 hours per week
R = required
E = elective
R/E = required-elective

Scientific and methods modules

Basic concepts in molecular spectroscopy (2018-B4)

02 / 03 May 2018,
written exam, 2 credit points, yearly recurrence with modification, 15 participants

This module for physicists, chemists and biochemists introduced the basic concepts in molecular spectroscopy, i.e. Infrared (IR), (surface enhanced) Raman- with imaging options and Broadband Dielectric Spectroscopy (BDS), Nuclear Magnetic Resonance Spectroscopy, Optical Microscopy, Superresolution Microscopy, Single Molecule Fluorescence Detection.

Responsible Scientists:
Prof. Dr. K. Asmis, Prof. Dr. F. Cichos, Prof. Dr. D. Huster, Prof. Dr. F. Kremer

Contents:
⇒ The quantum mechanical foundation of Infrared Spectroscopy
⇒ Experimental principles of Fourier Transform Infrared Spectroscopy
⇒ The principle of Broadband Dielectric Spectroscopy
⇒ Modern applications of Broadband Dielectric Spectroscopy
⇒ Discussion of the chemical shift Hamiltonian with isotropic and anisotropic parts in NMR spectroscopy
⇒ The influence of sample orientation and molecular dynamics on the NMR signals
⇒ Magic angle spinning
⇒ Requirements for single molecule fluorescence detection at low and room temperature
⇒ Optical microscopy
⇒ Schemes as well as microscopic detection beyond the diffraction limit

Smart Molecules – Supramolecular anions chemistry (2018-T1)

20 - 21 September 2018,
writen exam, 2 credit points, bi-yearly recurrence with modification, 14 participants

This module provided an overview of recent developments in the field of anion recognition and links it to topics in supramolecular chemistry, biomedical applications and nanochemistry. The doctoral researchers will gain insight into specific syntheses and modifications of anion receptors, their specific functions and their integration into functional materials with optimized catalytic activity and adjustable physical, magnetic, electronic, biological and optical properties.

Responsible Scientists:
Prof. Dr. B. Kersting, Prof. Dr. H. Krautscheid

Lecturers:
⇒ Markus Albrecht (RWTH Aachen, Aachen, Germany)
⇒ Anthony P. Davis (University of Bristol, Bristol, UK)
⇒ Enrique García-España (Universidad de Valencia, Valencia, Spain)
⇒ Evgeny Kataev (TU Chemnitz, Chemnitz, Germany)
⇒ Harald Krautscheid (University of leipzig, Germany)
⇒ Stefan Kubik (TU Kaiserslautern, Germany)
⇒ Carmelo Sgarlata(University of Catania, Italy)

Contents:
Anion recognition chemistry has grown from its beginnings in the late 1960s and a variety of charged and neutral, cyclic and acyclic, inorganic and organic supramolecular host systems for the selective complexation, detection, and separation of anionic guest specieshave been developed. Recent developments include exciting advances in anion-templated syntheses, directed self-assembly, ion-pair recognition, the function of anions in supramolecular catalysis, anion recognition in aqueous systems, fluorescence sensing of anion, recognition of anions in metal-organic frameworks. The two-day module provided an introduction into the field and looked at recent developments, covering anion recognition based on biomolecules, polymers, and nanoparticles.

Methods:
⇒ Synthesis of macrocyclic receptors
⇒ Anion as templates in synthesis
⇒ Macrocyclic chemistry
⇒ Molecular spectroscopy (fluorescence spectroscopy, IR, NMR, UV-Vis,etc.)
⇒ Solution thermodynamics
⇒ Structural changes due to anion binding
⇒ Calculations (quantumchemistry)

Complex nanostructures – Dynamics and interactions of semiconductor nanowires for optoelectronics (2018-T3)

25 / 26 September 2018
written report, 2 credit points, 8 participants

This module was organized as part of the FOR1616 research unit group meeting which took place in Weimar. The talks and interdisciplinary discussions focused on understanding light properties in nanostructures smaller than the light wavelength and how to control them.

Responsible Scientists:
Prof. Dr. M. Grundmann

Speakers:
⇒ Thomas Schäpers, FZ Jülich: *Preparation and Transport Experiments on Nanowire-Superconductor Hybrid Structures*
⇒ Jesper Wallentin, University Lund, *Using X-ray beams as in operando pump and probe of single nanowire devices*
⇒ Werner Prost, University Duisburg/Essen, *Electrically stimulated nanowire light sources*
⇒ Lutz Geelhaar, PDI Berlin) *Excitonic Aharonov-Bohm oscillations in core-shell nanowires*
⇒ Dennis Franke, University Bremen, *First principles investigations on the electronic and optical properties of mercaptocarboxylic acids on ZnO surfaces*
⇒ Tobias Voss, TU Braunschweig, S*emiconductor nanowires for hybrid optoelectronic devices*
⇒ Alois Lugstein, TU Wien, *Ultrascaled and –strained nonowires for optoelectronics*
⇒ Carsten Ronning, University Jena, L*ight-nanowire interaction: from lasing and tunnel excitation to hard X-ray generation*
⇒ Jos Haverkort, TU Eindhoven, *Nanophotonic solar cells: fundamental limits*
⇒ Hao Zhou, TU Braunschweig, *MOCVD of core-shell nanorod LEDs*
⇒ Maria Timofeeva, ETH Zürich, *III-V nanowires as building blocks for nonlinear photonics*
⇒ Artur Zrenner, University Paderborn, *Coherent optoelectronics with single quantum dots*
⇒ Rüdiger Schmidt-Grund, University Leipzig, *Coherent states in Nano- and Microstructure Microcavities*
⇒ Rupert Oulton, Imperial Collage London, *Exploiting plasmonic nanofousing on semiconductor photonics platforms*

Scientific minisymposium

Chemical biology and biophysics of cancer (2018-A2)

25 - 26 September 2018

The BuildMoNa minisymposium was organised by the research group of Prof. Dr. J. Käs The module focused on how molecular and materials science can provide a new perspective in oncology. Molecular biology shows the complexity and ambiguity that arises from the variability of tumours. Nevertheless, some biochemical and biophysical changes are universal to solid tumour progression and may provide both, novel diagnostic as well as therapeutic concepts. The state of the art in diagnostics and therapeutics was discussed to identify the current needs.

Speakers:
⇒ I. Thievessen, Friedrich Alexander University Erlangen-Nuremberg, Germany
The cancer-associated adhesion-protein β-parvin functions as mechanoresponsive signaling hub that regulates cell size, shape, and contractility
⇒ C. Broedersz, Ludwig Maximilians University Munich, Germanyy
Feeling the tension: cell-induced stresses in the extracellular matrixo
⇒ P. Janmey, University of Pennsylvania, USA
Role of phosphoinositide signaling in mechanoresponse of liver cancer cells
⇒ K. Pogoda, Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
Microenvironmental mechanics contribute to glioblastoma cell behaviour
⇒ R. Leube, RWTH Aachen University, Germany
Focal adhesion - hemidesmosome crosstalk in migrating keratinocytes
⇒ O. Otto, University of Greifswald, Germany
Virtual fluidic channels: from single cell rheology to tissue mechanics
⇒ C. Leduc, The Institut Pasteur, France
Polarized dynamics of intermediate filament in glial cell migration
⇒ A. Tijore, TNational University of Singapore, Singapore
Mechanical cyclic stretching inhibits cancer cell growth but promotes normal cell growth
⇒ A.-C. Reymann, Institute of Genetics and Molecular and Cellular Biology, France
Modulation of cortical actin assembly dynamics
⇒ A.-S. Smith, Friedrich Alexander University Erlangen-Nuremberg, Germany

Physics of cell adhesion: The role of the membrane in the protein recognition process

⇒ J. Kayser, University of California, Berkeley, USA
Collective motion attenuates natural selection in crowded cellular populations

⇒ V. Vogel, ETH Zurich, Switzerland
New peptide probes to map the tensional states of ECM fibers in tumour tissues

⇒ F. Rehfeldt, University of Göttingen, Germany
Mechanics matters for cells: From extracellular matrix via cytoskeleton to the nucleus

⇒ P. Roca - Cusachs, Institute for Bioengineering of Catalonia, Spain
Control of mechanosensitivity by integrin-ECM binding and nucleocytoplasmic shuttling kinetics

⇒ J. Bobrowska, Polish Academy of Sciences, Krakow, Poland
Biochemical and nanomechanical fingerprints of melanoma development

⇒ H. Rieger, Saarland University, Germany
Search and kill - the immune response to cancer cells

⇒ M. Kreysing, Max Planck Institute of Molecular Cell Biology and Genetics, Germany
Probing the physiology of physical transport inside cells and developing tissues

⇒ L. Sorokin, University of Münster, Germany
Mechanisms of cellular penetration of vascular basement membranes - how biophysics could help us better understand this process

⇒ A. Patteson, University of Pennsylvania, Philadelphia, USA
Loss of vimentin increases motility and nuclear damage in confined spaces

⇒ D. Riveline, Institut de Genetique et de Biologie Moleculaire et Cellulaire, France
Ratchetaxis and cytokinesiss

⇒ B. Austin, Princeton University, USA
PC3-epi prostate cancer cells become polyploid, resistant and mesenchymal on a docetaxel gradient

⇒ D. Bi, Northeastern University, USA
Different modes of fluidization in Human Bronchial Epithelial Cells -- the Unjamming Transition vs. the Epithelial-Mesenchymal Transition

⇒ T. Zielinski, Polish Academy of Sciences, Krakow, Poland
Biomechanics of glioblastoma cells by atomic force microscopy

⇒ B. Wolf, University Hospital Leipzig, Germany
Cancer resection within morphogenetic fieldss

⇒ M. Aliee, Friedrich-Alexander University of Erlangen-Nuremberg, Germany
Coordination of tissue growth by cell mechanics

⇒ S. Huang, Institute for Systems Biology, USA
Why cancer treatment can backfire - From non-linear dynamics to single-cell transcriptomics of cell state transitions to preclinical studies

⇒ C. Mark, Friedrich-Alexander University Erlangen-Nuremberg, Germany
Collective forces of tumor spheroids in three-dimensional biopolymer networks

⇒ B. Aktas, University Hospital Leipzig, Germany
Catch me if you can: Circulating and disseminated tumor cells in breast cancer patients

⇒ R. Osellame, University of Milan, Italy
Integrated optofluidic devices for cancer cell analysis and imaging

Transferable skills workshops

Presentation Workshop

Dr. Frank Lorenz,
09 / 22 March 2018 in combination with the Annual BuildMoNa Conference,
8 participants

How to give successful oral presentations in the natural and related sciences? The workshop (held in English language throughout) aimed at an improvement of the presentation skills of doctoral candidates. Besides a short review of the basic foundations of successful oral presentations, the workshop covered advanced methods and techniques for preparing and performing oral presentations with special focus on the particular setting at international scientific conferences. As a major element of the workshop, the attendees jointly prepared and practiced their yearly progress report presentation in front of their colleagues and advisors. The presentation at the report meeting was monitored by video and thoroughly analysed in group and plenary discussions with the colleagues on the second workshop day.

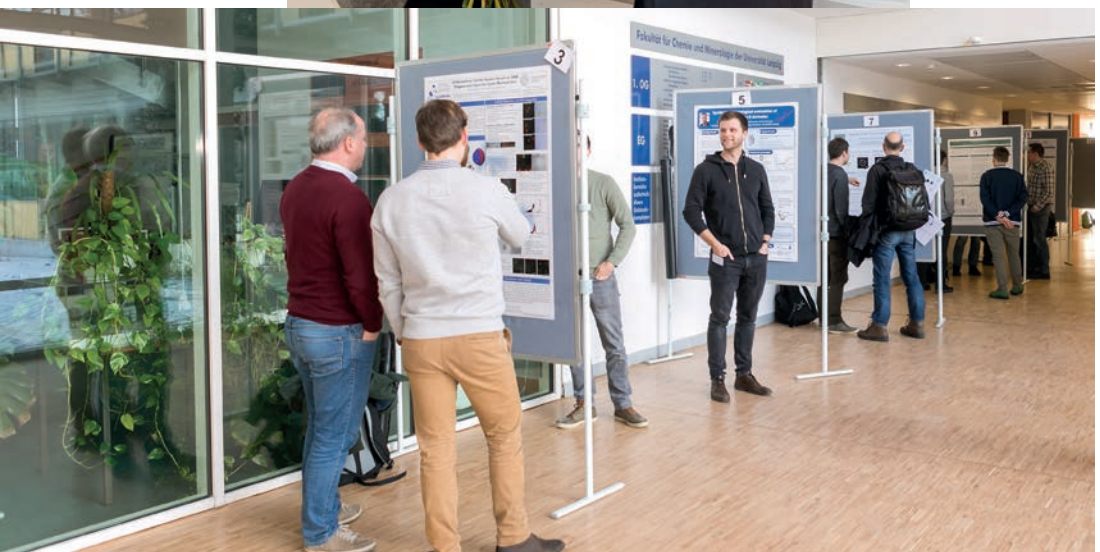
Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Hansjörg Grützmacher	*ETH Zürich*	Fun with Funny Phosphorus Molecules	18 January 2018	*Faculty of Chemistry and Mineralogy*
Dr. Lars Renner	*Leibniz-Institut für Polymerforschung, Dresden*	Engineering Bacteria Cells: Bacterial cell shape regulation under mechanical stress	23 January 2018	*Faculty of Life Sciences*
Prof. Dr. Kathrin Lang	*Technische Universität München*	Expanding the Genetic Code – Chemistry in Living Systems	17 April 2018	*Faculty of Life Sciences*
Dr. Ünal Coskun	*Paul-Langerhans-Institut, Dresden*	Membrane Lipids as determinants for controlled cell signaling	15 May 2018	*Faculty of Life Sciences*
Prof. Dr. Markus Weingarth	*Utrecht University*	Magic bullets to fight antimicrobial resistance	13 November 2018	*Faculty of Life Sciences*

Annual BuildMoNa Conference

The sixth annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held at the Faculty of Chemistry and Mineralogy on 19 and 20 March 2018.

A special feature of this year's conference was the celebration of the 10-year anniversary of BuildMoNa. To mark this jubilee the current speaker Prof. Dr. M. Grundmann presented a retrospective and expressed his gratitude, on behalf of all members, to the former speaker Prof. Dr. Dr. h. c. mult. E. Hey-Hawkins for her commitment during the last ten years. Besides, special contributions were made by the Vice-Rector for Research and Young Academics Prof. Dr. E. Schröger and by former BuildMoNa members, who gave short presentations on how the Graduate school influenced their further career.



⇑ Participants of the Annual BuildMoNa Conference 2018.

The following renowned guest speakers gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Knut Asmis, University Leipzig
Cryogenic ion vibrational spectroscopy: more than a structural characterization tool for gas phase clusters

⇒ Dr. ir. Henk Huinink, Technical University Eindhoven
Towards a thermal battery – utilizing solid-solid transitions in crystal hydrates

⇒ Prof. Dr. Claudia Blindauer, University of Warwick
Metal-sensing proteins and regulatory molecular switches: the mechanics of zinc homeostasis

⇒ Prof. Dr. Silke Christiansen, Helmholtz-Zentrum Berlin
3D nanoarchitectures of organic and inorganic nature – enhancing functionality and understanding through correlative microscopy

⇒ Dr. Donald MacLaren, University of Glasgow
Mapping the nanoscale functionality of advanced materials using analytical electron microscopy

During the poster session, doctoral candidates presented their scientific topics and discussed them with the international guests, receiving further inspiration for their work at the Graduate School BuildMoNa.

⇑ Winners of the BuildMoNa Awards 2018: Steffen Richter, Robert Kuhnert and Stefanie Riedel (from left to right).

The BuildMoNa Awards were given to doctoral candidates to recognise their outstanding scientific achievements.

Steffen Richter (Felix Bloch Institute for Solid State Physics) received one the two first prizes for his work on anisotropic microcavities published as:
Exceptional points in anisotropic planar microcavities
S. Richter, T. Michalsky, C. Sturm, B. Rosenow, M. Grundmann, R. Schmidt-Grund / Phys. Rev. A (2017) **95** 023836

Robert Kuhnert (Institute of Inorganic Chemistry) received the other first prize for his work on Carborane-based Lipoxygenase Inhibitors published as:
CarbORev-5901: The First Carborane-Based Inhibitor of the 5-Lipoxygenase Pathway
R. Kuhnert, M.-B. Sárosi, S. George, P. Lönnecke, B. Hofmann, D. Steinhilber, B. Murganic, S. Mijatovic, D. Maksimovic-Ivanic and E. Hey-Hawkins / ChemMedChem (2017) **12** 1081

Stefanie Riedel (Leibniz Institute of Surface Engineering) received the third price for her research on a gelatin-based bioactuator published as:
Programming stimuli-responsiveness of gelatin with electron beams: basic effects and development of a hydration-controlled biocompatible demonstator
S. Riedel, B. Heyart, K.S. Apel and S.G. Mayr / Sci. Rep. (2017) **7** 17436

Beside the poster session, several doctoral candidates presented their scientific results with short talks. Presentations covered the whole research profile of the graduate school: Development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. Mechanisms of material formation from building blocks, e.g. self-organisation, were also included. For the 8 participants of the Presentation Workshop by Dr. Frank Lorenz this was the opportunity to directly apply their newly acquired knowledge in that area. Their talks were filmed and critically discussed afterwards. At the end of the workshop a jury selected the three best presentations given by the doctoral candidates. The first prize was awarded to Paul Räcke for his presentation "Deterministic ion implantation: how to count single ions", the second to Rafaella Precker for her presentation "BioMOFs as drug carriers in cancer therapy" and the third prize to Dennis Worm for his talk "Selective neuropeptide Y conjugates with high carbaborane loading as potential boron delivery agents for BNCT".

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference together with the Speaker of the Graduate School: Dennis Worm, Prof. Dr. Marius Grundmann, Rafaella Precker and Paul Räcke (from left to right).

Funding of doctoral candidates