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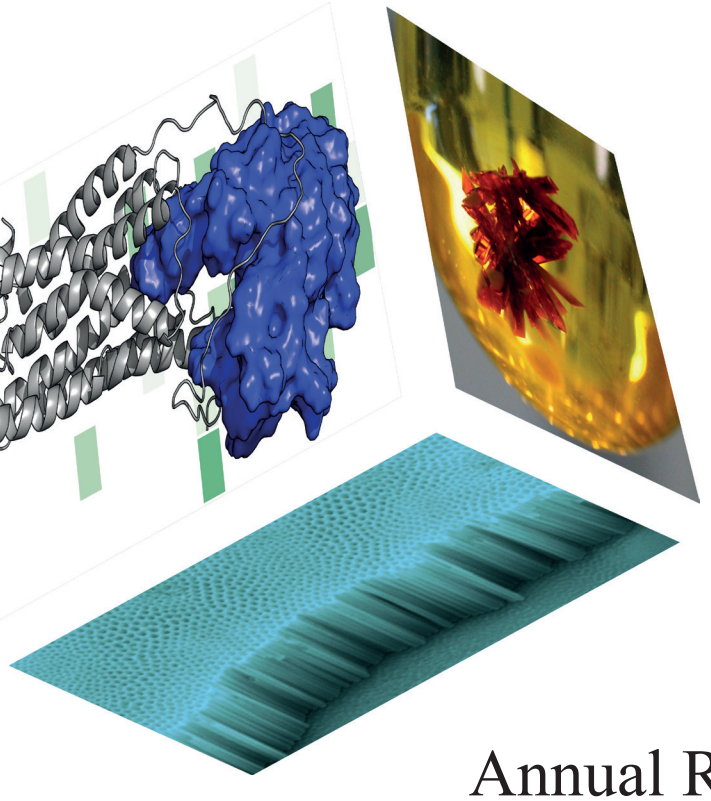
BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2019

Cover image:
⇒ *Left:* Investigation of G protein-coupled receptors: *in silico* contact prediction for the determination of novel contact sites.
⇒ *Right:* Crystals of a redox-active ferrocene-based tris-phosphane.
⇒ *Bottom:* SEM image of TiO_2 nanotube substrates.

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Annual Report 2019

Founded as DFG Graduate School 185 in 2007

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Leipzig School of Natural Sciences – the twelfth 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

The Leipzig School of Natural Sciences – Building with Molecules and Nano-objects (BuildMoNa) has supported interdisciplinary doctoral studies of young scientists in the twelfth year now. Excellent research conditions, training of scientific key competencies for broadening the horizon, acquisition of soft skills, as well as support for various activities such as stays abroad and conference contributions provide an excellent and stimulating scientific and professional network 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.

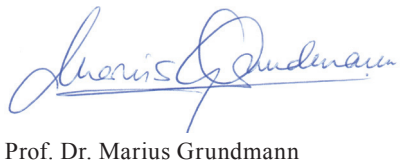
Since the establishment of the Graduate School in 2007, 157 young scientists have finished their doctoral studies with a certificate of the Graduate School. In 2019, 66 doctoral researchers have been enrolled as members of BuildMoNa. Most of them were employed through third-party funded research projects.

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

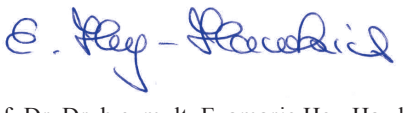
Each year, one of the advanced modules is organised as an international symposium. In 2019, the symposium "Transparent Conductive Oxides – Fundamentals and Applications" (TCO2019) was organised by Prof. Marius Grundmann together with Dr. Holger von Wenckstern of the Semiconductor Physics Group and brought together researchers in the field of transparent materials. These materials are used for ohmic applications such as transparent contacts in displays or solar cells. Furthermore, semiconducting transparent oxides for diodes and transistors have gained tremendous interest due to applications in transparent and flexible active electronics. TCO2019 was also supported by the Deutsche Forschungsgemeinschaft.

Science-related events included the Annual BuildMoNa Conference in March, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School. The doctoral researchers of the Graduate School took the opportunity to present the progress made in the individual research projects and to obtain direct feedback from an interdisciplinary audience. Renowned guest speakers, selected and invited by the doctoral researchers of BuildMoNa, covered current topics in engaging presentations. Also on this occasion, the annual BuildMoNa Awards were given to three doctoral candidates for their excellent scientific publications resulting from their doctoral research.

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

RESEARCH ACADEMY LEIPZIG ADVISORY BOARD

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Universität Graz

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Radboud University

RESEARCH ACADEMY LEIPZIG

RESEARCH ACADEMY DIRECTORATE OF THE GRADUATE CENTRE MATHEMATICS/COMPUTER SCIENCE AND NATURAL SCIENCES

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Dr. Alexandra Hildebrand

Multilingual Secretary
Johanna Lendewig

BOARD

Speaker of the Graduate School
Prof. Dr. Marius Grundmann

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

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M.Sc. Phys. Astrid Weidt
M.Sc. Phys. Florian Scheffler

Deputies
M.Sc. Phys. Martin Fränzl
M.Sc. Phys. Patrick Irmisch

Representatives of Principal Investigators
Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Prof. Dr. Daniel Huster
Prof. Dr. Roger Gläser
Prof. Dr. Bernd Abel
Prof. Dr. Annette G. Beck-Sickinger
Prof. Dr. Frank Cichos
Prof. Dr. Marius Grundmann
Prof. Dr. Andreas Schmid
Prof. Dr. Felix Otto

The Graduate School BuildMoNa is a graduate school 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 Astrid Weidt 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.

The major tasks of the BuildMoNa Board 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 BuildMoNa Board 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 represent the doctoral candidates within the BuildMoNa Board.

The BuildMoNa Office consists of a professional scientific manager (half-time position) and a multilingual secretary (half-time position), who support the BuildMoNa Board. 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	Thesis Advisory Committee	Working title of doctoral thesis
M.Sc. Chem. Ken Luca Abel	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid / Dr. J. Titus	*Rational design of catalysts for the methanation of carbon dioxide*
M.Sc. Phys. Alice Abend	Prof. Dr. M. Zink / Prof. Dr. R. Seidel / Prof. Dr. M. Zink	*Interaction of neuronal cells with electrode materials*
M.Sc. Chem. Angela Aleksovska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Coordination polymers and metal-organic frameworks for electro-catalysis*
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. Chem. Sebastian Braun	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Dr. F. Hansen	*Multi-target enzyme inhibitors in cancer therapy*
M.Sc. Phys. Henrik Christiansen	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Nonequilibrium investigation of (bio-)physical systems*
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. Biochem. Anne Sophie Czerniak	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe / Prof. Dr. I. Coin	*Chemerin's structure and activity relationship*
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. Chem. Zeno Fickenscher	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting / Prof. Dr. K. Zeitler	*Investigation of heterobimetallic complexes in homogeneous catalysis*
M.Sc. Phys. Alexander Fischer	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Feedback controlled active particle assemblies*
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 chalcogenides*
M.Sc. Phys. Martin Fränzl	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Thermoelectric effects at the nanoscale*
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. Chem. Florian Harth	Prof. Dr. R. Gläser / Prof. Dr. A. Schmid	*Valorisation of glycolate by heterogeneous catalysis in aqueous phase*
M.Sc. Phys. Anna Hassa	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Deep UV photodetector arrays based on large bandgap oxides*
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. Chem. Benjamin Hoffmann	Prof. Dr. K. Asmis / Prof. Dr. J. Meijer / Prof. Dr. B. Abel	*Action spectroscopy on single nanoparticles*
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*
M.Sc. Chem. Dilara Issayeva	Prof. Dr. R. Gläser / Prof. Dr. B. Kersting / Dr. I. Titus	*Hydrogenation of CO_2 to methanol under dynamic reaction conditions: a novel concept for carbon capture and utilisation*
M.Sc. Phys. Tanja Jawinski	Prof. Dr. M. Grundmann / Prof. Dr. C. Schnohr/ Dr. habil. H. von Wenckstern	*Preparation and analysis of intermediate band solar cells*
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. Chem. Aleksandr Kazimir	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Dr. F. Hansen	*Organometallic compounds in dual anticancer therapy*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
M.Sc. Phys. Max Kneiß	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Combinatorial pulsed laser deposition employing radially-segmented targets: exploring orthorhombic $(In_xGa_{1-x})_2O_3$ and $(Al_xGa_{1-x})_2O_3$ towards superlattice heterostructures*
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. Phys. Evgeny Krüger	Prof. Dr. M. Grundmann / Prof. Dr. B. Rosenow / Dr. C. Sturm	*Topological effects in anisotropic dielectric photonic structures*
M.Sc. Phys. Astrid Kupferer	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*
M.Sc. Phys. Oliver Lahr	Prof. Dr. M. Grundmann / Dr. habil. H. von Wenckstern / Prof. Dr. C. Schnohr	*High-frequency, flexible, bendable electronics for wireless communication systems based on amorphous oxide semiconductors*
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. Chem. John Popp	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*P-Stereogenic dendritic ferrocenyl phosphines for redox-switchable catalysis*
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. Chem. Ivana Predarska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. G. Kaluderovic / Prof. Dr. B. Kersting	*Development of novel dual-acting antitumour agents*
M.Sc. Chem. Kyzgaldak Ramazanova	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis of P-chiral bidentate phosphane ligands for applications in stereoselective catalysis*
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. Biochem. Veronika Riedl	Prof. Dr. T. Pompe / Prof. Dr. A. G. Beck-Sickinger / Dr. Dr. J. T. Heiker	*Immobilisation of enzyme structures for soft-colloidal particle biosensors*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
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 centres*
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. Phys. Nicola Söker	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Thermo-osmosis for manipulating microscopic liquid flow fields*
M.Sc. Chem. Philipp Stockmann	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Prof. Dr. B. Kersting	*Carborane-containing molecules for medical applications*
M.Sc. Phys. Tillmann Stralka	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer / Dr. habil. H. von Wenckstern	*Correlation of electrical and topographical properties in copper iodide thin films*
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. Xiaoya Su	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Frequency-dependent noise temperature of hot Brownian motion*
M.Sc. Phys. Lukas Trefflich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Fabrication and characterisation of carbon-nanodot-based planar microcavities*
M.Sc. Chem. Liridona Useini	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis of carboranyl analogues of nonsteroidal anti-inflammatory drugs (NSAIDs)*
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*

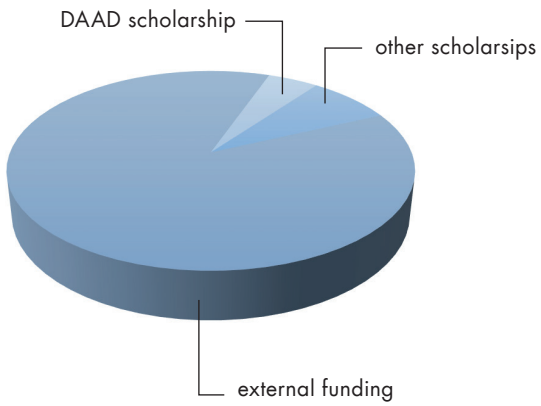
Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
M.Sc. Nanoscience Muhammad Ayman Zaheer	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Studying of diffusion in reacting catalytic systems by means of NMR spectroscopic methods*
Dipl.-Math. Heinrich-Gregor Zirnstein	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Topological aspects of Dirac fermions in condensed matter systems*

Alumni 2019

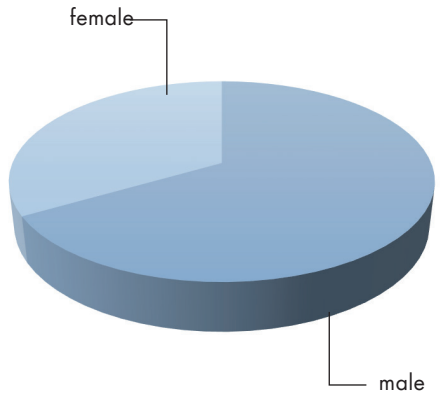
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Peter Coburger	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*A carborane-substituted 1,2-diphosphetane as building block for the development of new ligands with potential application in homogeneous catalysis*
Dr. rer. nat. 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*
Dr. rer. nat. Marta Gozzi	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Ruthenacarborane complexes as building blocks for the design of novel anti-tumour agents*
Dr. rer. nat. Susann Liedtke-Grüner	Prof. Dr. Dr. h.c. B. Rauschenbach / Prof. Dr. J. Meijer	*Sculptered metal films*
Dr. rer. nat. Felix Link	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Diesel exhaust catalyst deactivation by biofuel-originated poisons and hydrothermal treatment*
Dr. rer. nat. Georgia Mhanna	Prof. Dr. R. Gläser / Prof. Dr. A. G. Beck-Sickinger	*Hexagonal mesoporous silicates for immobilisation of multi-enzyme conjugates*
Dr. rer. nat. Stefanie Riedel	Prof. Dr. S. G. Mayr / Prof. Dr. J. Käs	*Radiation assisted modification of gelatin and collagen for biomedical applications*
Dr. rer. nat. Benedikt Schwarze	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. G. Beck-Sickinger	*Development of tamoxifen-based vectors as novel targeting antitumour agents by conjugation with molybda- and ruthenacarborane or rhenium complexes*

Statistics

FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



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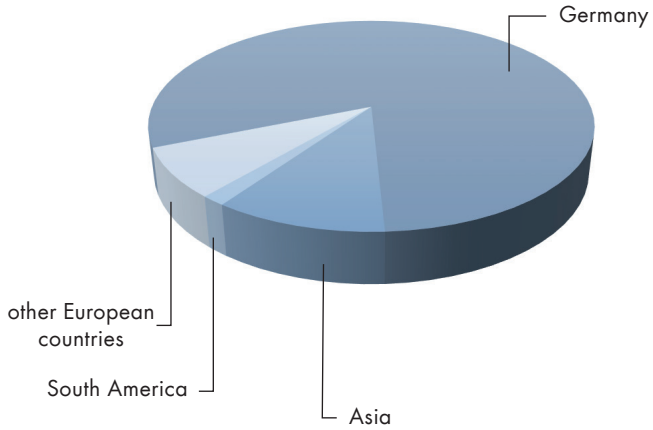
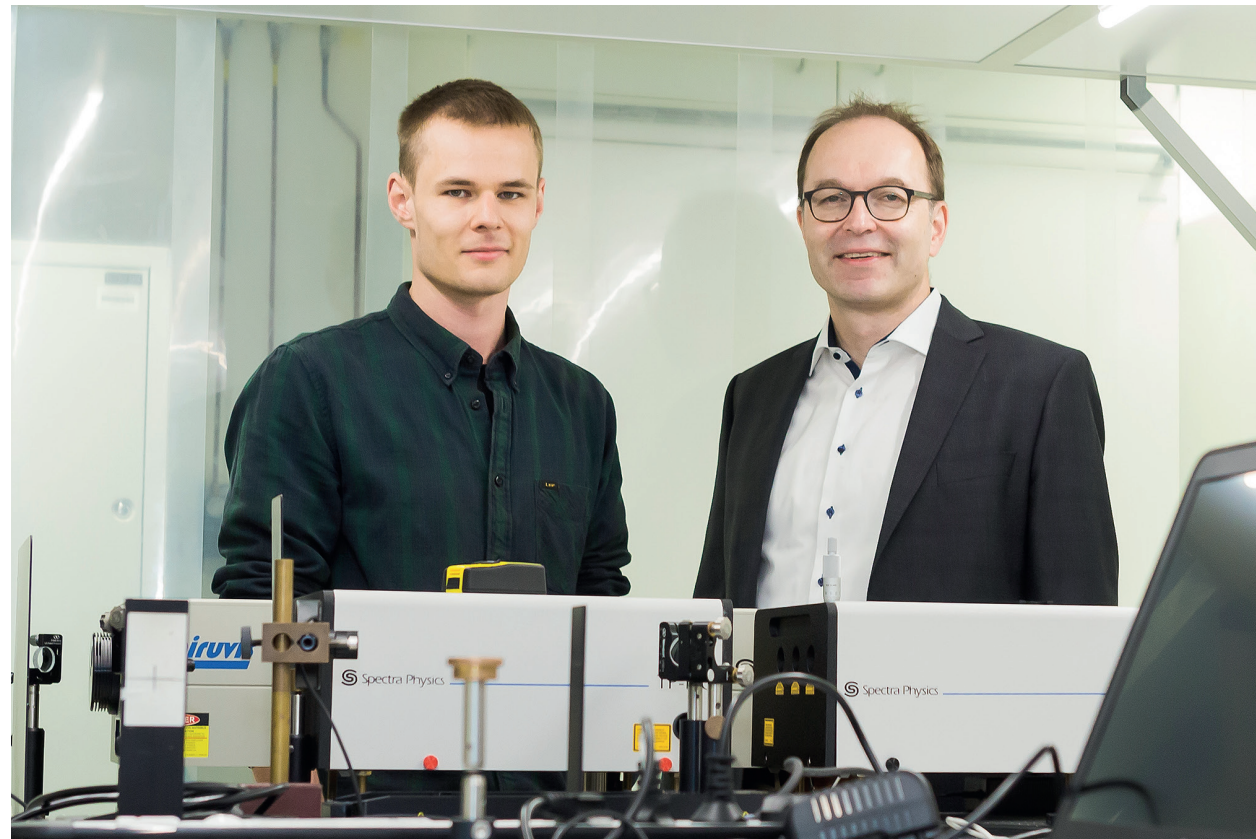


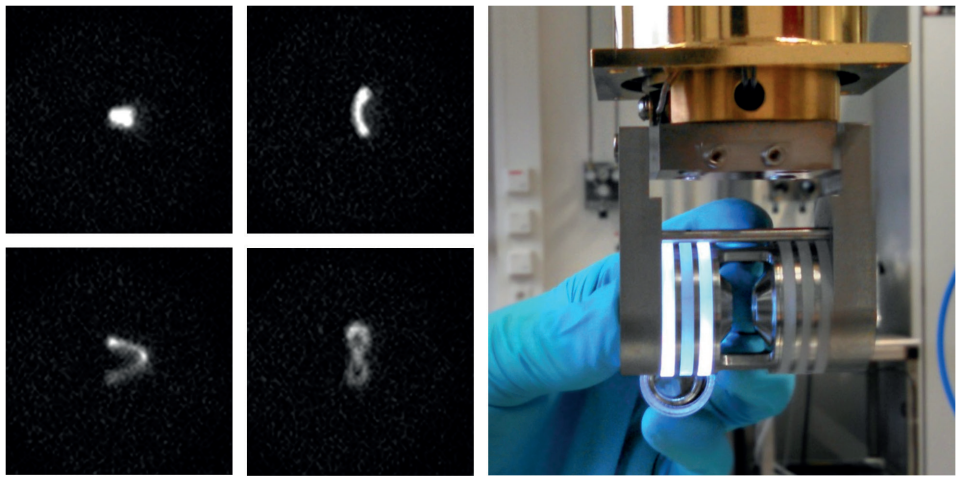
Single nanoparticle spectroscopy in a cryogenic ion trap

Prof. Dr. Knut Asmis
M.Sc. Chem. Benjamin Hoffmann

Research on nanoparticles (NPs) is motivated by gaining an understanding of the dependence of their optical, electrical and magnetic properties on their size, shape and surface chemistry. However, detailed information on the intrinsic properties of NPs remains challenging to obtain, because macroscopic samples typically exhibit chemical as well as physical heterogeneity. Consequently, their characterisation by spectroscopic ensemble techniques always suffers from inhomogeneous line broadening and single NP methods are required to avoid averaging over an ensemble of NPs. However, the traditional single NP approaches all rely on deposited NPs, *i.e.*, NPs that interact with a surface (and possibly other nearby NPs). Probing truly intrinsic properties requires isolating NPs in an inert matrix or, ideally, in the gas phase.



Direct absorption spectroscopy is typically not sensitive enough to probe single isolated NPs and therefore alternative methods are required, in which the absorption of photons is detected indirectly by way of action spectroscopy. For this purpose, Benjamin Hoffmann is developing a new technique: a single NP is trapped in a custom made, temperature-controllable quadrupole ion-trap that allows to non-destructively monitor the absolute mass of a single NP by means of light scattering; cooling allows for precisely controlled adsorption of messenger compounds at the NPs surface; absorption of electromagnetic radiation is detected by monitoring changes in the gas adsorption kinetics. This allows for insight into the electronic structure and surface properties of the NP and ultimately contributes to bridging the information gap between molecular clusters and macroscopic bulk samples.



⇑ Characteristic oscillations of a trapped 100 nm particle in the ion trap (left) and image of the custom made quadrupole ion trap (right).

⇒ *A cryogenic single nanoparticle action spectrometer*
T. K. Esser, B. Hoffmann, S. Anderson, K. R. Asmis / Rev. Sci. Instrum. (2019) **90** 125110

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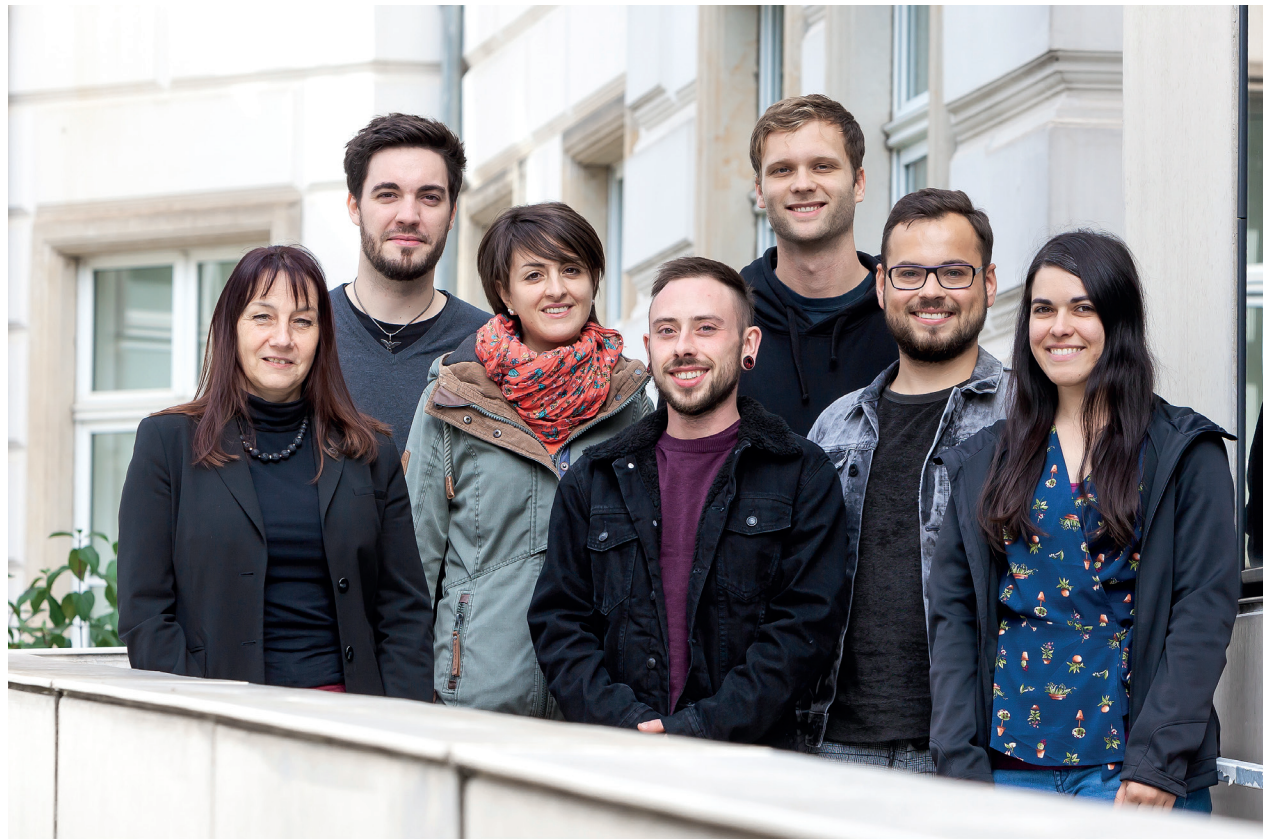
Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger
M.Sc. Biochem. Anne Sophie Czerniak, M.Sc. Chem. Jan Sebastian Dirks, M.Sc. Chem. Jan-Patrick Fischer, M.Sc. Biochem. Tobias Fischer, M.Sc. Chem. Kevin Kretzschmer, M.Sc. Biotech. Chiara Rugirello, M.Sc. Biochem. Philipp Wolf

The common aim of the projects includes the synthesis and characterisation of chemically modified peptides and proteins to modulate their function. This includes proteins involved in tumour targeting, proteins for nanomedicine or biomaterial development. Peptides are synthesised by solid phase peptide synthesis. Proteins are expressed recombinantly and fused to the peptides by native chemical ligation or click chemistry.

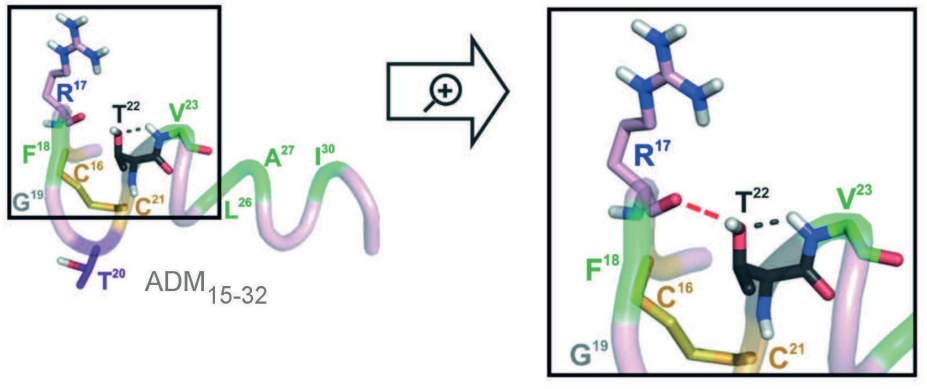
In 2019 Jan-Patrick Fischer successfully finished his doctorial work. He worked successfully on the identification of the binding and activation site of adrenomedullin and developed novel, active and very stable analogues of this 52 amino acid protein. Furthermore, Jan-Patrick Fischer explores the field of selectivity of the adrenomedullin and its interaction with its receptor system. He aims to stabilise different structural ele-



-ments of the molecule and to evaluate their impact on the selectivity of these peptides. Furthermore, he developed a number of disulphide bond mimetics and tested them for stability and activity.

Tobias Fischer and Anne Czerniak work in the field of chemerin. Tobias Fischer identified small chemerin peptides that bind to their respective receptors with high affinity and great stability. Furthermore, he spent some time in Vanderbilt in the laboratory of Jens Meiler to be introduced into the programme Rosetta and the modelling of the chemerin receptors. This significantly advanced his work. Anne Czerniak worked on the characterisation of chemerin-peptides for drug shuttling selectively into cells of the immune system.

Protein expression and chemical modification of enzymes was pursued by Jan Dirks. He works on the engineering of BM3-P450 protein, a 110 kDa large member of the cytochrome family consisting of three domains. He succeeded in expression and aims to modify this with a photoactivatable linker to induce activity by light. Kevin Kretschmer also is interested in chemical modification of proteins by light. However, he uses photoactivatable interaction partners to crosslink peptides to their interacting proteins. Subsequently, he characterises the interaction sites by mass spectrometry after enzymatic digestion and affinity purification. Philipp Wolf is interested in the chemical modification of proteins in living cells. He managed to chemically label endothelin receptors that belong to the family of GPCR with fluorophors, and monitor trafficking.



⇑ Structure of adrenomedullin 15-32 with hydrophobic residues marked in green, dislufide bond in yellow. Jan-Patrick Fischer identified the important role of threonine 22 for selectivity of adrenomedullin for AM1 receptor versus CGRP receptor.

In addition to current members, several papers of former BuildMoNa-members have been published, including Sylvia Els-Heindl, Sven Hofmann and Dennis Worm. Work was achieved during their PhD project but was delayed in publication owing to collaborators.

⇒ *Identification and stabilisation of a highly selective gastrin-releasing peptide receptor agonist*
P. Hoppenz, S. Els-Heindl, A. G. Beck-Sickinger / J. Pept. Sci. (2019) **25** e3224

⇒ *Modular triazine-based carborane-containing carboxylic acids - synthesis and characterisation of potential boron neutron capture therapy agents made of readily accessible building blocks*
M. Kellert, D. J. Worm, P. Hoppenz, M. B. Sárosi, P. Lönnecke, B. Riedl, J. Koebberling, A. G. Beck-Sickinger, E. Hey-Hawkins / Dalton Trans. (2019) **48** 10834

⇒ *Adrenomedullin disulfide bond mimetics uncover structural requirements for AM1-receptor activation*
J. P. Fischer, R. Schönauer, S. Els-Heindl, D. Bierer, J. Koebberling, B. Riedl, A. G. Beck-Sickinger / J. Pept. Sci. (2019) **25** e3147

⇒ *Chemical modification of neuropeptide Y for human Y1 receptor targeting in health and disease*
S. Hofmann, K. Bellmann-Sickert, A. G. Beck-Sickinger / Biol. Chem. (2019) **400** 299

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Active particle feedback control with a single-shot detection convolutional neural network

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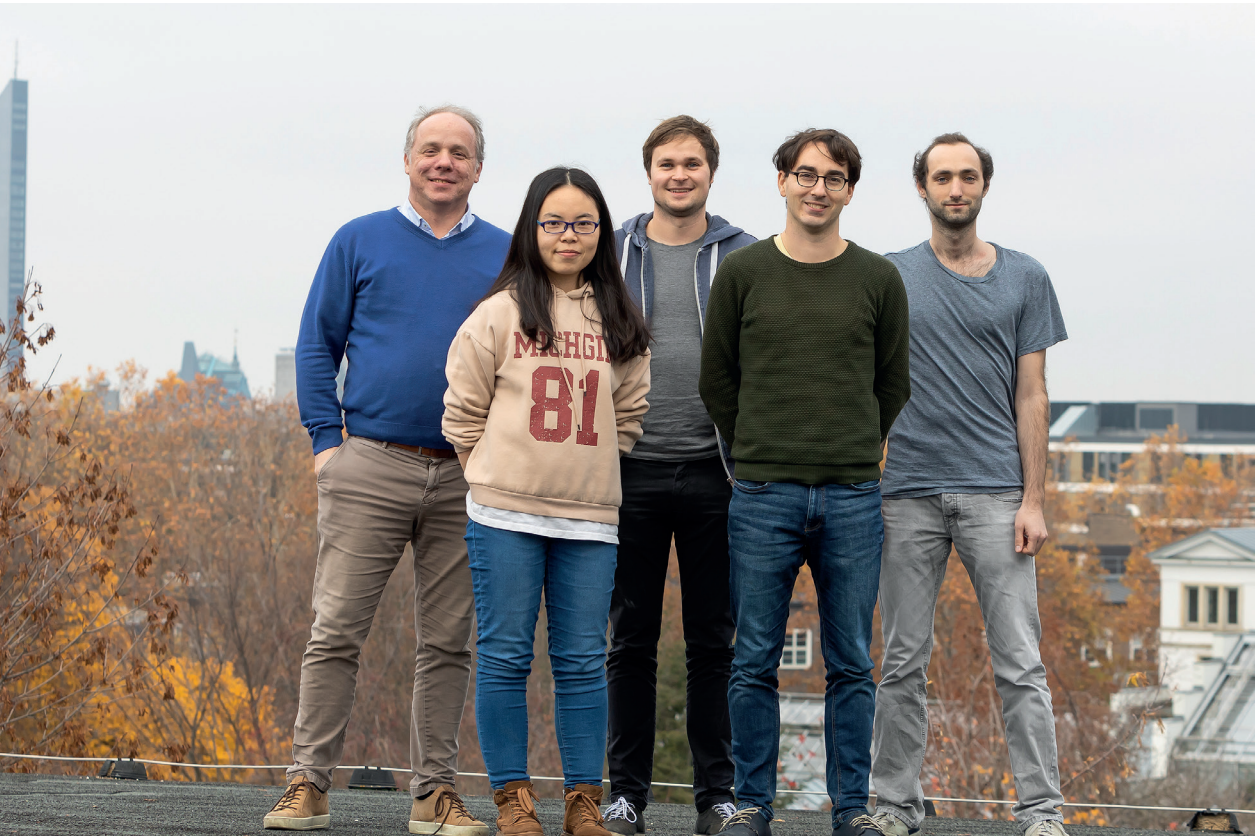
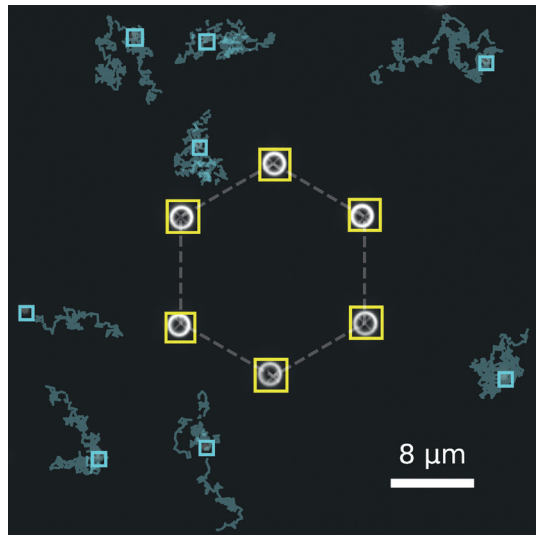
Synthetic active particles serve as simple microscopic model systems for living objects. They mimic the propulsion of bacteria without the complexity of physical properties and chemical networks in living objects, yet with the fluctuations due to Brownian motion. Active particles convert local energy to propel persistently and as such they have given considerable insight into collective behaviours of active materials including motility-induced phase transitions. With their bare function of self-propulsion, they are, however, missing the important ingredients of sensing, information processing and feedback, which most living objects from cells up to whole organisms have in common. All of their living relatives have sensorial capabilities which they use to gain information about the environment and to self-organise into collective states such as swarms, flocks or tissue.



The Molecular Nanophotonics Group has developed active particles that self-propel in liquids by converting light into heat with the help of plasmonic nanostructures on polymer surfaces. These particles are completely symmetric in their structure but break the time reversal symmetry by a local heat release due to light being focused on just one side of the particle. This allows us to introduce a precise feedback control that can mimic social interactions as in living systems. To extend these information-based interactions to particle systems with different size and optical contrast, we have developed advanced machine learning techniques to localise and classify objects in microscopy images in real time. The convolutional neural network employs a single-shot approach to detect individual particles in a single pass. The network can be trained to recognise several hundred different object shapes with a high localisation accuracy. We have demonstrated video-rate feedback control in heterogeneous samples of active particles and passive polymer colloids. The network is currently used to study critical behaviour in ensembles of active particles based on delayed interactions.



⇐ Real-time localisation and classification of objects in a darkfield microscopy image by a single-shot convolutional neural network (YOLOTrack). The boxes surround gold nanoparticle coated polymer active particles (2.19 µm diameter, green) and passive polymer particles (0.5 µm diameter, white).

⇒ *Thermophoretic trap for single amyloid fibril and protein aggregation studies*
M. Fränzl, T. Thalheim, J. Adler, D. Huster, J. Posseckardt, M. Mertig, F. Cichos / Nature Methods (2019) **16** 611

⇒ *Thermophoretic trap for single amyloid fibril and protein aggregation studies*
F. Cichos, M. Fränzl, T. Thalheim, J. Adler, D. Huster, J. Posseckardt, M. Mertig / Protocol Exchange (2019)

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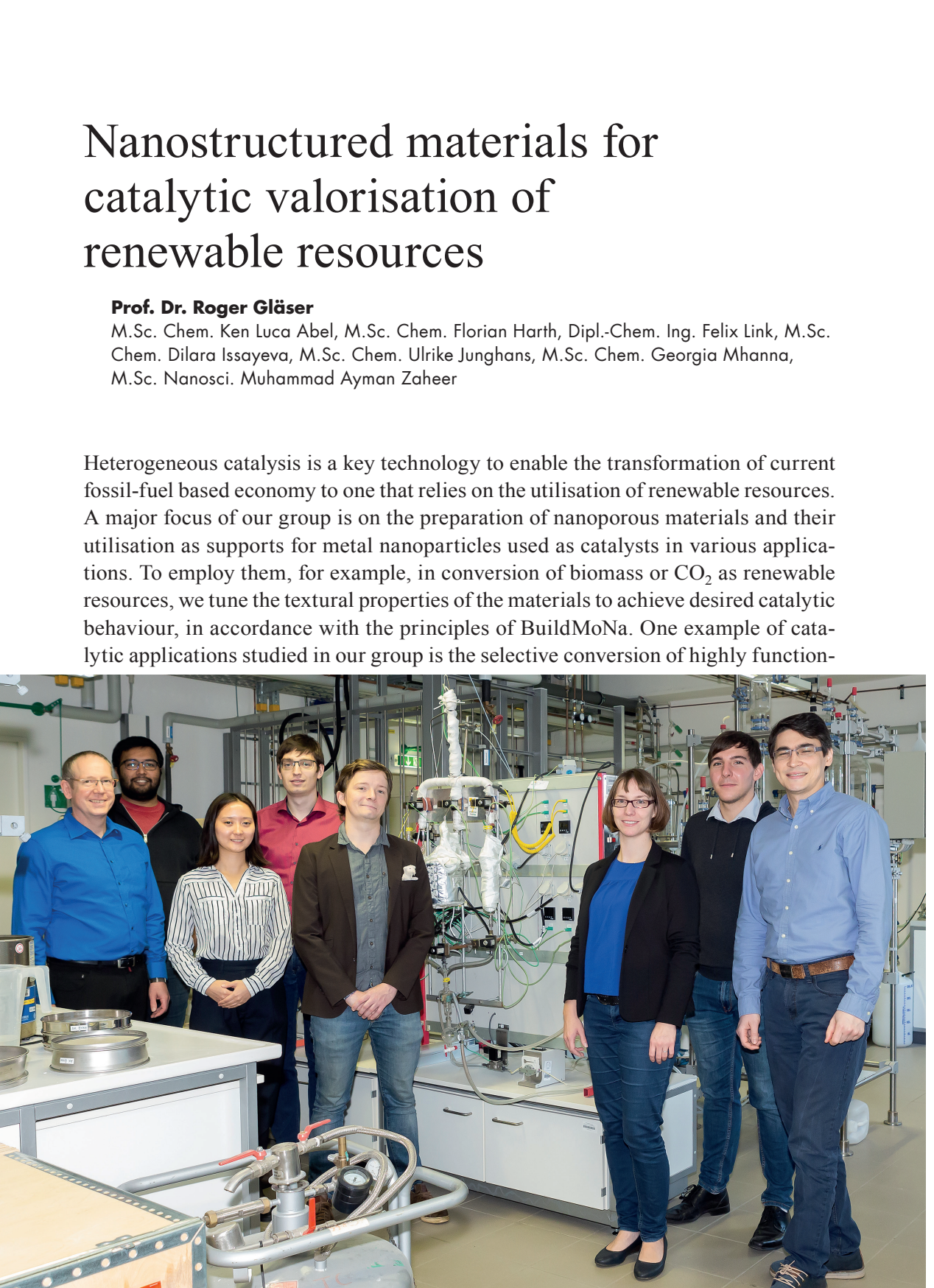
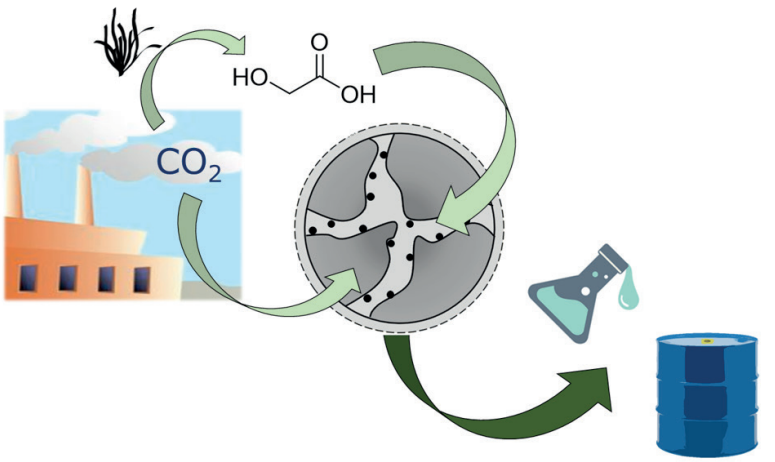
Nanostructured materials for catalytic valorisation of renewable resources

Prof. Dr. Roger Gläser
M.Sc. Chem. Ken Luca Abel, M.Sc. Chem. Florian Harth, Dipl.-Chem. Ing. Felix Link, M.Sc. Chem. Dilara Issayeva, M.Sc. Chem. Ulrike Junghans, M.Sc. Chem. Georgia Mhanna, M.Sc. Nanosci. Muhammad Ayman Zaheer

Heterogeneous catalysis is a key technology to enable the transformation of current fossil-fuel based economy to one that relies on the utilisation of renewable resources. A major focus of our group is on the preparation of nanoporous materials and their utilisation as supports for metal nanoparticles used as catalysts in various applications. To employ them, for example, in conversion of biomass or CO_2 as renewable resources, we tune the textural properties of the materials to achieve desired catalytic behaviour, in accordance with the principles of BuildMoNa. One example of catalytic applications studied in our group is the selective conversion of highly functionalised biomass-based molecules, e.g., functionalised organic acids like algae-derived glycolic acid, into value-added chemicals with lower oxygen content. This is done by studying the influence of various supports, active metal components, and promoters. Another case of modifying the textural properties of porous supports is the introduction of mesopores into microporous titanosilicate, which generates hierarchically structured ETS-10-based catalyst. This catalyst has higher activity in the conversion of fatty acid methyl esters (FAME) compared to purely microporous titanosilicate. These materials are also used for other challenging conversions such as CO_2 utilisation. In this regard, porous silica materials are functionalised with amines, which allow CO_2 to be chemisorbed on the surface in the form of carbamates. Textural characteristics of porous silica influences the amount of chemisorbed CO_2 as well as CO_2 adsorption kinetics. Chemisorbed CO_2 can be further converted to methanol with the help of metal nanoparticles loaded onto the porous silica. Moreover, the synthesis of monolithic oxide materials (Al_2O_3, ZrO_2) with a hierarchical meso-/macropore structure is investigated. These materials are used as a catalyst support for the methanation of CO_2 with H_2, with expected benefits in heat- and mass transfer properties.





⇑ Schematic representation of the biomass conversion and CO_2 utilisation strategies using nanostructured catalysts.

⇒ *Synthesis of highly active ETS-10-based titanosilicate for heterogeneously catalyzed transesterification of triglycerides*
M. A. Zaheer, D. Poppitz, K. Feyzullayeva, M. Wenzel, J. Matysik, R. Ljupkovic, A. Zarubica, A. A. Karavaev, A. Pöppl, R. Gläser, M. Dvoyashkin / Beilstein J. Nanotechnol. (2019) **10** 2039

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Combinatorial acceleration of material research

Prof. Dr. Marius Grundmann
M.Sc. Phys. Anna Hassa, M.Sc. Phys. Oliver Herrfurth, M.Sc. Phys. Tanja Jawinski, M.Sc. Phys. Max Kneiß, M.Sc. Phys. Evgeny Krüger, M.Sc. Phys. Oliver Lahr, M.Sc. Phys. Tillmann Stralka, M.Sc. Phys. Lukas Trefflich, M.Sc. Phys. Antonia Welk

At the very core of semiconductor technology lies the possibility to combine different materials into so-called heterostructures. This concept, often termed 'band-gap engineering' is the basis for modern electronic and photonic devices such as high electron mobility transistors and light emitting diodes and laser. 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/optimisation 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 stabilised. The latter has the potential advantage of high polarisation 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-$(Al_xGa_{1-x})_2O_3$ alloy system was investigated [R1-R4]. As can be seen in Fig. 1, the aluminum concentration x, as determined by EDX (energy-dispersive X-ray analysis in the scanning electron microscope), varies almost linearly over the 2 inch wafer. The correlation of the locally measured X-ray diffraction scans with the aluminum concentration (Fig. 2) reveals the continuous shift of the lattice constant up to the phase boundary (at about x=0.5). This way a complete alloy system can be investigated with just one sample.

The XPS (X-ray photoelectron spectroscopy) technique has been used for the investigation of our samples in cooperation [R1, R5, R6]. The Al-content agrees with that measured via EDX in the electron microscope (Fig. 1b). Additionally, XPS allows to determine the band-offsets of the material system relative to the semiconductors. This is essential information for the design of heterostructures as discussed

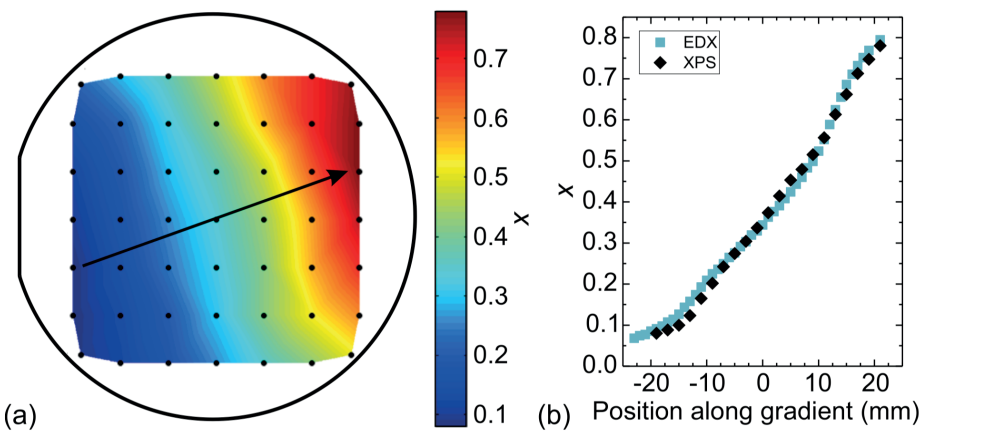
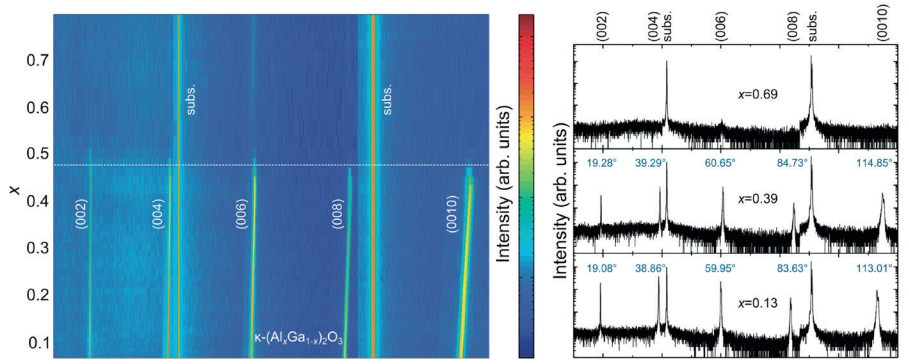


Fig. 1: (a) False colour representation of the aluminum content x of a $(Al_xGa_{1-x})_2O_3$ thin film grown on a 2 inch diameter c-plane sapphire substrate. The black dots indicate measurement spots, data in between was interpolated. The solid black line indicates the gradient direction. (b) Al-concentration along the gradient arrow in (a) using EDX and XPS chemical analysis.

above. In references [R5, R6], the offsets against MgO are reported.

Work of other BuildMoNa students concerns fabrication and characterisation of electronic devices based on the amorphous semiconductor zinc-tin-oxide [R7, R8]. Such devices avoid any expensive or rare metals and provide excellent properties. The fabrication is entirely at room temperature and thus works even when made on flexible substrates (work funded within DFG SPP 1796 FFlexCom).



⇑ Fig. 2: (a) False colour map of 2θ-ω scans of orthorhombic κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ recorded along the composition gradient indicated in Fig. 1(a). (b) XRD patterns for x = 0.13, x = 0.39, and x = 0.69. Peak positions of the (0 0 2n) lattice planes as well as the substrate (subs.) reflection are labeled.

⇒ [R1] *Solubility limit and material properties of a κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin film with a lateral cation gradient on (00.1) Al$_2$O$_3$ by tin-assisted PLD*
A. Hassa, C. Sturm, M. Kneiß, D. Splith, H. von Wenckstern, T. Schultz, N. Koch, M. Lorenz, M. Grundmann / APL Mater. (2020) **8** 021103:1

⇒ [R2] *Control of phase formation of (Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin films on c-plane Al$_2$O$_3$*
A. Hassa, C. Wouters, M. Kneiß, D. Splith, C. Sturm, H. von Wenckstern, M. Albrecht, M. Lorenz, M. Grundmann / J. Phys. D: Appl. Phys. (2020) **53** 485105:1

⇒ [R3] *Growth, structural and optical properties of coherent κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/κ-Ga$_2$O$_3$ quantum well superlattice heterostructures*
M. Kneiß, P. Storm, A. Hassa, D. Splith, H. von Wenckstern, M. Lorenz, M. Grundmann / APL Mater. (2020) **8** 051112:1

⇒ [R4] *Anisotropic strain relaxation through prismatic and basal slip in α-(Al,Ga)$_2$O$_3$ on R-Plane Al$_2$O$_3$*
M. Grundmann, M. Lorenz / APL Mater. (2020) **8** 021108:1

⇒ [R5] *Band offsets at κ-([Al,In]$_x$Ga$_{1-x}$)$_2$O$_3$/MgO interfaces*
T. Schultz, M. Kneiß, P. Storm, D. Splith, H. von Wenckstern, M. Grundmann, N. Koch / ACS Appl. Mater. Interfaces (2020) **12** 8879

⇒ [R6] *Changes in band alignment during annealing at 600°C of ALD Al$_2$O$_3$ on (In$_x$Ga$_{1-x}$)$_2$O$_3$ for x=0.25-0.74*
C. Fares, M. Xian, D.J. Smith, M.R. McCartney, M. Kneiß, H. von Wenckstern, M. Grundmann, M. Tadjer, F. Ren, S.J. Pearton / J. Appl. Phys. (2020) **127** 105701:1

⇒ [R7] *Low-voltage operation of ring oscillators based on room-temperature-deposited amorphous zinc-tin-oxide channel MESFETs*
O. Lahr, S. Vogt, H. von Wenckstern, M. Grundmann / Adv. Electron. Mater. (2020) **5** 1900548:1

⇒ [R8] *Full-swing, high-gain inverters based on ZnSnO JFETs and MESFETs*
O. Lahr, Z. Zhang, F. Grotjahn, P. Schlupp, S. Vogt, H. von Wenckstern, A. Thiede, M. Grundmann / IEEE Transact. Electr. Dev. (2019) **66** 3376

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

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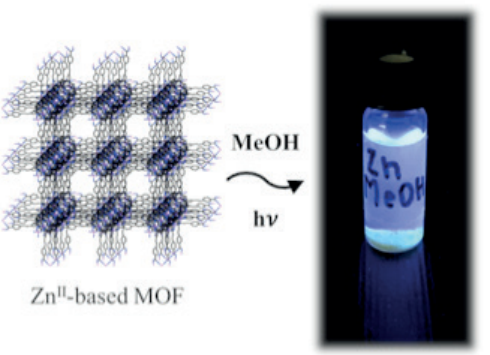
The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carborane clusters and antitumour drugs).

Smart Catalysts

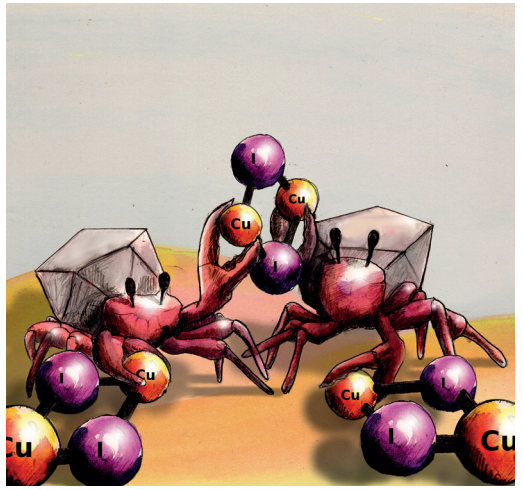
Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups (ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way ”switchable“ phosphines for catalytic applica-



⇐ Fig. 1: Methanol sensing by a luminescent zinc(II)-based metal-organic framework.

tions (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, S. Baweja, K. Ramazanova).



⇐ Fig. 2. Supramolecular self-assembly of Cu_2I_2 units bridged by the first *nido*-carborane-substituted diphosphetane, as symbolised by the crabs, forming a one-dimensional coordination polymer (design: Dr. Christoph Selg (Leipzig University)).

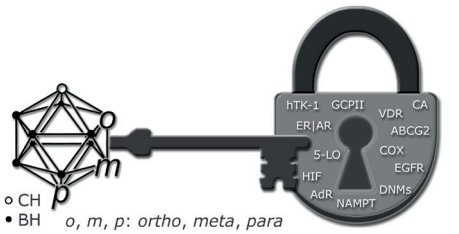
From Molecules to Novel Materials

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) (Fig. 1). Selected examples of functionalised building blocks for organometallic or phosphorus-based polymers are: strained phosphorus-based rings (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 redox-active coordination polymers or MOFs (A. Aleksovska).

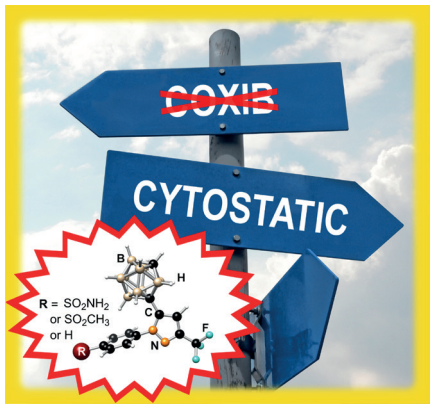
Molecular precursors: Binary metal phosphides MP_x often exhibit interesting optical, electronic and magnetic properties and thus have a wide range of applications, such as corrosion resistors, catalysts, semiconductors, electrode materials in lithium-ion batteries, etc. We have developed an approach to this class of compounds starting with volatile phosphorus-rich metal complexes (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 (Fig. 3) in cyclooxygenase (COX) (L. Useini) (Fig. 4) or other enzyme inhibitors (S. Braun, P. Stockmann) for boron neutron capture therapy (BNCT) as conjugates with tumour-targeting entities.
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. COX inhibitors (I. Predarska), tamoxifen (B. Schwarze, A. Kazimir)). 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, A. Kazimir).



⇑ Fig. 3: New keys for old locks: Carborane-containing drugs as platforms for mechanism-based therapies.



⇑ Fig. 4: The carborane-based analogues of celecoxib, which is a potent COX-2-selective inhibitor (COXIB), do not act as COXIBs, but showed a selective and high cytostatic effect on specific cancer cell lines.

⇒ *Half- and mixed-sandwich metallacarboranes for potential applications in medicine*
M. Gozzi, B. Schwarze, E. Hey-Hawkins / invited contribution, Pure Appl. Chem. (2019) **91** 563

⇒ *Carborane-based analogues of 5-lipoxygenase inhibitors co-inhibit heat shock protein 90*
R. Kuhnert, M.-B. Sárosi, S. George, P. Lönnecke, B. Hofmann, D. Steinhilber, S. Steinmann, R. Schneider-Stock, B. Murganić, S. Mijatović, D. Maksimović-Ivanić, E. Hey-Hawkins / ChemMedChem (2019) **14** 255

⇒ *Group 6 metal carbonyl complexes of cyclo-(P_3Ph_3)*
D.M. Yufanyi, T. Grell, M.B. Sárosi, E. Hey-Hawkins / Pure Appl. Chem. (2019) **91** 785

⇒ *Making and breaking of phosphorus–phosphorus bonds*
T. Grell, D.M. Yufanyi, A.K, Adhikari, M.B. Sárosi, P. Lönnecke, E. Hey-Hawkins / Pure Appl. Chem. (2019) **91** 103

⇒ *Carboranyl analogues of celecoxib with potent cytostatic ability against human melanoma cell lines*
A. Buzharevski, S. Paskas, M.B. Sárosi, M. Laube, P. Lönnecke, W. Neumann, S. Mijatović, D. Maksimović-Ivanić, J. Pietzsch, E. Hey-Hawkins / ChemMedChem (2019) **14** 315

⇒ *Selective laser sintering of metal-organic frameworks*
E. Lahtinen, R.L.M. Precker, M. Lahtinen, E. Hey-Hawkins, M. Haukka / ChemPlusChem (2019) **84** 222

⇒ *Methanol sensing by a luminescent zinc(II)-based metal-organic framework*
S. Durini, N. Ilić, K. Ramazanova, T. Grell, P. Lönnecke, E. Hey-Hawkins / ChemPlusChem (2019) **84** 307

⇒ *Unusual reactivity of cyclo-(P_5Ph_5): Oxidative addition at a group 6 metal carbonyl and insertion of acetonitrile into a P–P bond*
D.M. Yufanyi, T. Grell, E. Hey-Hawkins / special issue, "Advances in Fundamental and Applied Phosphorus Chemistry", Eur. J. Inorg. Chem. (2019) 1557

⇒ *Rhodium(I) complexes with carborane-substituted P,N ligands: Investigations of electronic structure and dynamic behaviour*
P. Coburger, G. Kahraman, A. Straube, E. Hey-Hawkins / invited contribution to Dalton Transactions themed issue: d Block Chemistry, Dalton Trans. (2019) **48** 9625

⇒ *Spectroscopic and electronic properties of molybdacarborane complexes with non-innocently acting ligands*
B. Schwarze, S. Sobottka, R. Schiewe, B. Sarkar, E. Hey-Hawkins / Chem. Eur. J. (2019) **25** 8550

⇒ *Carboranyl analogues of ketoprofen with cytostatic activity against human melanoma and colon cancer cell lines*
A. Buzharevski, S. Paskas, M. Laube, P. Lönnecke, W. Neumann, B. Murganić, S. Mijatović, D. Maksimović-Ivanić, J. Pietzsch E. Hey-Hawkins / ACS Omega (2019) **4** 8824

⇒ *Accessing the first nido-carborane-substituted diphosphetane: A ligand and synthon for nido-carboranylphosphanes*
P. Coburger, P. Bielytskyi, D. Williamson, E. Rys, A. Kreienbrink, P. Lönnecke, J. Matysik, E. Hey-Hawkins / Chem. Eur. J. (2019) **25** 11456

⇒ *New keys for old locks: Carborane-containing drugs as platforms for mechanism-based therapies*
P. Stockmann, M. Gozzi, R. Kuhnert, M.B. Sárosi, E. Hey-Hawkins / Chem. Soc. Rev. (2019) **48** 3497

⇒ *On the aqueous solution behaviour of C-substituted ruthenacarboranes*
M. Gozzi, B. Schwarze, P. Coburger, E. Hey-Hawkins / invited contribution to the special issue on "Metal Complexes Containing Boron Based Ligands", Inorganics (2019) **7** 91

⇒ *Direct synthesis of an anionic 13-vertex closo-cobaltacarborane cluster*
T.M. Maier, P. Coburger, N.P. van Leest, E. Hey-Hawkins, R. Wolf / Dalton Trans. (2019) **48** 15772

⇒ *Targeting autophagy: Dual mode of action of quinoline-conjugated ruthenacarboranes against glioblastoma cells*
M. Gozzi, B. Murganić, D. Drača, J. Popp, P. Coburger, D. Maksimović-Ivanić, S. Mijatović, E. Hey-Hawkins / ChemMedChem (2019) **14** 2061

⇒ *2,2'-Bipyridine-modified tamoxifen: A versatile vector for molybdacarboranes*
B. Schwarze, S. Jelača, L. Welcke, D. Maksimović-Ivanić, S. Mijatović, E. Hey-Hawkins / ChemMedChem (2019) **14** 2075

⇒ *Facile arene ligand exchange in p-cymene ruthenium(II) complexes of tertiary P chiral ferrocenyl phosphines*
J. Popp, S. Hanf, E. Hey-Hawkins / ACS Omega (2019) **4** 22540

⇒ *Inorganic polymers for potential medicinal applications*
A. Valente, R.L.M. Precker, E. Hey-Hawkins / in: Smart Inorganic Polymers: Synthesis, Properties, and Emerging Applications in Materials and Life Sciences, ed. E. Hey-Hawkins and M. Hissler, ISBN:9783527819140, Wiley-VCH Verlag GmbH & Co. KGaA, (2019) 243

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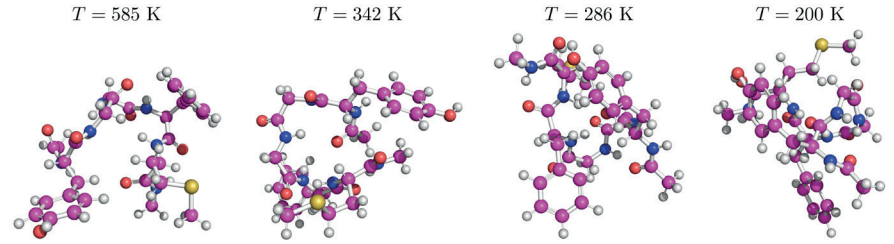
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
M.Sc. Phys. 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 generalised ensemble methods such as multicanonical, parallel-tempering (sometimes also called replica-exchange), and more recently also population annealing 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) 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. While in the previous work only uncorrelated disorder was considered, in the present project also the effects of long-range power-law correlated disorder are investigated. One of the main objectives is to investigate by means of a "breadth-first" chain-growth algorithm to what extent the disorder can be effectively described by a "renormalised" bending stiffness of the macromolecules.

(ii) 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 behaviour can be investigated by analysing related two-time correlation functions. For an Ising spin model with long-range power-law interactions, he has verified for the first time a theoretical prediction for the growth law of the ordered structures and recently also determined their aging characteristics. The main goal of such studies is to elucidate the dynamic scaling laws governing the kinetics of complex physical systems. Along another line he generalised the population annealing method first proposed and applied for MC simulations to molecular dynamics studies and demonstrated its efficiency by simulations of the optiate peptide Met-enkephalin.



⇑ Population annealing molecular dynamics (PAMD) simulations of the opiate peptide Met-enkephalin: Conformation snapshots at different temperatures, decreasing from left to right. The atoms are colour-coded as pink: carbon, white: hydrogen, red: oxygen, blue: nitrogen, and yellow: sulfur.

⇒ *Phase ordering kinetics of the long-range Ising model*
H. Christiansen, S. Majumder, W. Janke / Physical Review E (2019) **99** 011301(R)

⇒ *Accelerating molecular dynamics simulations with population annealing*
H. Christiansen, M. Weigel, W. Janke / Physical Review Letters (2019) **122** 060602

⇒ *Dissipative dynamics of a single polymer in solution: A Lowe-Andersen approach*
S. Majumder, H. Christiansen, W. Janke / Journal of Physics: Conference Series (2019) **1163** 012072

⇒ *Coarsening in the long-range Ising model: Metropolis versus Glauber criterion*
W. Janke, H. Christiansen, S. Majumder / Journal of Physics: Conference Series (2019) **1163** 012002

⇒ *Population annealing molecular dynamics with adaptive temperature steps*
H. Christiansen, M. Weigel, W. Janke / Journal of Physics: Conference Series (2019) **1163** 012074

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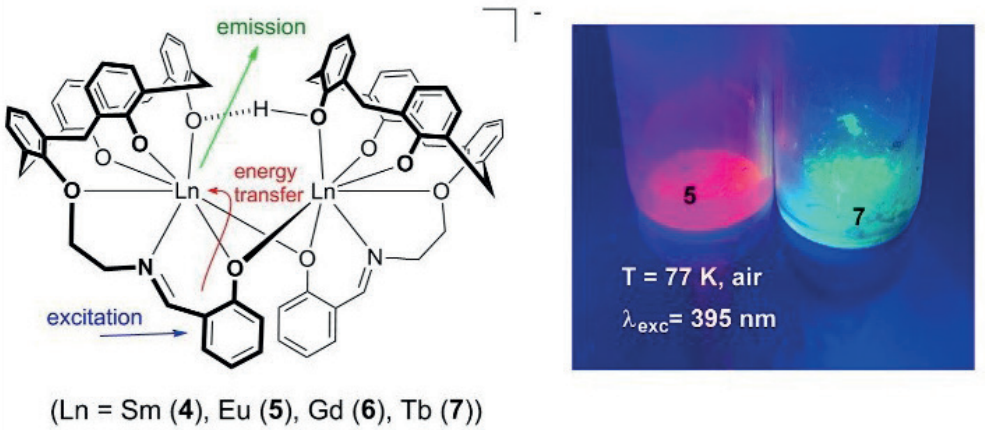
Coordination compounds in supramolecular chemistry and materials chemistry

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

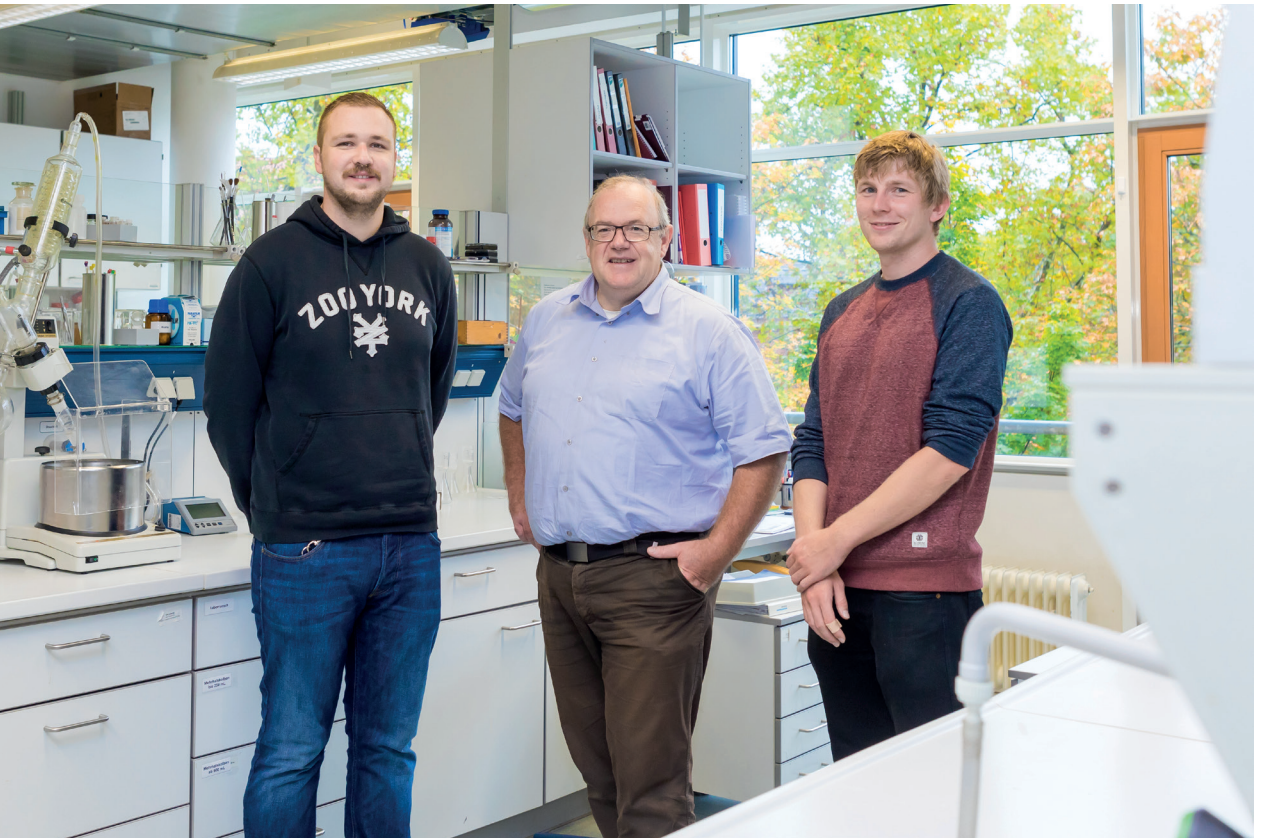
Our research focuses on the coordination chemistry of macrocyclic ligands based on calixarene and thiophenolate units capable of coordinating to a range of d- and f-block metals. The optical and magnetic properties of the corresponding complexes are studied by luminescence spectroscopy, SQUID magnetometry 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.

Two papers can be mentioned. In the first, the synthesis, structures and properties of a new calix[4]arene ligand with an appended salicylaldimine unit (H_4L = 25-[2-((2-methylphenol)imino)ethoxy]-26,27,28-trihydroxy-calix[4]arene) and four lanthanide complexes $(HNEt_3)[Ln_2(HL)(L)]$ (Ln = Sm^{III} (**4**), Eu^{III} (**5**), Gd^{III} (**6**), and Tb^{III} (**7**)) have been reported (Fig. 1). X-ray crystallographic analysis (for **4** and **6**) reveals an isostructural series of dimeric complexes with a triply-bridged $NO_3Ln(\mu\text{-}O)_2(OH\cdots O)LnO_3N$ core and two seven coordinated lanthanide ions. According to UV-vis spectrometric titrations in MeCN and ESI-MS the dimeric nature is maintained in solution. The apparent stability constants range between log K = 5.8 and 6.3. The appended salicylaldimines sensitise Eu^{III} and Tb^{III} emission (λ_{exc} 311 nm) in the solid state or immersed in a polycarbonate glass at 77 K (for **5**, **7**) and at 295 K (for **7**).



(Ln = Sm (**4**), Eu (**5**), Gd (**6**), Tb (**7**))

Fig. 1: Stuctures of dinuclear lanthanide complexes supported by a hybrid Schiff-base calix[4]arene ligand.



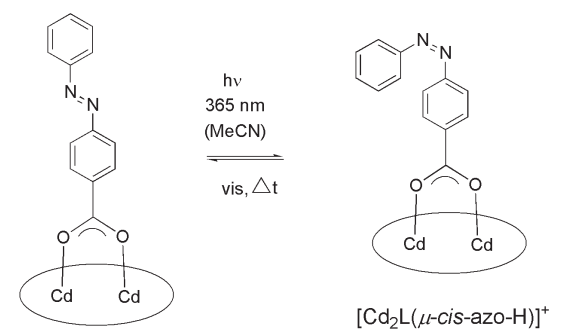


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Fig. 2: *Cis*/*trans* isomerisation process of the bound azo-carboxylato coligand in $[Cd_2L(\mu\text{-azo-H})]ClO_4$ (**1**) in cetonitrile mediated by irradiation with 365 nm UV light. The amino-thiophenolato ligand is shown as an ellipse for clarity.

The synthesis of mixed-ligand complexes of the type $[M_2L(\mu\text{-}L')]^+$, where L represents a 24-membered macrocyclic hexaaza-dithiophenolate ligand, L' is an azobenzene carboxylate coligand, and M = Cd^{II}, Ni^{II} or Zn^{II}, is reported. A series of new complexes were synthesised, and fully characterised. The crystal structures display an isostructural series of compounds with bridging azobenzene carboxylates in the trans form. The paramagnetic Ni complexes reveal a weak ferromagnetic exchange interaction with magnetic exchange coupling constant values between 21 and 23 cm^{-1} ($H = -2JS_1S_2$). Irradiation of the cadmium complex at λ = 365 nm reveals a photoisomerisation of the coligand from the *trans* to the *cis* form.

⇒ *Dinuclear lanthanide complexes supported by a hybrid salicylaldiminato/calix[4]arene-ligand: Synthesis, structure, magnetic and luminescence properties of $(HNEt_3)[Ln_2(HL)(L)]$ ($Ln = Sm^{III}, Eu^{III}, Gd^{III}, Tb^{III}$)*
S. Ullmann, P. Hahn, L. Blömer, A. Mehnert, C. Laube, B. Abel, B. Kersting / Dalton Trans. (2019) **48** 3893

⇒ *Coordination chemistry and photoswitching of dinuclear macrocyclic cadmium-, nickel-, and zinc complexes containing azobenzene carboxylato coligands*
J. Klose, A. Jeremies, T. Severin, D. Fuhrmann, J. Bergmann, J. Griebel, B. Abel, B. Kersting / Beilstein. J. Org. Chem. (2019) **15** 840

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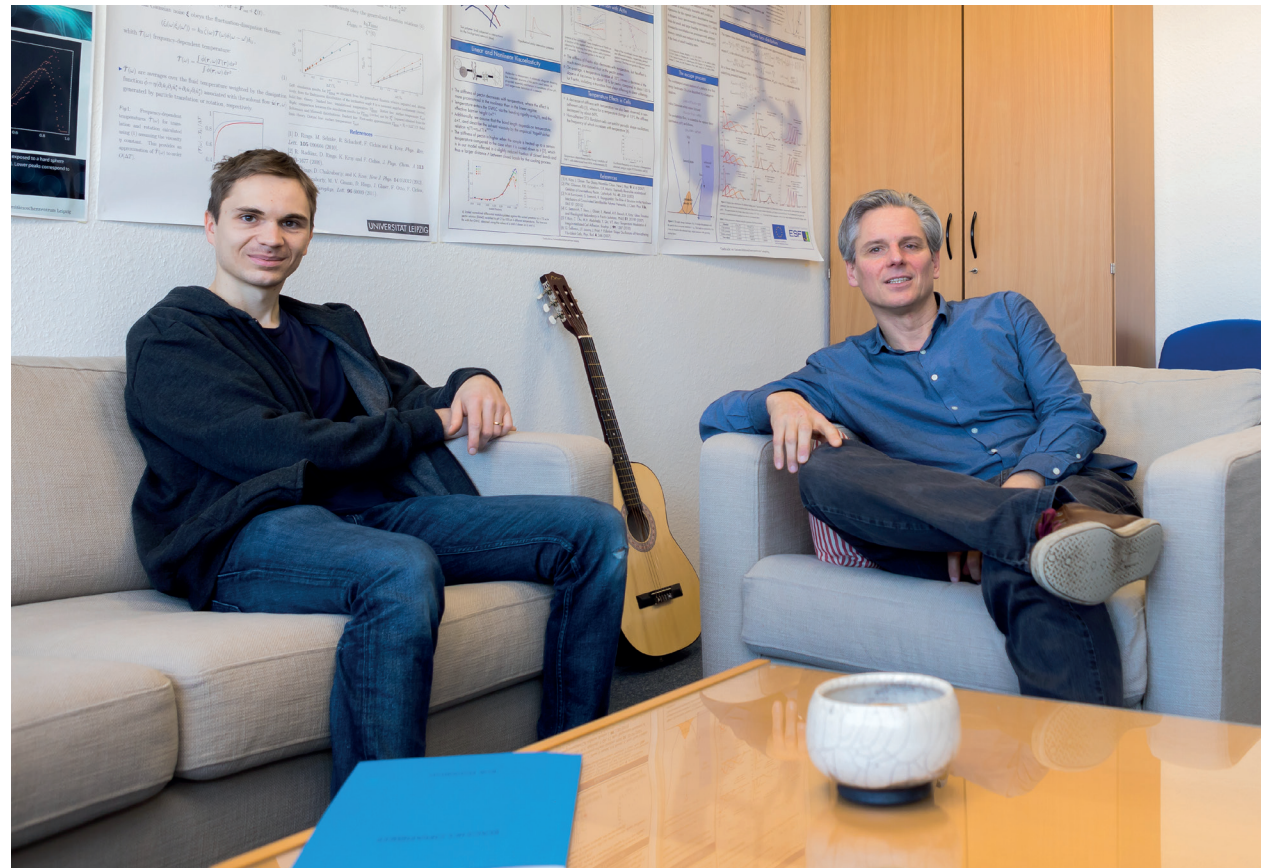
Bottom-up inelastic mechanics of cytoskeletal networks

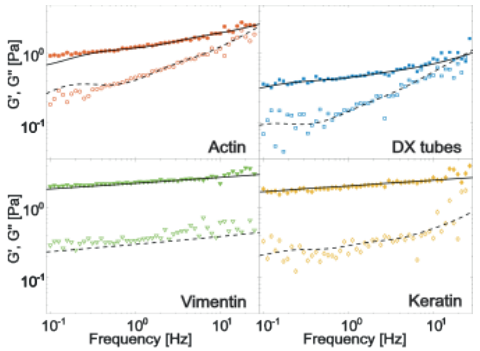
Prof. Dr. Klaus Kroy
M.Sc. Phys. Constantin Huster

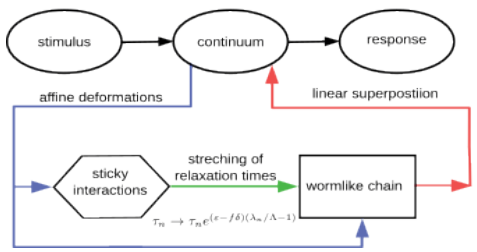
In our modelling approach to the mechanics of cytoskeletal networks we combine two important concepts in bio-mechanics. First, the bottom-up approach to biomechanics that traces back the mechanical response of living matter to its macromolecular constituents. And secondly, the idea that the mechanics 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 bonds. A general framework for inelastic biomechanics 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 analysed and compared. We thereby aim at a unfied minimalistic description of the universal rheological properties of biomaterials in



the linear 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 continuum model employing integration and distribution rules.

Models constructed within this scheme are currently used to interpret and describe experimental data measured in various biophysics labs. For example, we employed our framework to model the linear and non-linear rheology of various biopolymer networks [1]. We provided evidence that the influence of molecular details mediated by inter-filament interactions on the bulk rheology can not be ignored, but can be captured quantitatively by a single model parameter of the glassy wormlike chain model (GWLC). This parameter can be interpreted as a polymer specific stickiness, which provides a consistent interpretation of observations from macrorheological measurements and reptation behaviour.





⇐ Fig. 1. **Top:** Typical storage modulus G' (solid symbols) and loss modulus G'' (open symbols) versus frequency for actin, vimentin, keratin and synthetic DNA nanotube networks. Black lines are the result of fitting with the GWLC model. Although the curves roughly resemble a rubber plateau, they in fact follow weak power laws with power law exponents determined by the polymer specific stickiness. Figure adapted from [1]. **Bottom:** Schematic illustration of the glassy wormlike chain model when viewed in the context of the inelastic bottom-up framework to describe rheological properties of biopolymer networks. For the description of the network a wormlike chain model for the polymers is combined with a trap model for weak reversible bonds representing inter-filament interaction.

⇒ [1] *The role of stickiness in the rheology of semiflexible polymers*
T. Golde, M. Glaser, C. Tutmarc, I. Elbalasy, C. Huster, G. Busteros, D.M. Smith, H. Herrmann, J.A. Käs, J. Schnau / Soft matter (2019) **15** 4865

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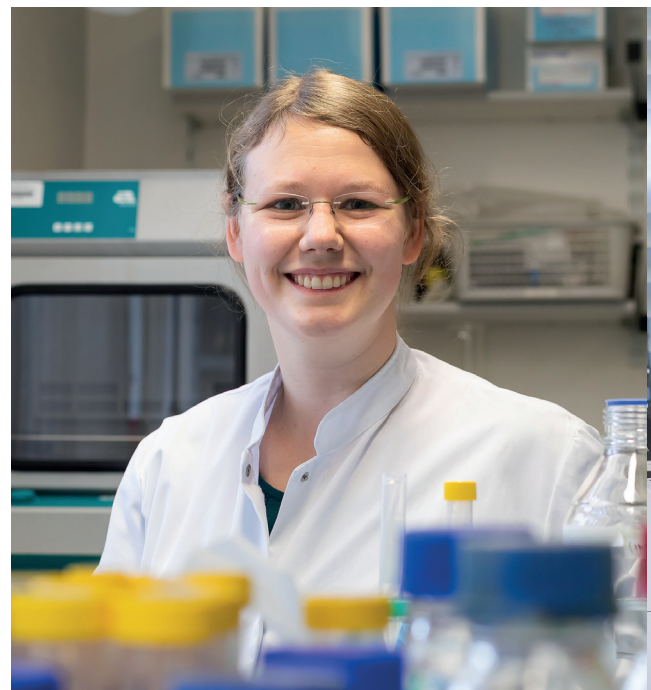
Cellular adhesion on tailored soft and hard materials

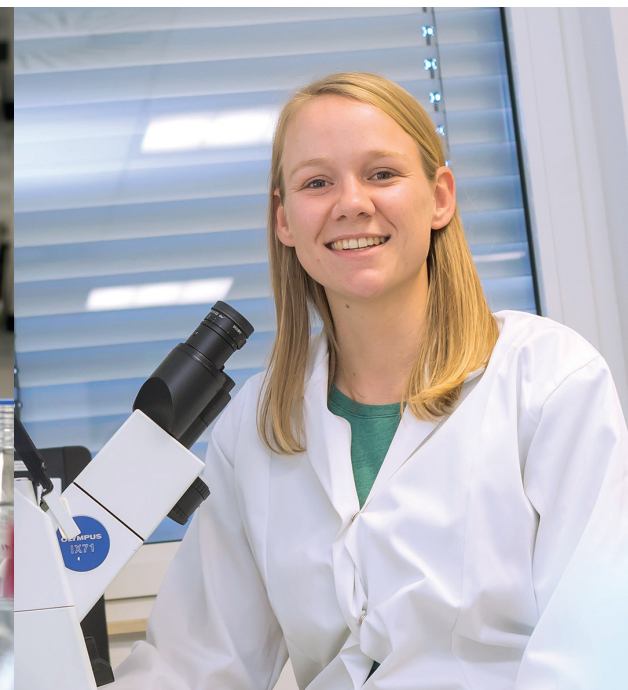
Prof. Dr. Stefan G. Mayr
M.Sc. Phys. Astrid Kupferer, Dr. Stefanie Riedel

Specific adsorption of proteins and an exceptional adhesion of cells facilitate the integration of foreign materials in the human body. In order to prevent rejection reactions, the development and design of new smart soft and hard materials with excellent biocompatibility and tailored surface characteristics is highly relevant. The aim of the division Surface Physics is to provide such enhanced materials with outstanding properties and to investigate the interactions of materials, proteins and cells.

On one hand, we focus on soft materials mimicking the extracellular matrix (ECM). Gelatin and collagen represent such polymers. They are derived from mammalian tissues, and, hence, provide an eminent biocompatibility. In this way, they serve as an attractive basis to study cell invasion, diseases or new drugs. Using electron irradiation, the mechanical properties of these hydrogels can be adjusted without the need of chemical crosslinkers.

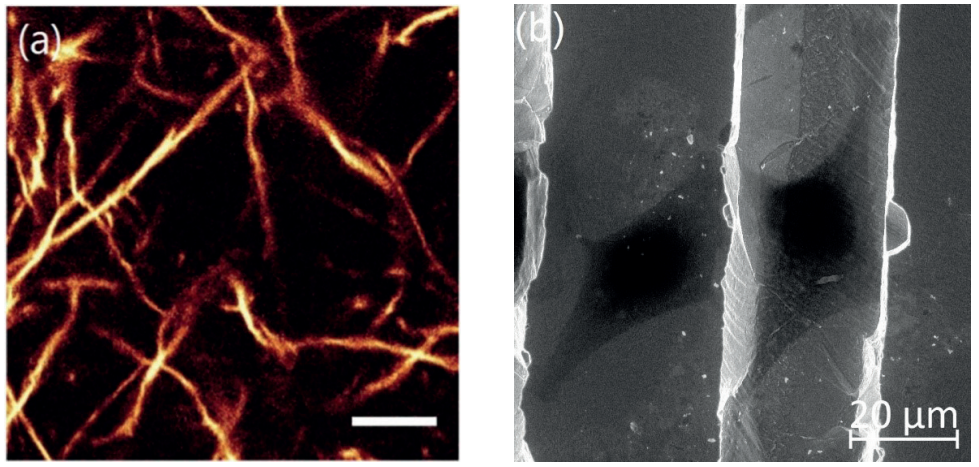
Riedel and Hietschold et al. provide a comprehensive overview on the design and characteristics of electron-irradiated collagen hydrogels.[1] In detail, the modification of the network structure, the stiffness as well as viability of cells was investi-





gated and showed a prospective use as ECM model system. In addition, Tadsen et al. describe the option of surface patterning for gelatin hydrogels.[2] Here, a micro-moulding technique and subsequent electron irradiation was applied to enhance cell adhesion and to induce contact guidance.

On the other hand, hard materials as metals and metal oxides are commonly used for protheses and orthopedic implants. For successful integration into the human body, a suitable microstructure is required to promote cell adhesion and bone formation. Weidt, Mayr and Zink show, that cellular contact guidance on microstructured titanium specifically depends on protein adsorption.[3] In fact, fibronectin predominantly adsorbs to the edges of the ridges of grooved patterns and mediates early cell adhesion.



⇑ (a) Confocal laser scanning microscopy image of a collagen network, from [1]. (b) NIH 3T3 fibroblasts on fibronectin-coated microstructured titanium, imaged with environmental scanning electron microscopy, from [2].

⇒ [1] *Design of biomimetic collagen matrices by reagent-free electron beam induced crosslinking: Structure-property relationships and cellular response*
S. Riedel, P. Hietschold, K. Krömmelbein, T. Kunschmann, R. Konieczny, W. Knolle, C. Mierke, M. Zink, S. G. Mayr / Materials & Design (2019) **168** 107606

⇒ [2] *Contact guidance by microstructured gelatin hydrogels for prospective tissue engineering applications*
M. Tadsen, R. P. Friedrich, S. Riedel, C. Alexiou, S.G. Mayr / Appl. Mat. & Interf. (2019) **11** 7450

⇒ [3] *Influence of topological cues on fibronectin adsorption and contact guidance of fibroblasts on micro-grooved titanium*
A. Weidt, S. G. Mayr, M. Zink / ACS Applied Bio Materials (2019) **2** 1066

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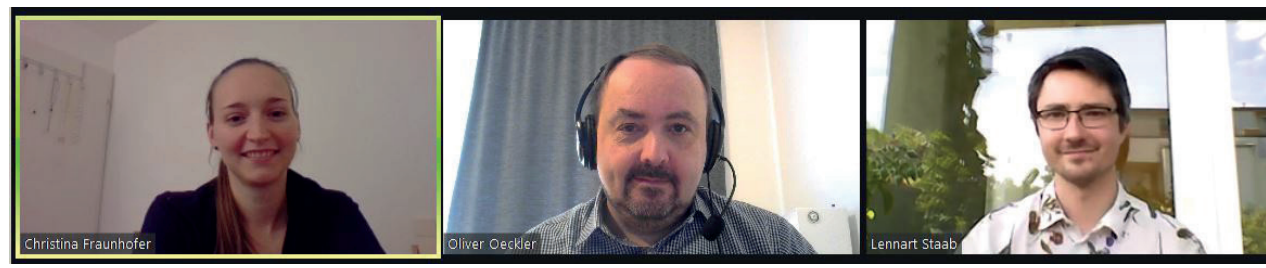
Stability of thermoelectric materials with mobile atoms under application oriented conditions

Prof. Dr. Oliver Oeckler
M.Sc. Chem. Christina Fraunhofer, M.Sc. Chem. Lennart Staab

Thermoelectrics make use of the voltage induced by the Seebeck effect in materials under a temperature gradient. Thermoelectric materials need to have high Seebeck coefficients but also high electrical and low thermal conductivities. These transport properties are strongly interrelated, thus, their design is a continuing challenge.

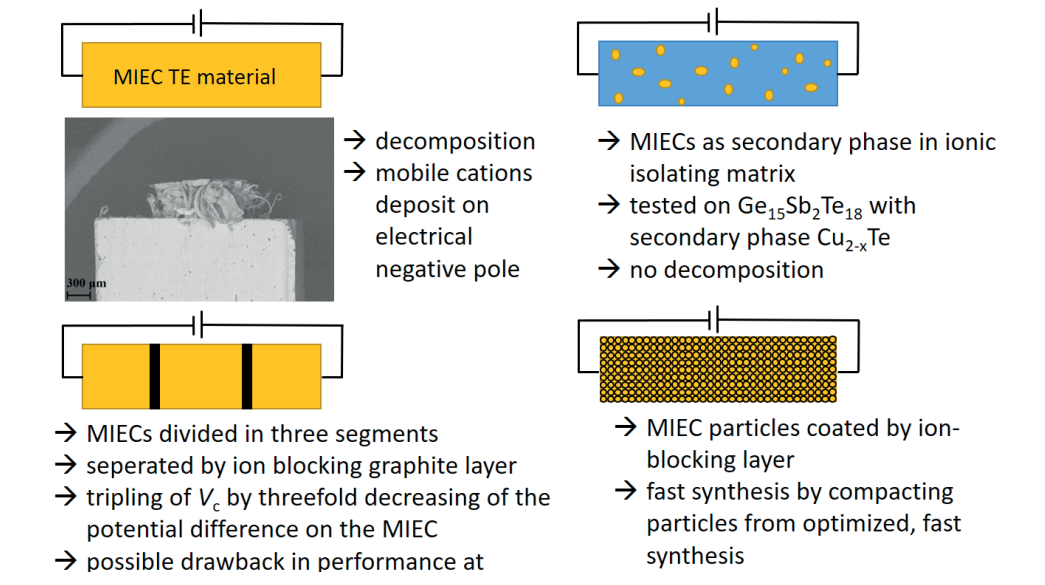
Thermoelectric materials with mixed ionic and electronic conduction (MIECs) have recently been studied intensely due to their high zT values and the abundance and low toxicity of the elements they contain. However, they often suffer from decomposition under electrical currents and temperature gradients, which makes them unsuitable for long-term application. Adding additional phases in composite materials may mitigate such problems. For instance, experiments with composites containing Cu_2Se and carbon nanoparticles have shown that metal deposition is inhibited and that zT values increase. Decomposition may even be suppressed on a macroscopic level by introducing an electronic conductor that does not allow ion migration between segments of bulk material.

To ensure low cost, easy reproducibility and robustness, MIECs can be milled to microparticles, coated with ion-insulating materials such as graphite or other layered compounds and pressed to pellets as a simple way of producing composites without the need for nanoparticle synthesis. The stability and properties of such composites have been studied under current flow in various temperature gradients. Different coating processes, grain sizes and thermoelectric components have been tested; the resulting samples are studied by means of scanning and high-resolution transmission electron microscopy. The electrical and thermal transport proper-



ties are compared to those of the pristine materials to evaluate the improvement achieved.

In addition, several copper iron chalcogenides and copper bismuth chalcogenides turned out to be cheap and eco-friendly alternatives to currently employed thermoelectric materials. They exhibit complex crystal structures that were investigated by resonant X-ray diffraction and electron microscopy. Their properties can be enhanced by diverse possibilities of substitution with transition metals.



⇑ Scheme showing the concepts pursued in order to suppress atom migration in MIEC materials.

⇒ *Cobalt germanide precipitates indirectly improve the properties of thermoelectric germanium antimony tellurides*
D. Souchay, S. Schwarzmüller, H. Becker, S. Kante, G.J. Snyder, A. Leineweber, O. Oeckler / J. Mater. Chem. C (2019) **7** 11419

⇒ *Layered manganese bismuth tellurides with $GeBi_4Te_7$- and $GeBi_6Te_{10}$-type structures: towards multifunctional materials*
D. Souchay, M. Nentwig, D. Günther, S. Keilholz, J. de Boor, A. Zeugner, A. Isaeva, M. Ruck, A.U.B. Wolter, B. Büchner, O. Oeckler / J. Mater. Chem. C (2019) **7** 9939

⇒ *Structures and transport properties of metastable solid solutions $(NaSbTe_2)_{1-x}(GeTe)_x$*
S. Schwarzmüller, F. Yang, O. Oeckler / J. Alloys Compd. (2019) **806** 774

⇒ *The sodium antimony telluridogermanate(III) $Na_9Sb[Ge_2Te_6]_2$*
S. Schwarzmüller, V. H.-T. Tran, F. Yang, O. Oeckler / Z. Anorg. Allg. Chem. (2019) **645** 1037

⇒ *Chemical aspects of the candidate antiferromagnetic topological insulator $MnBi_2Te_4$*
A. Zeugner, F. Nietschke, A.U.B. Wolter, S. Gaß, R.C. Vidal, T.R.F. Peixoto, D. Pohl, C. Damm, A. Lubk, R. Hentrich, S.K. Moser, C. Fornari, C.H. Min, S. Schatz, K. Kißner, M. Ünzelmann, M. Kaiser, F. Scaravaggi, B. Rellinghaus, K. Nielsch, C. Heß, B. Büchner, F. Reinert, H. Bentmann, O. Oeckler, T. Doert, M. Ruck, A. Isaeva / Chem. Mater. (2019) **31** 2795

⇒ *$K_2Hg_2Te_3$: Straightforward and large-scale mercury-flux synthesis of a small-band-gap photoconducting material*
G. Thiele, P. Bron, S. Lippert, F. Nietschke, O. Oeckler, M. Koch, B. Roling, S. Dehnen / Inorg. Chem. (2019) **58** 4052

⇒ *$Cu_{9.1}Te_4Cl_3$: A thermoelectric compound with low thermal and high electrical conductivity*
A. Vogel, T. Miller, C. Hoch, M. Jakob, O. Oeckler, T. Nilges / Inorg. Chem. (2019) **58** 6222

⇒ *Low thermal conductivity in thermoelectric oxide-based multiphase composites*
M. Wolf, K. Menekse, A. Mundstock, R. Hinterding, F. Nietschke, O. Oeckler, A. Feldhoff / J. Electron. Mater. (2019) **48** 7551

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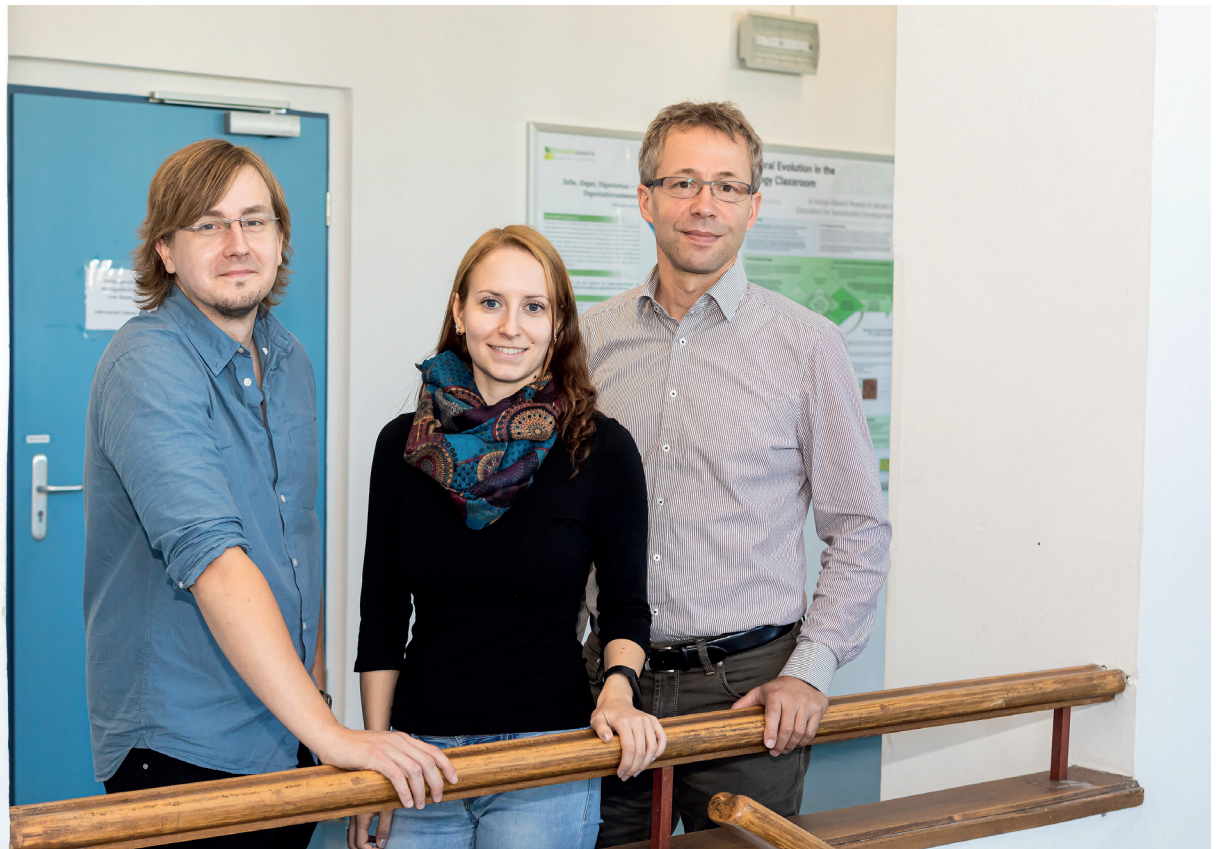
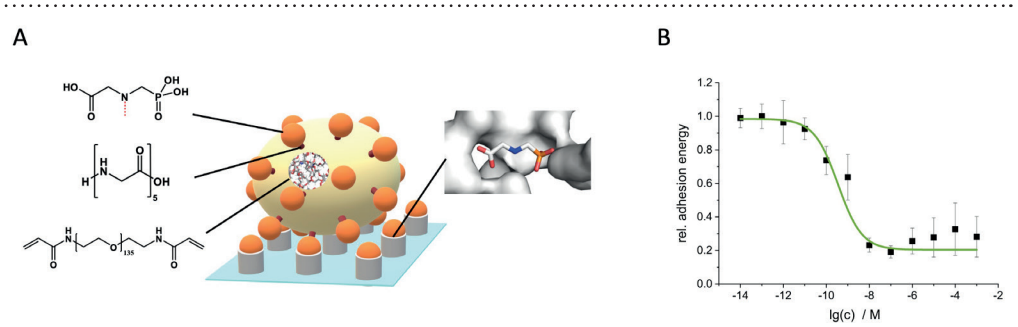
Soft colloidal probes as biomimetic sensors of low molecular weight analytes in aqueous solutions

Prof. Dr. Tilo Pompe
M.Sc. Chem. David Rettke, M.Sc. Chem. Veronika Riedl

One research area of our group is dedicated to 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 functionalised hydrogel microparticles and nanoparticles.

D. Rettke and V. Riedl specifically investigate biosensors to detect low molecular weight analytes in aqueous environments i.e. anthropogenic molecules like pesticides, hormones and antibiotics. The biomimetic sensing system utilises 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 functionalisation of SCP with biospecific ligands they are capable of interacting with capture binding sites presented on the 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 even in a pM range are developed. We already demonstrated the success of this biomimetic principle to detect the controversially discussed herbicide glyphosate using site-specific functionalisation of the SCP with the target molecule glyphosate and of the chip surface with hydrophobin fusion proteins of the natural glyphosate target enzyme 5-enolpyruvyl-shikimate-3-phosphate synthase. Furthermore, the detection principle is currently used to develop a sulfonamide antibiotics biosensor using dihydropteroate synthase as the capture site on the chip surface. Other options are investigated, too, in order to establish a platform technology to be commercialised.





⇑ **Picomolar sensitivity of the glyphosate biosensor. (A)** Scheme of the biosensor setup with site-specific coupling of glyphosate to the (polyethylene glycol)-SCP. **(B)** Picomolar sensitivity of the sensor as shown by the adhesion of functionalised SCP and chip surfaces in dependence of glyphosate concentration in aqueous solution.

⇒ *Radial profile detection of multiple spherical particles in contact with interacting surfaces*
J. Waschke, T. Pompe, D. Rettke, S. Schmidt, M. Hlawitschka / PLoS One (2019) **14** e0214815

⇒ *Surface functionalisation by hydrophobin-EPSPS fusion protein allows for the fast and simple detection of glyphosate*
J. Doring, D. Rettke, G. Rodel, T. Pompe, K. Ostermann / Biosensors-Basel (2019) **9** 104

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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).

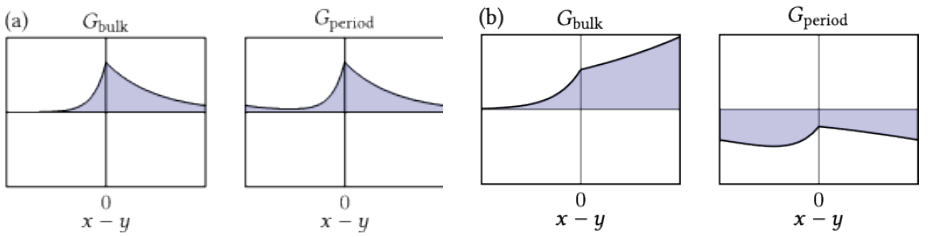
Topological insulators are an example of a topological quantum phase. There, the non-triviality manifests in the following way: A sample of such a material is insulating in the bulk, but due to quantum effects, perfectly conducting surface states emerge at the sample boundary. Moreover, these surface 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 realised 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.

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



⇑ 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.

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($iksx$) where the complex momentum ks 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.

⇒ *Bulk-boundary correspondence for non-Hermitian Hamiltonians via Green functions*
H.-G. Zirnstein, G. Refael, B. Rosenow / arXiv (2019) 1901.11241

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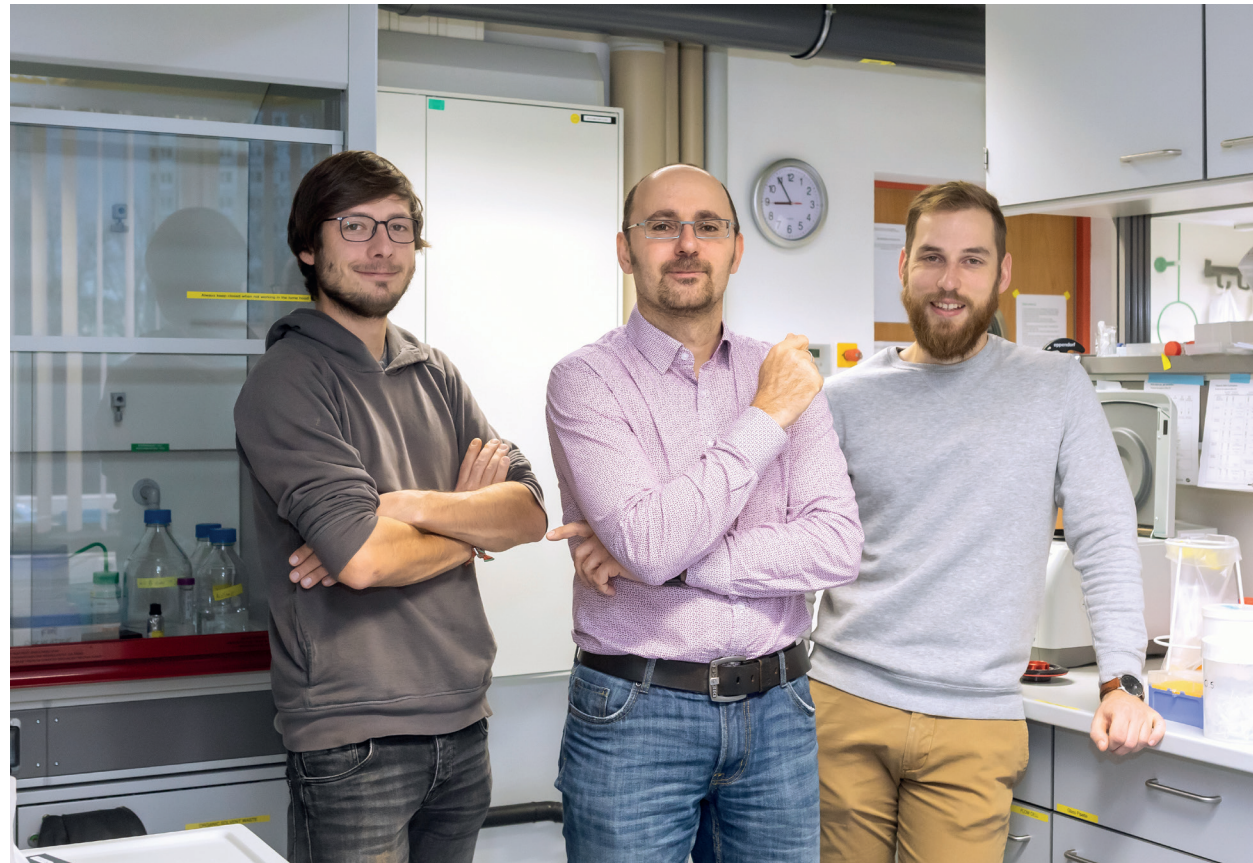
Modelling DNA-strand displacement reactions in the presence of base-pair mismatches

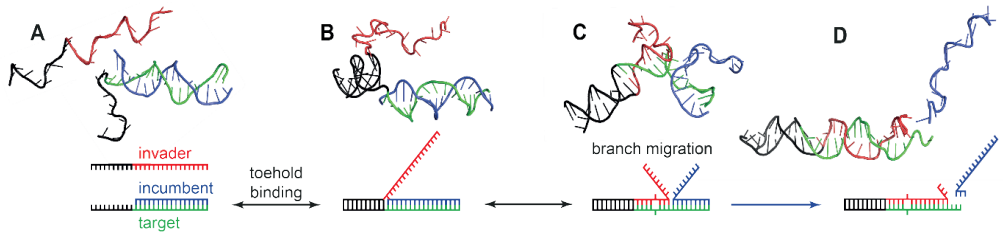
Prof. Dr. Ralf Seidel
M.Sc. Phys. Florian Scheffler, M.Sc. Phys. Patrick Irmisch

Toehold-mediated strand displacement is the most abundantly used method to achieve dynamic switching in DNA-based nanotechnology. An "invader" strand binds to the "toehold" overhang of a target strand and replaces a target-bound "incumbent" strand. Here, the complementarity of the invader to the single-stranded toehold provides the free energy bias of the reaction. Despite the widespread use of strand displacement reactions for realizing dynamic DNA nanostructures, variants on the basic motif have not been completely characterised. We introduced a simple thermodynamic model, which is capable of quantitatively describing the kinetics



of strand displacement reactions in the presence of mismatches, using a minimal set of parameters. Our model should provide a helpful tool for the rational design of strand-displacement reaction networks.[1]

Beyond strand displacement systems based on purified nucleic acids, our modeling also provides a useful reference for more complex systems such as CRISPR-Cas effector complexes. These enzymes recognise targets similarly to toehold mediated strand displacement reactions and gained an enormously growing interest in genome engineering. Developing rational, mechanism-based target predictors may help to avoid off targeting by these enzymes in biotechnological and medical applications.



⇑ Scheme of the toehold-mediated strand displacement reaction. (**A**) Start configuration. An incumbent strand (shown in blue) is hybridised to a target DNA strand (shown in black/green) leaving a ssDNA overhang called toehold (black). (**B**) Toehold binding. An invader strand that is complementary to the target binds first to the toehold. (**C**) Branch migration. The invader (red part) replaces the incumbent strand sequentially but reversibly in single base pair steps. It uses the fraying of the incumbent bases at the fork to hybridise with transiently unpaired target strand bases (green part of target). Mismatches between invader and target introduce an energetic penalty. (**D**) Incumbent dissociation. Incumbent dissociation that completes the reaction, occurs when only few incumbent–target base pairs are left.

⇒ [1] *Modeling DNA-strand displacement reactions in the presence of base-pair mismatches*
P. Irmisch, T.E. Ouldridge, R. Seidel / J. Am. Chem. Soc. (2020) **142** 11451

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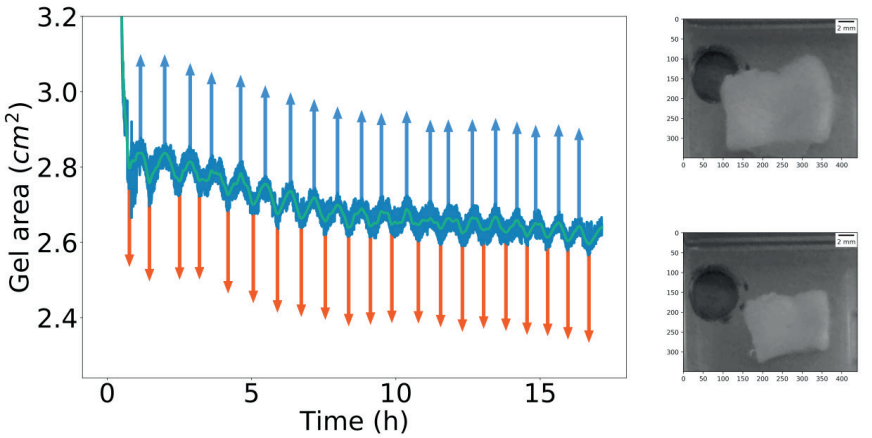
Cellular adhesion, proliferation and migration on artificial biomaterials

Prof. Dr. Mareike Zink
M.Sc. Chem. Alice Abend, M.Sc. Chem. Nils Wilharm

The interaction of cells with artificial biomaterials in terms of adhesion, proliferation, and network organisation is crucial for the performance and application of biomaterials. We investigate the behaviour of human neuronal cells on various electrode materials such as gold, indium tin oxide, and titanium nitride with and without nanostructured surface. To this end, we implemented computational methods to analyze the spatial organisation of neuronal cells grown on the electrode materials by applying a K-Means clustering algorithm combined with a radially averaged autocorrelation function to fluorescent images of cell networks. Recent experimental results indicate that cell clustering behaviour and pattern formation are characteristic for each substrate type.

Additionally, in collaboration with Prof. Dr. Stefan Mayr we study elastin/collagen gels as a novel biocompatible reversible thermal actuator in which the polymers were crosslinked using electron irradiation. This non-toxic technique couples amino acids via OH-radicals which are generated from water splitting. We obtained that the temperature of transition (37°C – 42°C) is inversely related to the irradiation dose. Furthermore, circular dichroism spectroscopy in collaboration with Prof. Dr. Annette Beck-Sickinger revealed that the irradiation process increases the amount of random coil structures in elastin and collagen on the expense of helical structures. Here, the elastin system drives the contraction process since only the elastin protein structure reacts to the temperature increase as opposed to collagen. This switchable and highly tunable gels offer great perspectives for biomedical applications, ranging from drug delivery systems to artificial tissues.



⇑ Heat induced multicycle switching of an electron irradiated compound gel made from elastin and collagen between 30°C and 42°C.

⇒ *Energetic electron assisted synthesis of highly tunable temperature-responsive collagen/elastin gels for cyclic actuation: macroscopic switching and molecular origins*
N. Wilharm, T. Fischer, F. Ott, R. Konieczny, M. Zink, A.G. Beck-Sickinger, S.G. Mayr / Scientific Reports (2019) **9** 12363

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Experiences

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

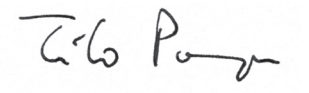
Prof. Dr. Tilo Pompe

The year 2019 was a very important and interesting year for the Graduate School BuildMoNa. In 2019 BuildMoNa successfully finished the transition process into the new concept of the Universität Leipzig. Large graduate schools in different research areas are now receiving permanent central support and are fully integrated within the Research Academy Leipzig. During the transition process, the rearrangements of the structure of BuildMoNa caused slight organisational problems and strong efforts of involved PIs and doctoral candidates.

A new board of PIs, new spokespersons, and a new postdoc assembly had to be set up. The permanent personal support of the Research Academy Leipzig had to be filled. The negotiations with Research Academy Leipzig and rectorate of the Universität Leipzig led to a reliable objective agreement with evaluation every 5 years. At the end of 2019, the new structure is now fully established and BuildMoNa is the first graduate school of the Universität Leipzig running in the new formal setting. By that BuildMoNa provided also a blueprint for the establishment of other graduate schools of the Universität Leipzig.

Now the Graduate School BuildMoNa continues to run its successful programme including the established set of modules and workshops and the annual BuildMoNa conference. With its focus in chemical, biochemical and physical sciences it integrates many important research areas of the strategic fields of the Universität Leipzig. This interdisciplinary character and the well-balanced module programme provide a good support for doctoral candidates to interact with neighbouring research fields, broadening their scientific expertise and extending their soft skills in scientific work. I feel that doctoral candidates benefit from this structure a lot. E.g. it allows them to learn to organise and perform on scientific conference, like the annual BuildMoNa conference, and it further supports scientific exchange at international conferences and internships by travel grants.

From my experience, the setting of BuildMoNa provides strong impulses for the education of the doctoral candidates and experiences for their later career in academia and industry, and additionally supports the involved doctoral candidates and PIs in their research.



Prof. Dr. Tilo Pompe

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

M.Sc. Phys. Florian Scheffler

The graduate school BuildMoNa offers an interdisciplinary training for doctoral candidates in the fields of physics, biology, chemistry, and biochemistry to obtain additional skills besides their daily lab work. The interdisciplinary education programme, offered by the graduate school, therefore provides a good opportunity to acquire professional skills useful for the lab work and soft skills such as project management, scientific writing, and teaching that are useful even beyond the academic career. Make use of these training programme requires additional time but sometimes also provides a new interdisciplinary point of view on the own research.

Next to the educational part the participation in these modules helps the doctoral candidates to get in touch with people from other fields of research. The steady exchange between young researchers from different departments is one of the main objectives of BuildMoNa. In addition to the scientific courses provided by the graduate school, the annual BuildMoNa conference offers a great opportunity to get in touch with other researchers. At this two day conference invited speakers, as well as the doctoral candidates of BuildMoNa, provide an overview over their field of research and often leads to vivid discussion about the topic.

Besides the provided professional training opportunities the graduate school BuildMoNa supports the doctoral candidates, e.g. by travel allowances to enable and encourage the participation in international conferences, workshops, and summer schools.

Even though the participation in BuildMoNa is an additional expenditure of time besides the daily lab work, it provides a great opportunity to acquire additional professional skills during the doctoral programme. The structured doctoral programme provided by BuildMoNa therefore helps the doctoral candidates to better prepare for a career within or outside the academic world.

M.Sc. Phys. Florian Scheffler

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 further graduate programmes of the Graduate Centres "Life Sciences" and "Mathematics, Computer Science and Natural Sciences" as well as 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

Chemical biology and biophysics of cancer (2019-A2)

25 - 27 September 2019,
written report, 2 credit points, yearly recurrence with modification, 14 participants

This module discussed how physics, chemistry, biochemistry, molecular and materials science can provide a new perspective on 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.

Responsible Scientist:
Prof. Dr. J. Käs

Lecturers:
J. Käs, Leipzig University, Germany; S. Köster, Georg-August University Göttingen, Germany; J. Guck, TU Dresden & MPI for Physics of Light, Erlangen, Germany; H.-G. Döbereiner, University of Bremen, Germany; A. Bernheim, Ben Gurion University, Israel; P. Janmey, University of Pennsylvania, USA; A. Janshoff, Georg-August University Göttingen, Germany; T. Büscher, Forschungszentrum Jülich GmbH; D. Bi, Northeastern University, USA; F. Jülicher, MPI for Physics of Complex Systems Dresden, Germany; A. Taubenberger, TU Dresden, Germany; T. Betz, University of Münster, Germany; A. Stylianou, University of Cyprus, Cyprus; K. Tanner, National Cancer Institute, USA; J. Ivaska, University of Turku, Finland; S. Gerecht, Johns Hopkins University, USA; C. Fischbach-Teschl, Cornell University, USA; R. Merkel, Forschungszentrum Jülich GmbH; T. Langenhan, Leipzig University, Germany; E. Fischer-Friedrich, TU Dresden, Germany; L. Spoerri, The University of Queensland, Brisbane, Australia; D. Discher, Syracuse University, USA; S. Kallendrusch, Leipzig University, Germany; I. Sack, Charité Berlin, Germany; J. Kayser, University of California, Berkeley, USA; K. Rottner, Technical University Braunschweig, Germany; X. Trepat, IBEC, Barcelona, Spain; I. Pajic-Lijakovic, University of Belgrade, Serbia; P. Katira, San Diego State University, San Diego, USA; G. Nader, Institut Curié, France; N. Gov, Weizmann Institute of Science, Israel; F. Lautenschläger, Saarland University Saarbrücken, Germany.

Contents:
⇒ Biomechanics (biopolymers, networks, rheology, cytoskeleton, cell shape)
⇒ Tumour progression (tumour growth and homeostasis, uncontrolled proliferation, invasion and metastasis, tumour induced alterations of the stroma, vascular system and immune system, role of chemical cues as well as active and passive forces in triggering cell division and apoptosis)
⇒ Diagnostics and screening (cytobrushes, imaging [CT, MRI], tumour markers, histology, tumour staging)
⇒ Therapy (surgery, radiation, chemotherapy [antineoplastic drugs, cytostatic molecules, protein kinase inhibitors])
⇒ Targeted tumour therapy (specific and unspecific shuttles, specific expression of cell surface proteins, internalisation of biomolecules into tumour cells, linkers for controlled release, etc.)
⇒ Personalised medicine and better tumour staging (single cell analysis, high throughput and content, genetic networks, tumour specificmtracers and their application by PET-imaging or fMRI-scanning, tumour cell biomechanics and adhesion)
⇒ Models of tumour growth (finite element-based models, differential adhesion hypothesis, glass-like behaviour)
⇒ Relapse (selective pressure and resistant tumour cells, dormant cancer cells, cancer stem cells)
⇒ Forces, motion, adhesion (cell motility, assembly, molecular motors)

Methods:
⇒ Hybrid molecules as novel or optimised drugs (advanced synthetic methods, combining organic, inorganic and biochemical approaches)
⇒ Imaging (CT, MRI, PET, fMRI)
⇒ Active and passive cell mechanics and adhesion (AFM-based cell rheology, cellhesion, magnetic bead rheology, optical stretcher)
⇒ Tumour cell migration (wound healing, migration through collagen gels, traction force microscopy)
⇒ Vital imaging of tumour cells

Chemometrics applied to spectroscopic data (2019-B6)

15 / 16 October 2019,
written exam, 2 credit points, 16 participants

This module aimed to develop an understanding of the application of chemometrics to spectroscopic data analysis, to gain a basic overview of how to process spectral data for multivariate analysis as well as to learn how to apply Principal Component Analysis, Partial Least Squares Discriminant Analysis and Partial Least Squares Regression to spectroscopic data using The Unscrambler.

Responsible Scientists:
Dr. B. Wood, Dr. P. Heraud, Monash, Australia

Contents:
⇒ Understand that the Universe is multivariate and applications of multivariate statistics
⇒ Explore types of data used in chemometrics Near-IR, Raman and IR, qualitative
⇒ Distinguish between classification (PCA) and regression modelling
⇒ Explain the difference between objects, variables including continuous and discrete variables
⇒ Describe ordinal, binary and category, dummy variables
⇒ Input data into Unscrambler
⇒ Plot line plots, bar plots, matrix plots
⇒ Identify noise and variance in spectra
⇒ Explain PCA and how it is used for data analysis
⇒ Understand and interpret scores and loadings plots
⇒ Recognise the difference between calibration, validation and test set
⇒ Explain “Explained Variance”
⇒ Define PCs, scores, loadings, residuals, variance and the PCA model equation
⇒ Know the pre-processing approaches for spectral data (baseline correction, derivatives, reduce average, mean centring, smoothing, normalisation, standard normal variate, Multiplicative scatter correction)
⇒ Be able to detect outliers
⇒ Partial Least Squares Discriminant Analysis
⇒ Partial Least Squares Regression Analysis

Smart molecules – Photochemistry and photophysics of metal complexes (2019-T1)

19 / 20 September 2019,
written report, 2 credit points, bi-yearly recurrence with modification, 12 participants

This module focused on current activities and research trends associated with the photophysical and photochemical properties of metal complexes ranging from synthesis through spectroscopy to applications.

Responsible Scientists:
Prof. Dr. K. Zeitler, Prof. Dr. B. Kersting

Lecturers:
L. DeCola, Strasbourg, France; D. Gryko, Warsaw, Poland; K. Heinze, Mainz, Germany; C. Hess, München, Germany; C. Piguet, Geneva, Switzerland; O. Reiser, Regensburg, Germany; B. Sarkar, Berlin, Germany; S. Schneider, Göttingen, Germany; A. Stefan, Dortmund, Germany; C. A. Strassert, Münster, Germany; S. Tunik, St. Petersburg, Russia; B. Weber, Bayreuth, Germany; O. Wenger, Basel, Switzerland; E. Zysman-Colman, St. Andrews, UK.

Contents:
⇒ Photochemistry: photoinduced catalysis, photochemistry, photocatalysis of earth-abundant metal complexes (incl. with $3d^6$ and $4d^6$ configuration), visible-light photoredox catalysis
⇒ Photophysics: luminescence properties and photophysics of earth-abundant metals, upconversion using linear optics in molecular metal complexes, ultrafast T_1 and TADF emitters, coordination compounds as fluorophores, sonophores and sensitisers of ROS, luminescent transition metal complexes in functional bioimaging, luminescence switching, strategies for tuning emission properties

From molecules to materials – Quantum mechanics at work: Quantum systems for applications (2019-T4)

10 / 11 October 2019,
poster presentation and discussion, 2 credit points, bi-yearly recurrence with modification, 7 participants

This module linked molecular sciences and materials science, teached how materials with optimised photocatalytic activity and adjustable magnetic, electronic, or optical properties are obtained from molecules, and provided an understanding of the properties and applications of these materials.

Responsible Scientists:
Prof. Dr. J. Meijer

Lecturers:
Prof. Kirsten Zeitler, Universität Leipzig; Dr. Roland Marschall, Justus-Liebig-University Giessen; Prof. Hartmut Herrmann, Universität Leipzig und IfT; Prof. Jennifer Strunk, Likat, Rostock; Prof. Detlef Bahnemann, Universität Hannover; Prof. Michael Wark, Universität Oldenburg; Prof. Christian Wilhelm, Universität Leipzig; Prof. Andreas Schmid, Universität Leipzig und UFZ

Contents:
⇒ Production and application of Quantum systems in solids: requirements to produce single qubits, methods and challenges of ion beam technology, an introduction to quantum optics, an introduction to quantum technology, quantum computers and quantum sensors
⇒ Topics: Atom-Light-WW, Laser, Photostatistics, Antbunching, Fockstate, Coherentstate, Squeezed light, Atom in cavities, Entangled states, Quantum cryptography Qubits, basics of computers, quantum computers, quantum error correction, adiabatic QC (D-WAVE), quantum sensors, practical realisation

Methods:
⇒ Confocal microscope, Quantum optics techniques: ODMR, HTB, single photons, single ion beam implantation, doping, annealing methods, single molecule spectroscopy, single molecule NMR, hyperpolarisation

Scientific symposium

Transparent conductive oxides – Fundamentals and applications (2019-A3)

24 / 25 September 2019
written report, 2 credit points, bi-yearly recurrence with modification, 14 participants

The BuildMoNa minisymposium was organised by the research group of Prof. Dr. M. Grundmann and dealt with the material class of transparent conductive materials, that has been discovered 1907 by Karl W. Baedeker in Leipzig. The module focused on modern transparent functional materials, from fabrication through material physics to applications. The speakers were:

⇒ P. Barquinha, Universidade Nova de Lisboa, Portugal
Towards autonomous flexible electronic systems with zinc-tin oxide thin films and nanostructures

⇒ S. B. Anooz, Leibniz Institute for Crystal Growth, Berlin, Germany
Optimisation of β-Ga_2O_3 film growth on miscut (100) β-Ga_2O_3 substrates by MOVPE

⇒ P. Mazzolini, Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany
Control over In-incorporation for monoclinic $(In_xGa_{1-x})_2O_3$ alloys on β-Ga_2O_3 substrates via molecular beam epitaxy

⇒ M. Kneiß, Universität Leipzig, Germany
Epitaxial stabilisation of κ-$(In_xGa_{1-x})_2O_3$ and κ-$(Al_xGa_{1-x})_2O_3$ layers up to $x_{In} \leq 0.28$ and $x_{Al} \leq 0.65$ by tin-assisted VCCS-PLD

⇒ F. Gunkel, FZ Jülich, Germany
Thermodynamic control of ionic-electronic structure in oxide thin films, heterostructures, and TCOs

⇒ M. Budde, Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany
Application potential of epitaxial, meta-stable p-type SnO: Temperature stability and pn-junction with Ga_2O_3

⇒ M. Himmerlich, CERN, Geneva, Switzerland
What to learn from surface spectroscopy about oxide layer functionality in electronic devices and particle accelerator components?

⇒ L. Grieger, Malvern Panalytical B.V., Almelo, The Netherlands
To swim or drown in XRD data - Measurement and Evaluation of 200 reciprocal space maps

⇒ G. Iannaccone, University of Pisa, Italy
Quantum Engineering of transistors based on 2D materials heterostructures

⇒ C. Di Valentin, University of Milan, Italy
Theory of oxide surfaces and interfaces

⇒ A. Schleife, University of Illinois, Urbana Champaign, USA
Excited electrons in TCOs: Dielectric screening and electron dynamics

⇒ T. Voss, TU Braunschweig, Germany
Controlled formation of hybrid functional ZnO/polymer junctions by oxidative chemical vapor deposition (oCVD)

⇒ M. Wagner, TU Berlin, Germany
Optical and thermal characteristics of Ga_2O_3 polymorphs

⇒ J. Feldl, Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany
Cubic $(In,Ga)_2O_3$ films studied by Raman scattering and spectroscopic ellipsometry

⇒ W. Walukiewicz, Lawrence Berkeley, USA
Materials design principles for transparent conductors

⇒ C. Yang, Universität Leipzig, Germany
Amorphisation of sputtered CuI thin films

⇒ H. Hosono, Tokyo Institute of Technology, Japan
Novel transparent oxide semiconductors: Design, property and application

Transferable skills workshops

Presentation workshop

Dr. Frank Lorenz,
14 / 21 March 2019 in combination with the Annual BuildMoNa Conference, 9 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 presentations were monitored by video during the Annual BuildMoNa Conference 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. Dorothea Fiedler	*Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany*	Inositol Pyrophosphate Signaling revealed with Chemical Tool	22 January 2019	*Faculty of Life Sciences*
Prof. Dr. Ramamoorthy Boomishankar	*Indian Institute of Science Education and Research, Pune, India*	Organic and Organic-Inorganic Hybrid Ferroelectric Materials Supported by Amino-phosphorus(V) Scaffolds	29 May 2019	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Banglin Chen	*University of Texas at San Antonio, USA*	Our Journey of Exploring Multifunctional Metal-Organic Framework Materials	12 June 2019	*Faculty of Chemistry and Mineralogy*

Annual BuildMoNa Conference

The annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nanoobjects" (BuildMoNa) was held at the Faculty of Chemistry and Mineralogy on 18 and 19 March 2019. The following renowned guest speakers gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Kirsten Zeitler, University Leipzig
Multicatalytic transformations with and without light
⇒ Prof. Dr. Siegfried R. Waldvogel, University Mainz
Electrifying organic synthesis
⇒ Dr. Irene Coin, University Leipzig
Genetically encoded chemical tools for studying membrane proteins
⇒ Ass. Prof. Peter Zijlstra, Technical University Eindhoven
Plasmon-enhanced single-molecule sensing
⇒ Dr. Eckhard Bill, Max Planck Institute for Chemical Energy Conversion, Mühlheim an der Ruhr
Spectroscopic properties and electron structure of low-valent iron nitrosyl complexes

⇑ Participants of the Annual BuildMoNa Conference 2019.

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. Furthermore, the BuildMoNa Awards were given to doctoral candidates to recognise their outstanding scientific achievements.

Max Kneiß (Felix Bloch Institute for Solid State Physics) received the first prize for for developing a novel process to fabricate gallia layers in a non-equilibrium phase, published as:
Tin-assisted heteroepitaxial PLD-growth of κ-Ga_2O_3 thin films with high crystalline quality
M. Kneiß, A. Hassa, D. Splith, C. Sturm, H. von Wenckstern, T. Schultz, N. Koch, M. Grundmann / APL Mater. (2018) **7**(2) 022516:1-11

Marta Gozzi and Benedikt Schwarze (Institute of Inorganic Chemistry) received the second prize for writing two review articles in different application areas of metallacarboranes, published as:
Half- and mixed-sandwich transition metal dicarbollides and nido-carboranes(–1) for medicinal applications
B. Schwarze, M. Gozzi, E. Hey-Hawkins / Boron-Based Compounds: Potential and Emerging Applications in Medicine, Wiley (2018), ISBN:978-1-119-27555-8
and

⇑ Winners of the BuildMoNa Awards 2019 together with the Speaker of the Graduate School: Benedikt Schwarze, Prof. Dr. Marius Grundmann, Marta Gozzi and Max Kneiß (from left to right).

Half- and mixed-sandwich metallacarboranes in catalysis
B. Schwarze, M. Gozzi, E. Hey-Hawkins / Handbook of Boron Science with Applications in Organometallics, Catalysis, Materials and Medicine, Volume 2: Boron in Catalysis, World Scientific Publishing Europe Ltd. (2018), ISBN-13: 978-1786344410

Doctoral candidates presented their scientific results with short talks. Presentations covered partly the research profile of the graduate school, e.g. development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers. For the 9 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 Martin Fränzl for his presentation “Single amyloid fibrils studied in a thermophoretic trap”, the second to Jan Schulz for his presentation “Carborane-based frustrated Lewis pairs” and the third to Sascha Becker for his talk “Photoelectrical readout of single nitrogen vacancy centres in diamond.“

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference: Martin Fränzl, Jan Schulz and Sascha Becker (from left to right).

Funding of doctoral candidates

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DAAD
Europäische Union
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