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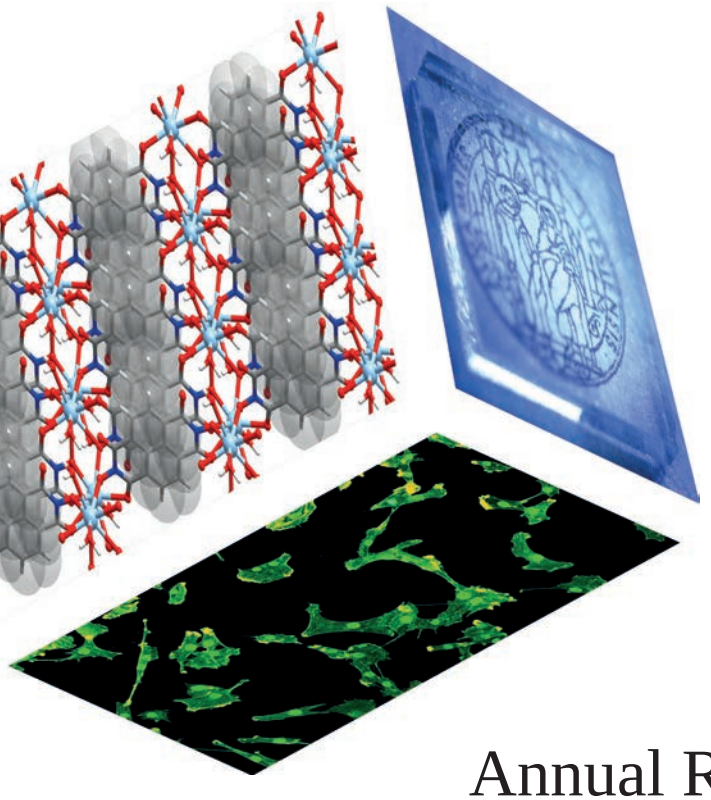
BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2020

Cover image:
⇒ *Left:* Electron transfer path in the coordination polymer $[Ca(ONDI)(H_2O)_2]_\infty$ (Ca-ONDI) obtained by reacting H_2ONDI (H_2ONDI = 2,7-dihydroxybenzo-[*lmn*][3,8]phenanthroline-1,3,6,8(2*H*,7*H*)-tetraone; NDI = naphthalene diamide) with alkaline earth metal ions (Ca^{2+}).
⇒ *Right:* Transparent oxide semiconductor electronics on glass. All-oxide and fully transparent metal-insulator-semiconductor field-effect transistors based on amorphous ZTO, comprising hafnium oxide as gate insulator and gallium zinc oxide as electrodes, exhibiting a total mean transmittance of 81% in the visible spectral range.
⇒ *Bottom:* Fluorescence microscopy image of glial cells grown on nanocolumnar titanium nitride. Actin fibers are green and cell nuclei are coloured yellow.

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Annual Report 2020

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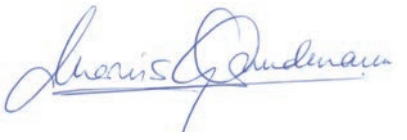
Preface
Prof. Dr. Marius Grundmann
Speaker of the Graduate School
Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Vice-Speaker of the Graduate School

The Graduate School Leipzig School of Natural Sciences – Building with Molecules and Nano-objects (BuildMoNa) focuses on interdisciplinary education of young scientists based on excellent research. The research concept follows the "bottom-up" strategy for the development of new materials. 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. 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.

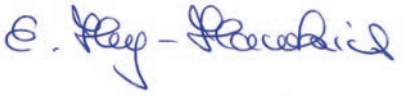
Since the establishment of the Graduate School in 2007, 163 young scientists have finished their doctoral studies with a certificate of the Graduate School. At the end of 2020, 72 doctoral researchers have been enrolled as members of BuildMoNa. Most of them were employed through third-party funded research projects.

The Graduate School provides a well-structured training program including multi-disciplinary scientific training and a transferable skills program in cooperation with the Research Academy Leipzig. The scientific training program consists of introductory modules to bridge interdisciplinary gaps, thematic modules and advanced modules linked to ongoing research and technological applications. A scientific conference is organised every year usually in March. Its goal is knowledge transfer in specific major research areas of the Graduate School. The conference comprises lectures held by invited national and international world-renowned speakers, industrial partners and graduate school members as well as oral and poster presentations by doctoral researchers.

During 2020 the Covid-19 pandemic had a great impact on the working and social life all over the world. Activities in many areas were affected and even disrupted. In spite of all efforts it was not possible to carry out the usual training program of the Graduate School. Less modules were organised in a virtual format, the planned symposium had to be postponed and the Annual BuildMoNa Conference was cancelled. It can only be hoped that the situation will get better and we look forward to getting back to some kind of normality and face-to-face meetings or conferences. We are eager to carry out further the sustained path established for BuildMoNa 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

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M.Sc. Phys. Oliver Lahr

Deputy
M.Sc. Chem. Lennart Staab

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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. J. A. Käs	*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. Biochem. Dennis Böhner	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe / Prof. Dr. I. Coin	*Generation and characterisation of biocompatible magnesium coatings*
M.Sc. Chem. Sebastian Braun	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Prof. 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*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
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. Benjamin Fanselow	Prof. Dr. F. Cichos / Prof. Dr. D. Huster/ Prof. Dr. R. Seidel	*Development of highly parallel trapping methods for the detection of protein aggregation with single molecule resolution*
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. Max Grellmann	Prof. Dr. K. Asmis / Prof. Dr. B. Abel / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Angle-resolved femtosecond-photoelectron spectroscopy on small cerium clusters*
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. Sebastian Henn	Dr. C. Sturm / Prof. Dr. B. Rosenow / Prof. Dr. F. Cichos	*Remanent switching of Bloch-polaritons*
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	*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*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
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. Aleksandr Kazimir	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Dr. F. Hansen	*Organometallic compounds in dual anticancer therapy*
M.Sc. Chem. Nils König	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Prof. Dr. B. Kersting	*Synthesis of new phosphole-containing π-systems and investigation of their photo-optical properties*
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. Catharina Krömmelbeim	Prof. Dr. S. Mayr / Prof. Dr. R. Seidel / Prof. Dr. J. A. Käs	*Development of electron beam irradiated granular hydrogels for biomedical and biotechnological applications*
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. Biochem. Paul Moritz List	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. I. Coin	*Development and characterisation of a shuttle system to therapeutic peptides*
M.Sc. Chem. Max Milewski	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A. Caminade / Prof. Dr. K. Zeitler	*Carboranyl phosphines meet dendrimers: Electron-deficient scaffolds for ligand design and applications in 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*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
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. 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*
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. Phys. Fabian Schöppach	Prof. Dr. M. Grundmann / Prof. Dr. C. Schnohr / Dr. habil. H. von Wenckstern	*Plasma treatment for enhancing electrical devices based on wide-bandgap semiconductors*
M.Sc. Chem. Jan Schulz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Carborane-based frustrated Lewis pairs for homogeneous catalysis*
M.Sc. Chem. Anastasiia Sherstiuk	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Prof. Dr. R. M. Sebastian Perez	*Photoswitchable phosphines for in situ modification of catalysts*
M.Sc. Phys. Nicola Söker	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Thermo-osmosis for manipulating microscopic liquid flow fields*
M.Sc. Chem. Lennart Staab	Prof. Dr. O. Oeckler/ Prof. Dr. H. Krautscheid / Dr. C. Benndorf	*Stability of thermoelectric materials at application oriented conditions - investigation with in-situ methods*
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. Phys. Xiaoya Su	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Frequency-dependent noise temperature of hot Brownian motion*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
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*
Dipl.-Math. Heinrich-Gregor Zirnstein	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Topological aspects of Dirac fermions in condensed matter systems*
M.Sc. Chem. Yong Yan	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser / Prof. Dr. B. Kersting	*Synthesis of luminescent coordination polymers*
M.Sc. Phys. Zhuolin Ye	Prof. Dr. K. Kroy / Prof. Dr. F. Cichos / Prof. Dr. J. Vollmer	*The optimisation of themodynamic devices*
M.Sc. Chem. Jingjing Yu	Prof. Dr. M. Grundmann / Prof. Dr. M. Lorenz / Prof. Dr. H. Krautscheid	*Disordered thin films of CuI and CuI-based alloys*

Alumni 2020

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Heterogeneously catalysed liquid phase oxidation of hydrocarbons over metal-organic frameworks*
Dr. rer. nat. 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 hetero-structures*
Dr. rer. nat. John Popp	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*P-Stereogenic dendritic ferrocenyl phosphines for redox-switchable catalysis*
Dr. rer. nat. Paul Räcke	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*High precision fabrication of quantum sensor arrays via ion implantation*
Dr. rer. nat. Axel Straube	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Tris(ferrocenyl)arene-based tris-phophanes: Coordination behaviour and application in redox-switchable catalysis*
Dr. rer. nat. 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*

Statistics

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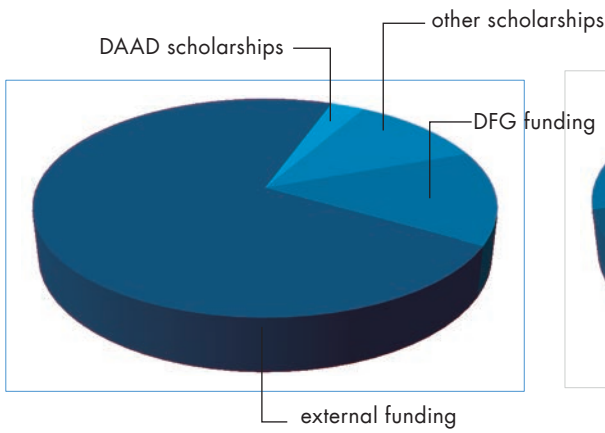

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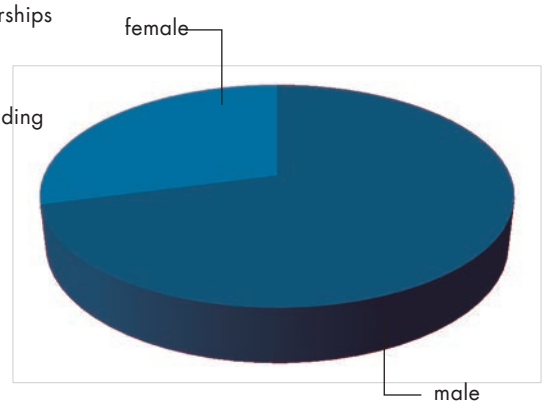

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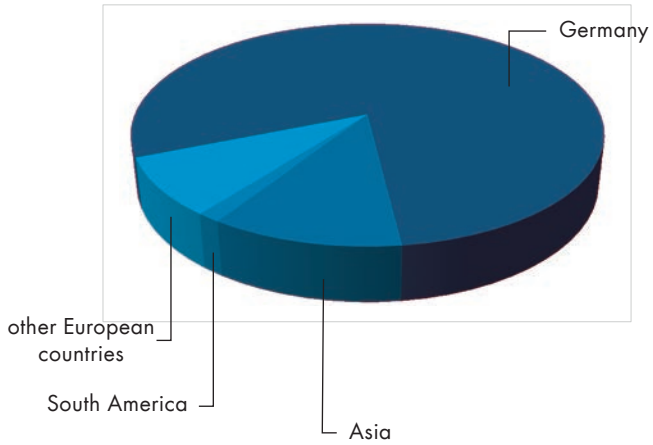


Bridging the gap between isolated nanoscale particles in the gas phase and condensed matter

Prof. Dr. Knut Asmis
M.Sc. Chem. Max Grellmann, M.Sc. Chem. Benjamin Hoffmann

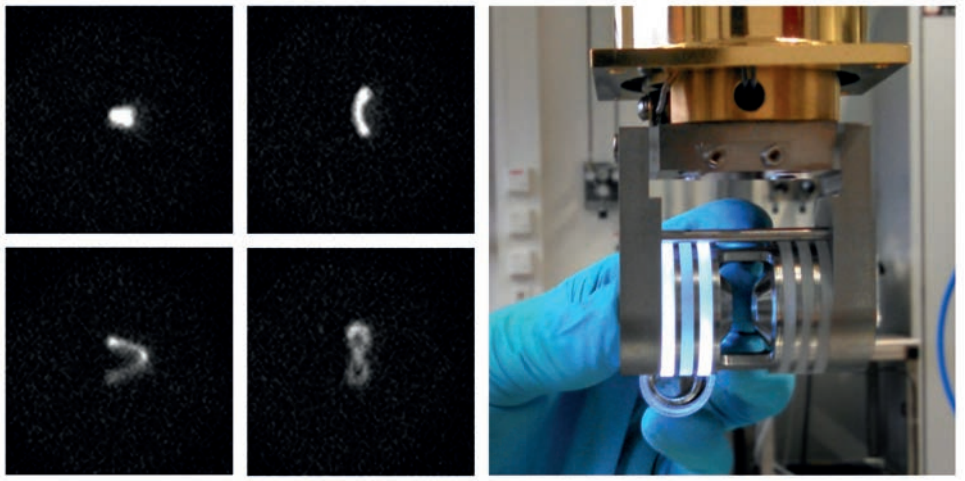
The research goal of the Asmis group is to bridge the information gap between the properties of small gas-phase clusters, nanoparticles (NPs) and bulk matter in order to gain insight into fundamental principles governing heterogeneous catalysis, aerosol nucleation, ion solvation and the rational design of functional materials. To this end, cutting-edge mass spectrometric as well as laser and particle spectroscopic methods are developed and refined in order to gain insight into the structure, reactivity and dynamics of size-selected clusters and NPs under precisely controllable conditions.

Single Nanoparticle Mass Spectrometry

Research on 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 nanoparticles (NPs) and therefore alternative methods are required, in which the absorption of photons is detected indirectly by way of action spectroscopy. To this end, 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-



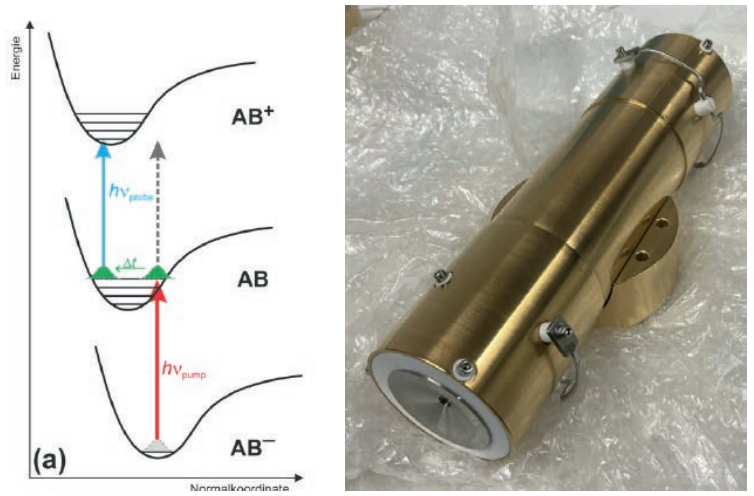
⇑ Characteristic oscillations of a trapped 100 nm particle in the ion trap (left) and image of the custom made quadrupole ion trap (right).

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.

fs-NeNePo Spectroscopy

Neutral gas phase clusters are usually difficult to access experimentally, since their manipulation and thus their mass-selection cannot be carried out by standard techniques. This problem is overcome in femtosecond Negative-Neutral-Positive spectroscopy (fs-NeNePo spectroscopy). Here, an electron is photodetached from mass-selected anions AB^- by means of an ultrashort laser pulse (pump pulse). The wave packet dynamics on the potential energy surface of the neutral ground (or excited) state AB are then interrogated using a second ultrashort laser pulse (probe pulse) after a variable time delay Δt, which photoionises AB and generates cations AB^+. The yield of mass-selected cations is measured as a function of Δt and plotted in the fs-NeNePo spectrum.

To enable this kind of spectroscopy to be carried out, Max Grellmann upgraded a triple quadrupole mass spectrometer with a custom-built quadrupole ion trap and coupled it with an amplified and broadly wavelength-tunable fs laser source. Currently, he is investigating the wave packet dynamics in small metal clusters, including aluminium, silver, copper and cerium clusters.



⇑ fs-NeNePo excitation scheme (left) and custom-built linear quadrupole ion trap (right)..

⇒ *Electronic action spectroscopy on single nanoparticles in the gas phase*
B. Hoffmann, T. K. Esser, B. Abel, K. R. Asmis / J. Phys. Chem. Lett. (2020) **11** 6051−6056

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Chemical modification of peptides and proteins

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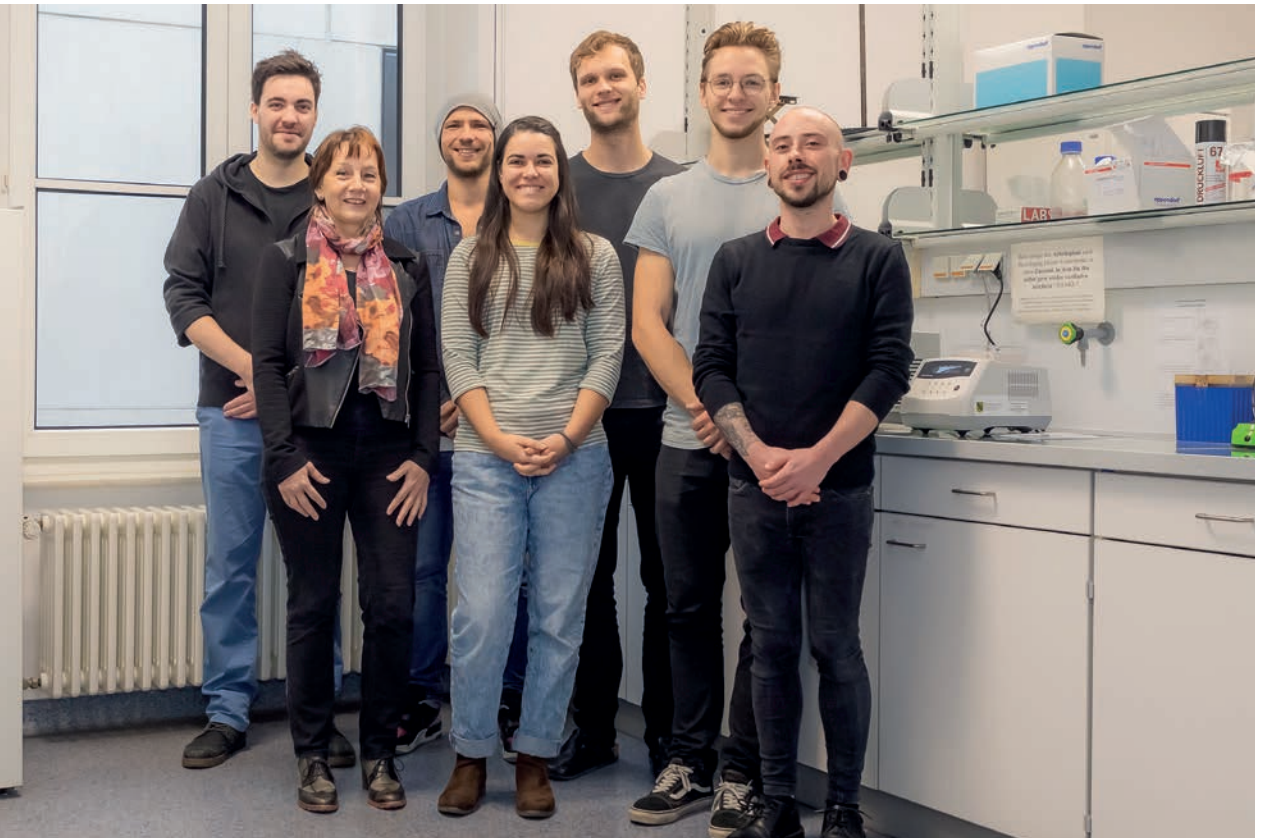
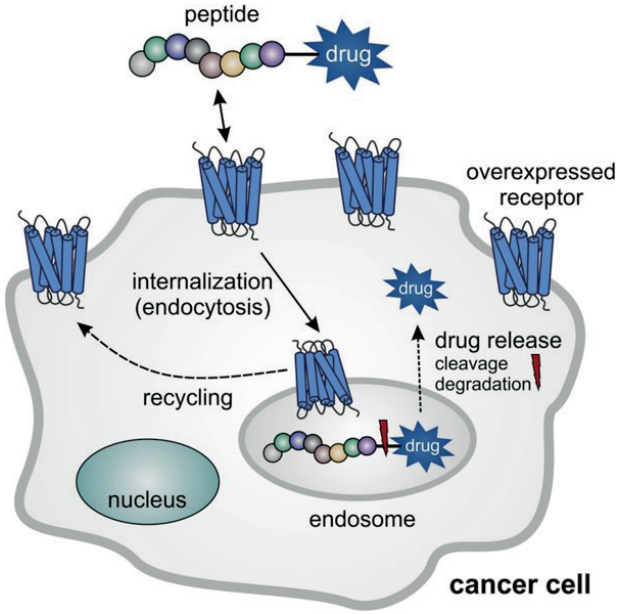
The synthesis and characterisation of chemically modified peptides and proteins to modulate their function is the common goal of the project. This includes proteins involved in tumour targeting, proteins for nanomedicine or biomaterial development. In this process, the peptides are synthesised by solid-phase peptide synthesis and the proteins are recombinant expressed and fused to the peptides by native chemical ligation or click chemistry.

In 2020, Philipp Wolf was in his last PhD-year and worked successfully on the chemical modification of proteins in living cells. He investigated the functional significance of variants in the LEPR gene. These mutations have been identified in two patients with severe early-onset obesity. The cause for the early onset obesity seems to be due to the complete loss of function of the p.Tyr411del-mutation. Philipp Wolf plans to finish his PhD-thesis in 2021.



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 at 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 works in the field of chemerin signalling. She characterised chemerin-peptides for drug shuttling to selectively address cells of the immune system. During her research she already obtained the first peptide drug conjugates for shuttling them into cell by the chemerin receptor CMKLR1. Furthermore, she achieved insights into the role of the chemerin receptor GPR1.



⇑ Schematic outline of targeting a tumour-expressed G protein-coupled receptor for anti-cancer drug delivery with a peptide-drug conjugate. The drug will be released intracellularly by intentionally using a cleavable linker or just by endo-lysosomal degradation of the peptide-drug conjugate:

Jan Dirks investigates protein expression and chemical modification of enzymes. He worked 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. Similarly, Kevin Kretschmer investigated the chemical modification of proteins by light. However, he used photoactivatable interaction partners to crosslink labelled peptides to their interacting protein partners. Subsequently, he characterised the interaction sites by mass spectrometry after enzymatic digestion and affinity purification. Moritz List joined the team in 2020 and also is interested in protein-protein interactions in cells. He works on the optimisation of a shuttle system for inhibitors of intracellular protein-protein interactions. It should become possible to selectively address a specific cell type through receptor-mediated endocytosis and subsequent

endosomal escape.

Dennis Böhner became a member of the Graduate School in 2019 and works in the field of biomaterial coating. He took a closer look on the preparation of a bio-inspired peptide coating for magnesium alloys and functionalisation of this coating with antimicrobial agents, e.g. antibiotics.

In addition to current members, several papers from former BuildMoNa-members have been published, including Sylvia Els-Heindl, Jan-Patrick Fischer and Kathrin Bellmann-Sickert. Joint publications of Dennis J. Worms who finished his thesis end of 2019 and different collaboration partners were finally published in 2020. Dennis investigated peptide-binding receptors for anticancer drug delivery, focusing on peptide ligands as active agents. An important contribution to the progress of the project was made as new knowledge was gained about the project.

⇒ *Targeting of peptide-binding receptors on cancer cells with peptide-drug conjugates*
D. J. Worm, S. Els-Heindl, A. G. Beck-Sickinger/ Peptide Science (2020) **112** e24171

⇒ *Identification of a novel leptin receptor (LEPR) variant and proof of functional relevance directing treatment decisions in patients with morbid obesity*
F. Voigtmann, P. Wolf, K. Landgraf, R. Stein, J. Kratzsch, S. Schmitz, R. Abou Jamra, M. Blüher, J. Meiler, A. G. Beck-Sickinger, W. Kiess, A. Körner / Metabolism (2021) **116** 154438

⇒ *Design, synthesis, and biological evaluation of a multifunctional neuropeptide-Y conjugate for selective nuclear delivery of radiolanthanides*
A. Chastel, D. J. Worm, I. D. Alves, D. Vimont, M. Petrel, S. Fernandez, P. Garrigue, P. Fernandez, E. Hindié, A. G. Beck-Sickinger, C. Morgat / EJNMMI Res (2020) **10** 16

⇒ *Selective neuropeptide Y conjugates with maximised carborane loading as promising boron delivery agents for boron neutron capture therapy*
D. J. Worm, P. Hoppenz, S. Els-Heindl, M. Kellert, R. Kuhnert, S. Saretz, J. Köbberling, B. Riedl, E. Hey-Hawkins, A. G. Beck-Sickinger / J Med Chem (2020) **63** 2358

⇒ *A selective carborane-functionalised gastrin-releasing peptide receptor agonist as boron delivery agent for boron neutron capture therapy*
P. Hoppenz, S. Els-Heindl, M. Kellert, M. Kuhnert, S. Saretz, H. G. Lerchen, J. Köbberling, B. Riedl, E. Hey-Hawkins, A. G. Beck-Sickinger / J. Org. Chem (2020) **85** 1446

⇒ *Tuning a modular system - synthesis and characterisation of a boron-rich s-triazine-based carboxylic acid and amine bearing a galactopyranosyl moiety*
M. Kellert, P. Hoppenz, P. Lönnecke, D. J. Worm, B. Riedl, J. Koebberling, A. G. Beck-Sickinger, E. Hey-Hawkins / Dalton Trans (2020) **49** 57

⇒ *Peptide-drug conjugates and their targets in advanced cancer therapies*
P. Hoppenz, S. Els-Heindl, A. G. Beck-Sickinger / Front Chem (2020) **8** 571

⇒ *Peptide-mediated surface coatings for the release of wound-healing cytokines*
F. Clauder, S. Möller, S. Köhling, K. Bellmann-Sickert, J. Rademann, M. Schnabelrauch, A. G. Beck-Sickinger / J Tissue Eng Regen Med (2020) **14** 1738

⇒ *Adrenomedullin - Current perspective on a peptide hormone with significant therapeutic potential*
J. P. Fischer, S. Els-Heindl, A. G. Beck-Sickinger / Peptides (2020) **131** 170347

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Thermohydrodynamic approaches to the manipulation of colloids

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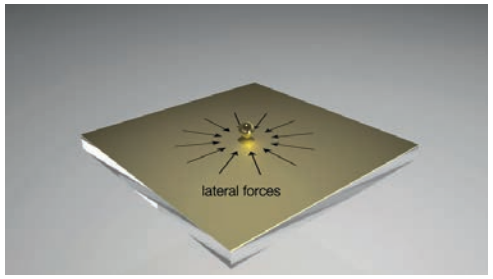
M.Sc. Phys. Alexander Fischer, M.Sc. Phys. Martin Fränzl, M.Sc. Chem. Benjamin Fanselow, M.Sc. Phys. Nicola Andreas Söker, M.Sc. Phys. Xiaoya Su

The control and manipulation of nano-objects is a key element for future nanophotonics, material science biotechnology or even quantum sensing. Analytes dissolved in liquids, for example, need to be delivered, concentrated, separated or locally confined for further studies to become eventually processed and removed. Photonic elements including plasmonic nano-structures require precise positioning or controlled rearrangements to serve as adaptive functional structures.

Key elements of the control at the micro- and nanoscale are often pressure driven fluidics transporting liquid volume and solutes as well as the generation of energy landscapes or force fields. The latter is achieved with optical and plasmonic tweezers, magnetic fields, or using electrokinetic or opto-electronic effects. Especially in the field of plasmonic tweezers and nanoantennas where light is used to excite collective electron motion in noble-metals, the Joule losses lead to the unavoidable

generation of heat at boundaries as an unwanted side effect. Nevertheless, such optically generated temperature fields seem also suitable for the manipulation of nano-objects in liquids, for example, for the trapping of nanoparticles and single molecules or protein aggregates as well as for manufacturing active particles.
The Molecular Nanophotonics group has recently developed processes to provide a versatile trapping and manipulation of nano-objects and fluids near surfaces in the simplest geometries. Contrary to most other techniques, our scheme is based on hydrodynamic flows generated by optically induced thermo-osmosis (Fig. 1). Thermo-osmosis relies on a perturbation of the interfacial interactions at a solid-liquid boundary and is present in all experiments involving temperature gradients in plasmonic structures including plasmonic tweezers. We have shown that local temperature gradients on a thin gold film induce strong interfacial flows of several 10 to 100 µm/s in its direct vicinity (10 nm) that results in a flow pattern reminiscent of convection. Based on a fully quantitative analysis of our experimental results we have revealed that these thermo-osmotic flows on gold-water interfaces are induced by a temperature-induced perturbation of the van der Waals (vdW) interactions. Nano-objects suspended in the liquid are therefore dragged by the hydrodynamic forces originating from these flows. Utilising attractive vdW interactions of the nano-object with the gold surface or temperature-induced depletion, we can trap and manipulate different types of nano-objects near the surface. The remote control of localised hydrodynamic flows paves the way for a machine learning controlled nano-fluidics [1] to seperate, assemble and manipulate tiny amounts of solutes in a new nanofluidics.



⇐ Fig. 1: Scheme of a radial thermos-osmotic flow generated by local heating of a thin gold film for the trapping of gold nanoparticles.

⇒ [1] *Active particle feedback control with a single-shot detection convolutional neural network*
M. Fränzl, F. Cichos / Scientific Reports (2020) **10** 12571

⇒ [2] *Emergent collective phenomena through active particle control by light*
S. Muiños-Landin, A. Fischer, N.A. Söker, F. Cichos / In: The 2020 Motile Active Matter Roadmap, Journal of Physics: Condensed Matter (2020) **32** 193001

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Nanostructured catalysts for the valorisation of renewable resources

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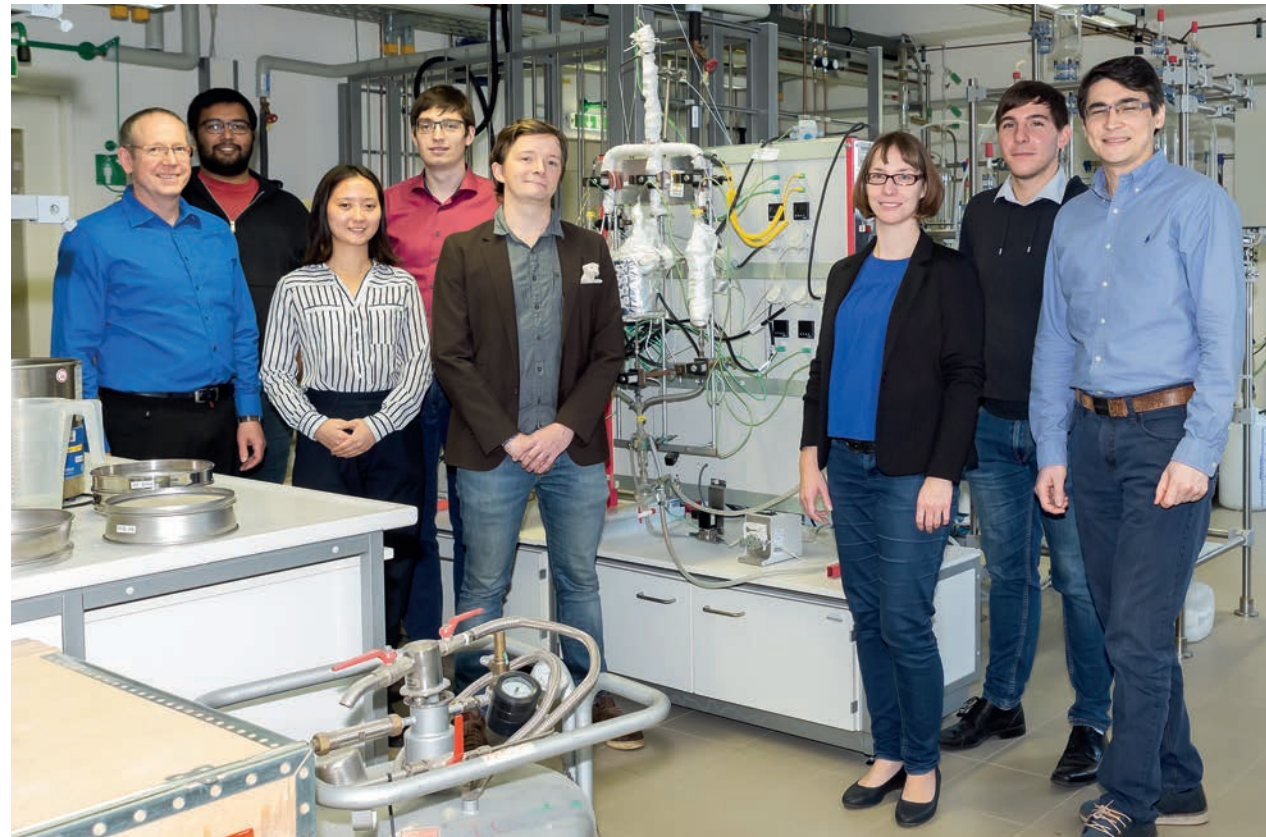
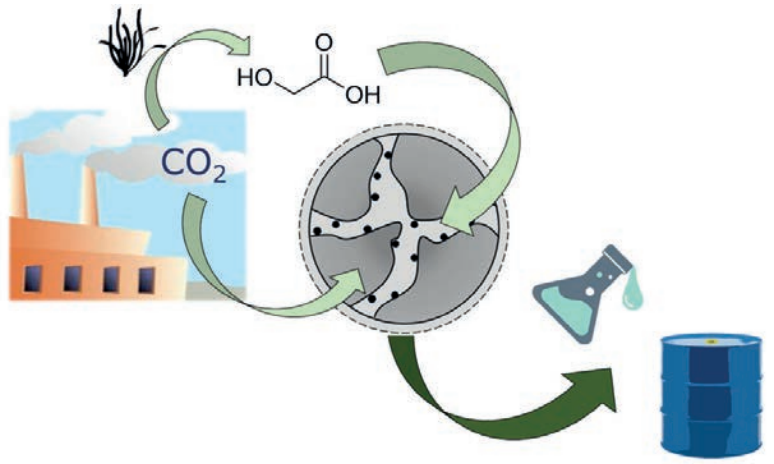
Heterogeneous catalysis is a key technology for the transition of the current fossil-fuel based value chain to a sustainable economy based on renewable resources. Therefore, the major focus of our group is on the preparation of nanoporous materials and their utilisation as catalysts, e.g., as supports for metal nanoparticles. We apply these catalysts in promising future catalytic conversions, such as the conversion of biomass or the reduction of CO_2 with H_2. In accordance with the principles of BuildMoNa, our goal is to adjust structural material properties on the nanoscale to achieve the desired catalytic properties. One catalytic application studied in our group is the conversion of sustainable algea-derived glycolic acid into value-added chemicals with lower oxygen content. Here, we focus on the influence of support materials and active components on catalytic activity as well as on the challenges emerging from additives in algea-derived feedstocks like nutrient salts and metabolic inhibi-



tors. Since increased levels of CO_2 in the atmosphere have a dramatic impact on the climate, our group investigates approaches for CO_2 utilisation through catalytic reduction of CO_2 with H_2 to chemicals and fuels, such as methanol and methane. Another focus area of our research is the direct air capture as a process to capture and utilise CO_2 directly from ambient air. This can be realised via amine- functionalised nanoporous silica. The uptake and sorption kinetics of chemisorbed CO_2 are studied and tuned by adjusting the textural characteristics of amine-functionalised porous silica. After loading with metal nanoparticles, the chemisorbed CO_2 is converted to methanol. For CO_2 methanation, we design monolithic catalysts based on Al_2O_3 and ZrO_2 with hierarchical nanoporosity in order to optimise mass and heat transport properties. This makes the solid catalysts not only highly active in the methanation reaction, but also able to cope with dynamic operation conditions which are a result of the increasing use of renewables in the chemical and energy industry.



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

⇒ *Porosity and structure of hierarchically porous Ni/Al_2O_3 Catalysts for CO_2 methanation*
S. Weber, K. L. Abel, R. T. Zimmermann, X. Huang, J. Bremer, L. Rihko-Struckmann, D. Batey, S. Cipiccia, J. Titus, D. Poppitz, C. Kübel, R. Gläser, T. L. Sheppard / Catalysts (2020) **10** 1471

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Amorphous oxide semiconductors for integrated devices

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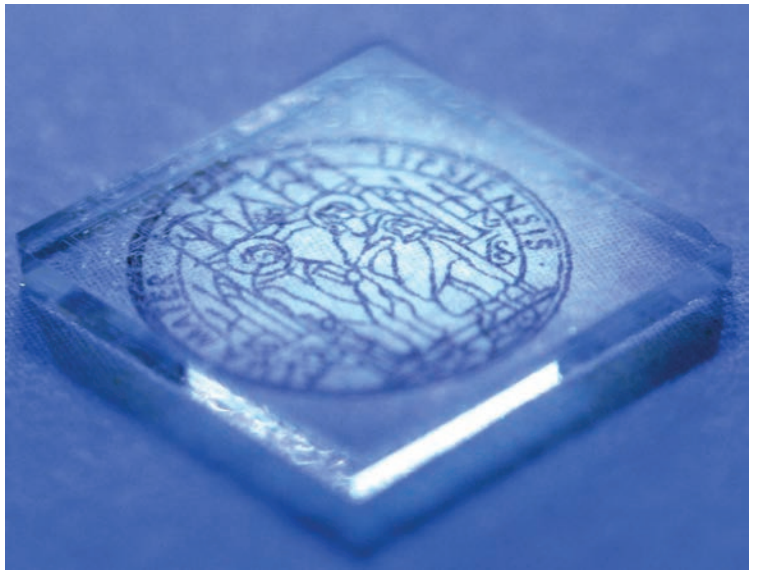
Amorphous semiconductors have rapidly gained in importance in recent years. They can be used to build transistors that function on glass as a substrate and are thus important for displays. Polymer substrate also allows the production of devices that are flexible and thus bendable. Indium gallium zinc oxide (IGZO) has become the most common material; however, indium is a critical raw material. Therefore, we are investigating indium-free materials that are similarly or even better suited for the fabrication of amorphous transistors. One of the promising candidates is zinc tin oxide (ZTO). We have established a fabrication process that takes place exclusively at room temperature and does not require post-deposition annealing steps. It is therefore very simple and also energy-saving. With the ZTO material, we have

succeeded in manufacturing and characterising the world's best field effect transistors (FET's) and inverters from this material [R1, R2]. This represents a significant advance and, in addition to individual transistors, we have already produced some integrated circuits. The devices are highly transparent in the visible spectral Range (Fig. 1). As special features, the devices are characterised by having extremely steep characteristics and their properties are very close to the thermodynamic limit (Fig. 2). This has been achieved by optimising the channel and contact materials themselves as well as the device design and layout. In addition, the manufacturing process is also very reliable and reproducible after some optimisations in photolithography and processing steps.

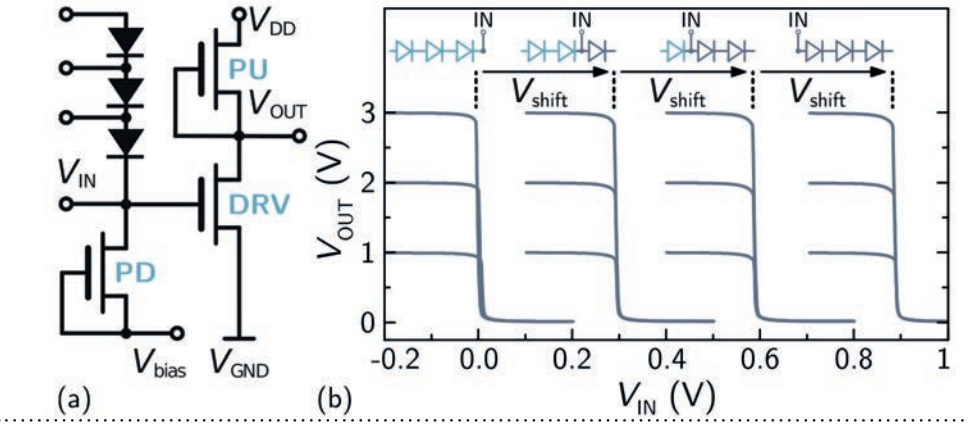
Another amorphous semiconductor material is zinc-oxinitrite (ZnON). Here, there is no mixing on the cation side but on the anion side. Obviously, nitrogen is a very cheap element; however, this is not the most important aspect. The mixing on the anion lattice results in less scattering for electrons due to the reduced disorder at the conduction band edge, so that the charge carrier mobility is even larger than in ZTO. The influence of Mg doping has been investigated and found to allow to control the charge carrier density, however, for the price of reduced electron mobility [R3]. Also pure zinc-nitride has been studied in detail [R4].

Our previous work on TCO's (transparent conductive oxides) with rather high electron concentration and thus electrical conductivity has borne fruit in the form of transparent electrodes for the coherent control of qubits. Indium-zinc-oxide (ITO) microwave strip lines directly deposited and structured on diamond were used to control NV colour centres and address individual spin states using circularly polarised microwaves [R5].



⇑ Fig. 1: Transparent oxide semiconductor electronics on glass. All-oxide and fully transparent metal-insulator-semiconductor field-efect transistors based on amorphous ZTO, comprising hafnium oxide as gate insulator and gallium zinc oxide as electrodes, exhibiting a total mean transmittance of 81% in the visible spectral range. Photo: Oliver Lahr, Daniel Splith, both Universität Leipzig.

While all of the oxide materials discussed above are of n-type, i.e., electron conducting, the quest for p-type semiconductor materials for thin film electronics is on. However, such materials are plagued by low hole mobility. An exception is copper iodide which is researched by us within DFG research Group FOR 2857. Copper iodide is the transparent p-type semiconductor that has the best figure of merit, i.e. the largest conductivity at the highest optical transparency. Stunning progress in growth control, surface morphology and hole mobility has been made in the fabrication of CuI thin films using both pulsed laser deposition (PLD) [R6] and sputtering [R7]. This will be the basis for fabricating p-type transparent FET's and subsequently complementary-type inverters.



⇑ Fig. 2: Schematic basic circuit layout of an Schottky diode FET logic (SDFL) inverter, employing a pull-down transistor (PD) and three ZTO/PtO_x Schottky barrier diodes for the level shifting of the output signal. DRV and PU denote the driving transistor and pull-up transistor, respectively. (b) Inverter characteristics without and with a series connection of up to three level-shifting diodes and operating at supply voltages VDD between 1 V and 3 V. Adapted from [R2].

Other work of our BuildMoNa doctoral candidates concerned growth and characterisation of thin films from sesquioxide alloys [R8-R12] and band offsets of such materials [R13, R14]. We investigated the dynamics of the dielectric function of ZnO using femto-second ellipsometry [R15] and the dynamics of the emission from carbon nanodots [R16]. Also, a novel material for solar energy harvesting, using the intermediate band principle, was investigated [R17].

⇒ [R1] *All-oxide transparent thin-film transistors based on amorphous zinc-tin-oxide fabricated at room temperature: Approaching the thermodynamic limit for sub-threshold swing*
O. Lahr, M. Bar, H. von Wenckstern, M. Grundmann / Adv. Electron. Mater. (2020) **6** 2000423:1–6

⇒ [R2] *Ultrahigh-performance integrated inverters based on amorphous zinc-tin-oxide deposited at room temperature*
O. Lahr, H. von Wenckstern, M. Grundmann / APL Mater. (2020) **8** 091111:1–8

⇒ [R3] *Tuning material properties of amorphous zinc oxynitride thin films by magnesium cationic substitutio*
A. Welk, A. Reinhardt, O. Herrfurth, T. Schultz, H. von Wenckstern, N. Koch, M. Grundmann / APL Mater. (2021) **9** 021120:1–8

⇒ [R4] *Epitaxial Zn_3N_2 thin films by molecular beam epitaxy: Structural, electrical and optical properties*
P. John, M. Al Khalfioui, C. Deparis, A. Welk, C. Lichtensteiger, R. Bachelet, G. Saint-Girons, M. Hugues, M. Grundmann, J. Zúñiga-Pérez / J. Appl. Phys. (2021) **130** 065104:1–11

⇒ [R5] *Method of full polarisation control of microwave fields in a scalable transparent structure for spin manipulation*
R. Staacke, R. John, M. Kneiß, C. Osterkamp, S. Diziain, F. Jelezko, M. Grundmann, J. Meijer / J. Appl. Phys. (2020) **128** 194301:1–9

⇒ [R6] *High mobility, highly transparent, smooth, p-type CuI thin films grown by pulsed laser deposition*
P. Storm, M. Bar, S. Selle, C. Yang, H. von Wenckstern, M. Grundmann, M. Lorenz / APL Mater. (2020) 8 091115:1–8

⇒ [R7] *Controllable growth of copper iodide by sputtering towards high-mobility thin films and self-assembled microcrystals*
C. Yang, E. Rose, W. Yu, T. Stralka, F. Geng, M. Lorenz, M. Grundmann / ACS Applied Electronic Materials (2020) **2** 3627–3632

⇒ [R8] *Growth , structural and optical properties of coherent* κ-$(Al_xGa_{1-x})_2O_3$/ κ-Ga_2O_3 *quantum Well superlattice heterostructures*
M. Kneiß, P. Storm, A. Hassa, D. Splith, H. von Wenckstern, M. Lorenz, M. Grundmann / APL Mater. (2020) **8** 051112:1–14

⇒ [R9] *Solubility limit and material properties of a* κ-$(Al_xGa_{1-x})_2O_3$ *thin film with a lateral cation gradient on (00.1)* Al_2O_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** 021103:1–7

⇒ [R10] *Control of phase formation of* $(Al_xGa_{1-x})_2O_3$ *thin films on c-plane* Al_2O_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** 485105:1–9

⇒ [R11] *Investigating the ranges of (meta)stable phase formation in* $(In_xGa_{1-x})_2O_3$*: Importance of the cation coordination*
C. Wouters, C. Sutton, L.M. Ghiringhelli, T. Markurt, R. Schewski, A. Hassa, H. von Wenckstern, M. Grundmann, M. Scheffler, M. Albrecht / Phys. Rev. Res. (2020) **4** 125001:1–10

⇒ [R12] *A review of the segmented-target approach to combinatorial material synthesis by pulsed-laser deposition*
H. von Wenckstern, M. Kneiß, P. Storm, M. Grundmann / Phys. Status Solidi B (2020) **257** 1900626:1-13

⇒ [R13] *Band offsets at* κ-$([Al,In]_xGa_{1-x})_2O_3$*/MgO interfaces*
T. Schultz, M. Kneiß, P. Storm, D. Splith, H. von Wenckstern, M. Grundmann, N. Koch / ACS Appl. Mater. Interfaces (2020) **12** 8879–8885

⇒ [R14] *Changes in band alignment during annealing at 600°C of ALD* Al_2O_3 *on* $(In_xGa_{1-x})_2O_3$ *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** 105701:1–8

⇒ [R15] *Ultrafast dynamics of hot charge carriers in an oxide semiconductor probed by femtosecond spectroscopic ellipsometry*
S. Richter, O. Herrfurth, S. Espinoza, M. Rebarz, M. Kloz, J.A. Leveillee, A. Schleife, S. Zollner, M. Grundmann, J. Andreasson, R. Schmidt-Grund / New J. Phys. (2020) **22** 083066:1–14

⇒ [R16] *Influence of the excitation conditions on the emission behaviour of carbon nanodot-based planar microcavities*
L. Trefflich, F. Dissinger, R. Schmidt-Grund, C. Sturm, S.R. Waldvogel, M. Grundmann / Phys. Rev. Res. (2020) **2** 043216:1–6

⇒ [R17] *Properties of epitaxially grown* In_2S_3*:V thin films for intermediate band solar cell application*
T. Jawinski, R. Scheer, H. von Wenckstern, M. Lorenz, M. Grundman / Proc. 47th IEEE Photovoltaic Specialists Conference (PVSC), (2020) p. 2663–2666

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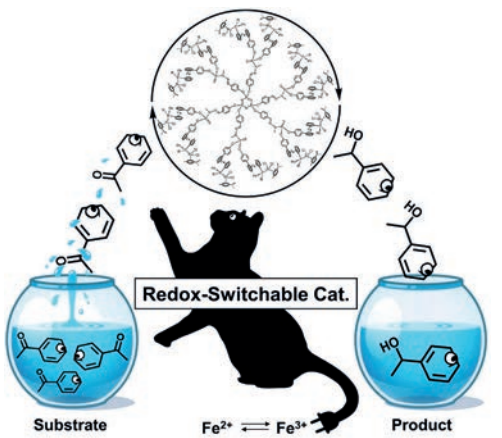
The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carborane clusters and antitumour drugs).

Smart Catalysts

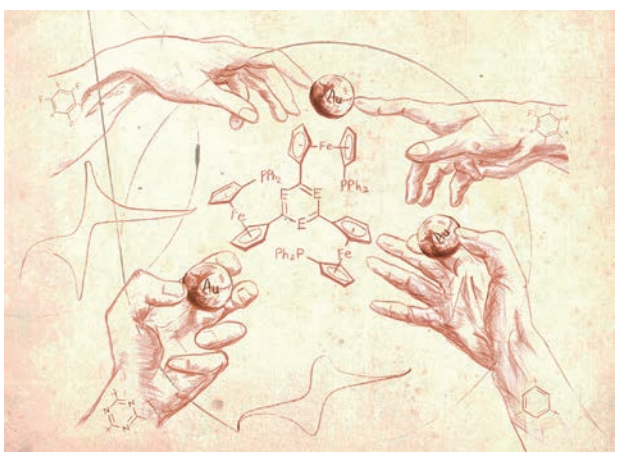
Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups (ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying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



⇐ Fig. 1: Will the fish reach the other side? Or will the redox-switchable cat catch a delicious treat? A single electron determines the fate of the fish. Depending on the redox state, the cat will let the fish pass to perform the hydrogen transfer to the product bowl (reduced state) or it will use its sharp claws to frighten them to remain in the substrate bowl (oxidised state).

cations (J. Popp (Fig. 1), M. Milewski, A. Sherstiuk). A new approach includes C3-symmetric (A. Straube (Fig. 2) and carborane-based (A. Straube, J. Schulz, M. Milewski) 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 (R. Clauß, S. Baweja, K. Ramazanova).



⇐ Fig. 2: Depending on the substitution of the central core, tris(1-phosphanyl-1'-ferrocenylene)arenes bind gold(I) in different coordination modes. The resulting complexes show stepwise activity changes in redox-switchable gold(I) catalysis (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). Selected examples of functionalised building blocks for organometallic or phosphorus-based polymers are: strained phosphorus-based rings (V. Eilrich) or (planar-chiral) ferrocene derivatives (A. Straube) and bis-, tris- and tetrakis-carboxylates of conjugated aromatic systems as ligands in redox-active coordination polymers or MOFs (A. Aleksovska), as well as phosphole derivatives showing aggregation-induced emission (AIE) properties (N. König).

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 (Fig. 3).

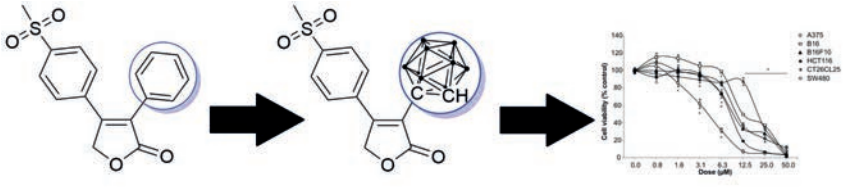
Inorganic Building Blocks in Medicinal Chemistry

Carboranes are highly hydrophobic and extremely stable icosahedral carbon-containing boron clusters. The cage framework of these clusters can easily be modified with a variety of substituents, both at the carbon and at the boron atoms and can either be used as pharmacophoric entities in cyclooxygenase (COX) (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

⇐ Fig. 3: Phosphorus-rich molecules are of special interest in coordination chemistry because of the presence of various donor atoms. Several fascinating transition metal complexes of an octaphosphine were obtained involving six different coordination modes (design: Dr. Christoph Selg, Leipzig University).

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 (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 (A. Kazimir).



⇑ Fig. 4: Carborane-containing derivatives of rofecoxib, a known COX-2-selective inhibitor, display remarkable cytostatic activity in the micromolar range with excellent selectivity for melanoma and colon cancer cell lines over normal cells. Furthermore, the introduction of a carborane cluster into the main structural motif of rofecoxib converts the cytotoxic into a cytostatic mode of action.

⇒ *Nanoparticle-based formulation of metallacarboranes with bovine serum albumin for application in cell cultures*
B. Schwarze, M. Gozzi, C. Zilberfain, J. Rüdiger, C. Birkemeyer, Irina Estrela-Lopis, E. Hey-Hawkins / J. Nanopart. Res. (2020) **22** 24

⇒ *Selective neuropeptide Y conjugates with maximised carborane loading as promising boron delivery agents for boron neutron capture therapy*
D. J. Worm, P. Hoppenz, S. Els-Heindl, M. Kellert, R. Kuhnert, S. Saretz, J. Köbberling, B. Riedl, E. Hey-Hawkins, A. G. Beck-Sickinger / J. Med. Chem. (2020) **63** 2358–2371

⇒ *Hybrid 2D nanofibers based on poly(ethylene oxide)/polystyrene matrix and poly(ferrocenylphosphinoboranes) as functional agents*
V.P. Nirwan, S. Pandey, E. Hey-Hawkins, A. Fahmi / J. Appl. Polym. Sci. (2020) 137:e49091

⇒ *A selective carborane-functionalised gastrin-releasing peptide receptor agonist as boron delivery agent for boron neutron capture therapy*
P. Hoppenz, S. Els-Heindl, M. Kellert, R. Kuhnert, S. Saretz, H.-G. Lerchen, J. Köbberling, B. Riedl, E. Hey-Hawkins, A.G. Beck-Sickinger / J. Org. Chem. (2020) **85** 1446–1457

⇒ *Unexpected isomerisation of hexa-tert-butyl-octaphosphane*
T. Grell, E. Hey-Hawkins / Chem. Eur. J. (2020) **26** 1008–1012

⇒ *Dynamic gold(I) complexes of hexa-tert-butyl-octaphosphane*
T. Grell, E. Hey-Hawkins / Europ. J. Inorg. Chem. (2020) 732–736

⇒ *Carboranyl derivatives of rofecoxib with cytostatic activity against human melanoma and colon cancer cells*
A. Buzharevski, S. Paskas, M.-B. Sárosi, M. Laube, P. Lönnecke, W. Neumann, B. Murganić, S. Mijatović, D. Maksimović-Ivanić, J. Pietzsch, E. Hey-Hawkins / Scientific Reports (2020) 10:4827

⇒ *Unusual racemisation of tertiary P-chiral ferrocenyl phosphines*
J. Popp, S. Hanf, E. Hey-Hawkins / Chem. Eur. J. (2020) **26** 5765–5769

⇒ *Tricoordinate coinage metal complexes with a redox-active tris(ferrocenyl)triazine backbone feature triazine–metal interactions*
A. Straube, P. Coburger, M.R. Ringenberg, E. Hey-Hawkins / Chem. Eur. J. (2020) **26** 5758–5764

⇒ *Redox-switchable transfer hydrogenations with P-chiral dendritic ferrocenyl phosphine complexes*
J. Popp, A.-M. Caminade, E. Hey-Hawkins / Eur. J. Inorg. Chem. (2020) 1654–1669

⇒ *Versatile coordination chemistry of hexa-tert-butyl-octaphosphine*
T. Grell, E. Hey-Hawkins / Inorg. Chem. (2020) **59** 7487–7503

⇒ *Zn- and Cd-based coordination polymers with a novel anthracene dicarboxylate ligand for highly selective detection of hydrogen peroxide*
A. Aleksovska, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2020) **49** 4817–4823

⇒ *Catalytic activity towards hydrogen evolution dependent of the degree of conjugation and absorption of six organic chromophores*
A. Aleksovska, P. Lönnecke, M. A. Addicoat, R. Gläser, E. Hey-Hawkins / ChemistryOpen (2020) **9** 405–408

⇒ *Metal-organic framework based on an anthracene tetracarboxylate ligand and cadmium or cobalt: Synthesis, structure analysis, stability and magnetic properties*
A. Aleksovska, H. Zaake-Hertling, P. Lönnecke, B. Schwarze, D. Gräsing, J. Matysik, L. Blömer, B. Kersting, E. Hey-Hawkins / ChemistrySelect (2020) **5** 6537–6540

⇒ *Silver(I) complexes of two flexible bis-phospholane ligands: Metallamacrocycles, polymeric chains and metallacryptands*
P. Boar, P. Lönnecke, E. Hey-Hawkinsf / Z. Anorg. Allg. Chem. (2020) **646** 915–922

⇒ *Facile synthesis of a nickel(0) phosphine complex at ambient temperature*
A. Straube, P. Coburger, L. Dütsch, E. Hey-Hawkins / Chem. Commun. (2020) **56** 7893–7896

⇒ *Triple the fun: Tris(ferrocenyl)arene-based gold(I) complexes for redox-switchable catalysis*
A. Straube, P. Coburger, L. Dütsch, E. Hey-Hawkins / Chem. Sci. (2020) **11** 10657–10668

⇒ *The core of the matter – arene substitution de-termines the coordination and catalytic behaviour of tris(1-phosphanyl-1'-ferrocenylene)arene gold(I) complexes*
A. Straube, P. Coburger, M. Michak, M. Ringenberg, E. Hey-Hawkins / Dalton Trans. (2020) **49** 16667–16682

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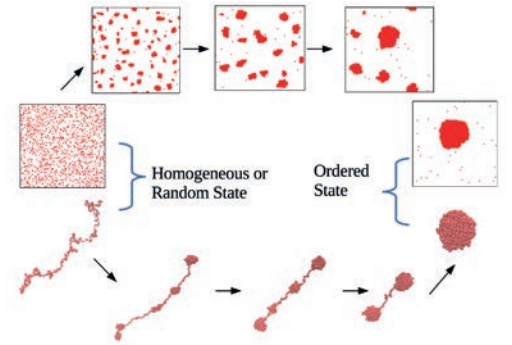
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
Dr. 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.



⇐ Illustration of the similarities between the usual coarsening kinetics of a particle or spin system and the collapse kinetics of a polymer when quenched from a completely disordered configuration at infinite temperature (left) to a low temperature below the phase transition point, i.e., into the ordered phase (right). The upper panel shows evolution snapshots for the droplet formation in a particle system modeled by the Ising lattice gas in two spatial dimensions. The lower panel illustrates the pearl-necklace picture of the time evolution of a polymer. Both data are obtained from Monte Carlo computer simulations.

⇒ *Understanding nonequilibrium scaling laws governing collapse of a polymer*
S. Majumder, H. Christiansen, W. Janke / European Physical Journal B (2020) **93** 142-1–19

⇒ *Aging in the long-range Ising model*
H. Christiansen, S. Majumder, M. Henkel, W. Janke / Physical Review Letters (2020) **125** 180601-1–7

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Coordination compounds in supramolecular chemistry and materials chemistry

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

The research of our group deals with the coordination chemistry of macrocyclic ligands based on calixarene and thiophenolate units capable of forming stable complexes with d- and f-block metals. The spectroscopic and magnetic properties of the synthesised complexes are studied by a range of methods including UV/vis, IR and 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.

The macrocyclic ligand H_6L_2 comprising two bis(iminomethyl)phenol and two calix[4]arene units provides dinuclear $[Ln_2(L_2)(MeOH)_2]$ complexes (Ln = La (1), Eu (2), Tb (3), and Yb (4)) in very good yield.[2] The seven coordinated lanthanide ions are in a distorted monocapped trigonal prismatic / octahedral coordination environment. UV-vis spectroscopic titrations show that a 2:1 (metal:ligand) stoichiometry is also present in solution. The ratio $\alpha = K_{11}/K_{21}$ of the stepwise formation constants for the mononuclear ($L^2 + M = ML^2$, log K_{11}) and the dinuclear complexes ($ML^2 + M = M_2L^2$, log K_{21}) is invariably smaller than unity indicating that the binding of the first Ln^{3+} ion augments the binding of the second Ln^{3+} ion. The present complexes are less luminescent than other seven-coordinated Eu and Tb complexes, which can be traced to vibrational relaxation of excited Eu^{III} and Tb^{III} states by the coligated MeOH and H_2O molecules and/or low-lying ligand-to-metal charge-transfer (LMCT) states.

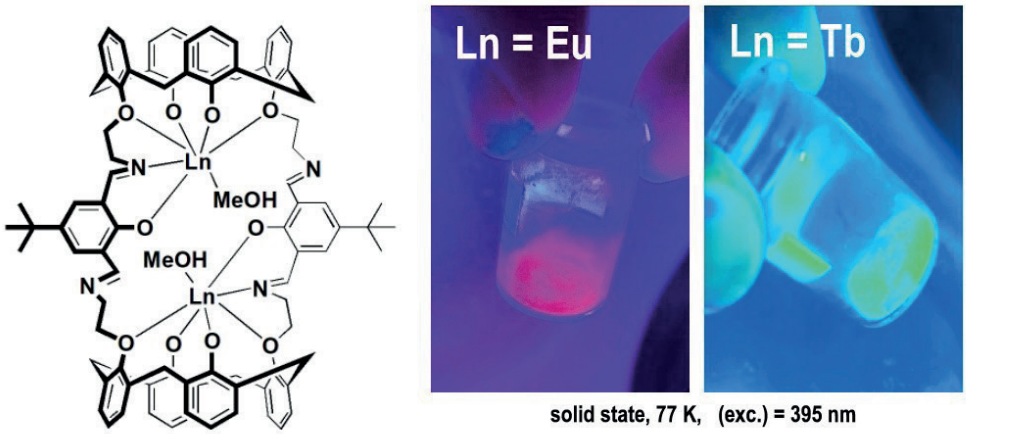
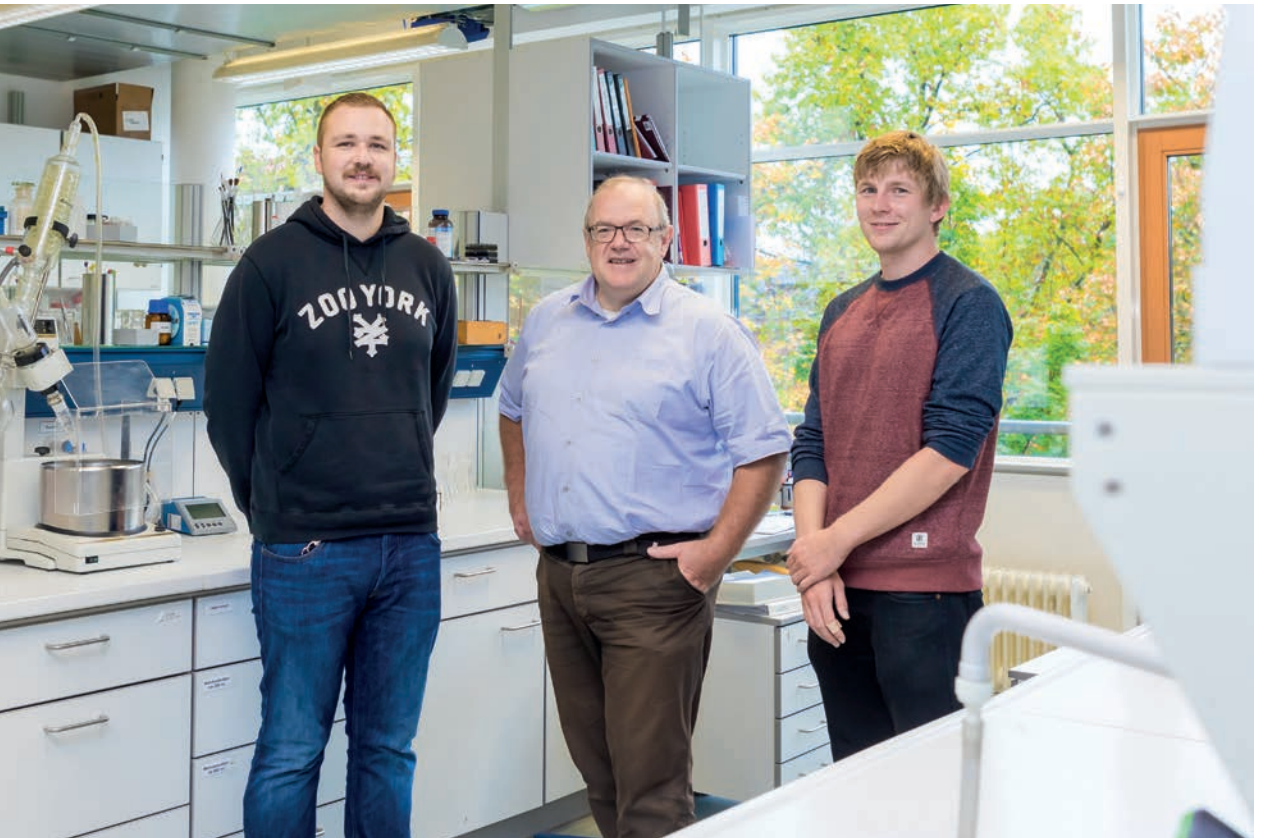


Fig. 1: Dinuclear lanthanide complexes supported by the hybrid Schiff-base calix[4]arene ligand H_6L^2.



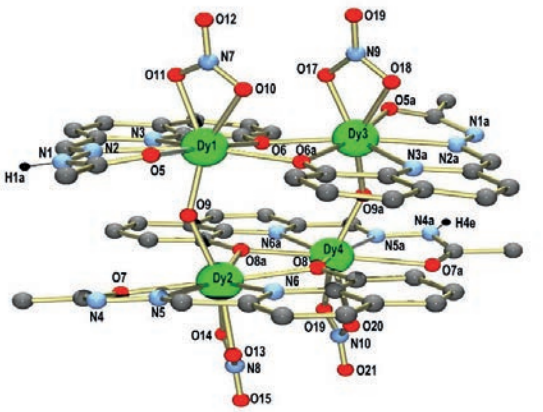


Fig. 2: Core structure of the teranuclear $[Dy_4(H_3L)_2(\mu\text{-}OH)_2(\eta^2\text{-}NO_3)_4]$ complex. The calixarene units and most H atoms are omitted for clarity.

The pendant 4-tert-butylcalix[4]arene ligand H_6L was also found to support an isostructural series of tetranuclear mixed-ligand complexes of composition $[Ln_4(H_3L)_2(\mu\text{-}OH)_2(\eta^2\text{-}NO_3)_4]$ (Ln = Tb, Dy, Yb). The complexes contain dinuclear $[Ln_2(H_3L)(OH)(NO_3)_2]$ subunits, which dimerise via the hydroxyquinoline O atoms to generate a central $[Ln_4(\mu\text{-}OH)_2(\mu\text{-}O^{Aryl})_4]$ core sandwiched between two calix[4] arene moieties. All complexes behave as paramagnetic systems, with very weak antiferromagnetic interactions. ESR experiments for a Dy complex revealed a significant g-factor anisotropy and only a small energy barrier for the spin reversal, which explains the absence of the single molecular magnet behaviour. The central cavities in both structures host additional coligands and warrants also more detailed investigations on the host-guest chemistry of these compounds.

⇒ *Dinuclear Tb and Dy complexes supported by hybrid Schiff-Base/calixarene ligands: Synthesis, structures and magnetic properties*
P. Hahn, S. Ullmann, J. Klose, Y. Peng, A. Powell, B. Kersting / Dalton Trans. (2020) **49** 10901–10908

⇒ *Mixed-ligand lanthanide complexes supported by ditopic bis(imino-methyl)-phenol/calix[4]arene macrocycles: synthesis, structures, and luminescence properties of $[Ln_2(L^2)(MeOH)_2]$ (Ln = La, Eu, Tb, Yb)*
S. Ullmann, P. Hahn, P. Mini, K. L. Tuck, A. Kahnt, B. Abel, M.E. Gutierrez Suburu, C. A. Strassert, B. Kersting/ Dalton Trans. (2020) 49 11179–11191

⇒ *Light controlled oxidation by supramolecular Zn(II) Schiff-base complexes*
C. Laube, J. Taut, J. Kretzschmar, S. Zahn, W. Knolle, S. Ullman, A. Kahnt, B. Kersting, B. Abel / Inorg. Chem. Front. (2020) **7** 4333–4346

⇒ *Tetranuclear lanthanide complexes supported by hydroxyquinoline-calix[4]arene-ligands: Synthesis, structure and magnetic properties of $[Ln_4(H_3L)_2(\mu\text{-}OH)_2(NO_3)_4]$ (Ln = Tb, Dy, Yb) and $[Dy_2(H_4L)_2(NO_3)](NO_3)$*
A. Jäschke, T. Stumpf, A. Aliabadi, B. Büchner, V. Kataev, T. Hahn, J. Kortus, B. Kersting / Eur. J. Inorg. Chem. (2020) **44** 4203–4214

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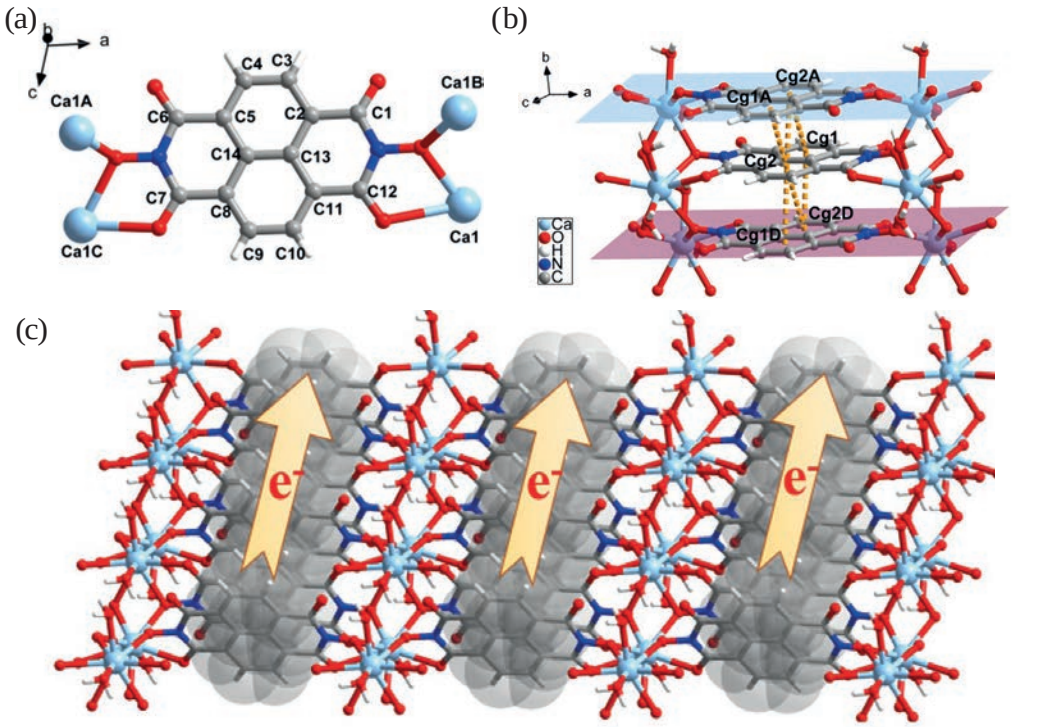
Semiconductive coordination polymers based on a redox-active hydroxamate linker

Prof. Dr. Harald Krautscheid
M.Sc. Chem. Yong Yan

Owing to their great potential in the field of electric sensors, electrocatalysis, batteries, and supercapacitors, semiconductive coordination polymers (CPs) have attracted huge attention recently. Although a few porous and conductive CPs with catecholate linkers have been constructed based on the approaches of ‘through bond’ and ‘through space’ conductivity, their specific crystal structures are not completely clear, which prevents setting up a relationship between structure and electrical conductivity. Hydroxamates feature a similar chelating behaviour as catecholates, but relevant reports are rare.

Our research focuses on the development of conductive CPs with redox-active hydroxamate linkers. By reaction of H_2ONDI (H_2ONDI = 2,7-dihydroxybenzo-

[*lmn*][3,8]phenanthroline-1,3,6,8(2*H*,7*H*)-tetraone; NDI = naphthalene diamide) with alkaline earth metal ions (Ca^{2+}, Sr^{2+}) we obtained two isostructural CPs $[Ca(ONDI)(H_2O)_2]_\infty$ (**Ca-ONDI**) and $[Sr(ONDI)(H_2O)_2]_\infty$ (**Sr-ONDI**). According to single crystal X-ray structure analyses, these CPs display continuous π-π stacking structures along the crystallographic b axis (Fig. 1). Results of DFT calculations reveal that the continuous π-stacking arrangement facilitates charge carrier mobility, which is beneficial for conductive performance. In electrical conductivity measurements both CPs show moderate conductivity of about 10^{-5} S/m.



⇑ (a) Fragment of the network and (b) continuous intermolecular π-πinteractions in **Ca-ONDI**; (c) electron transfer path in **Ca-ONDI**.

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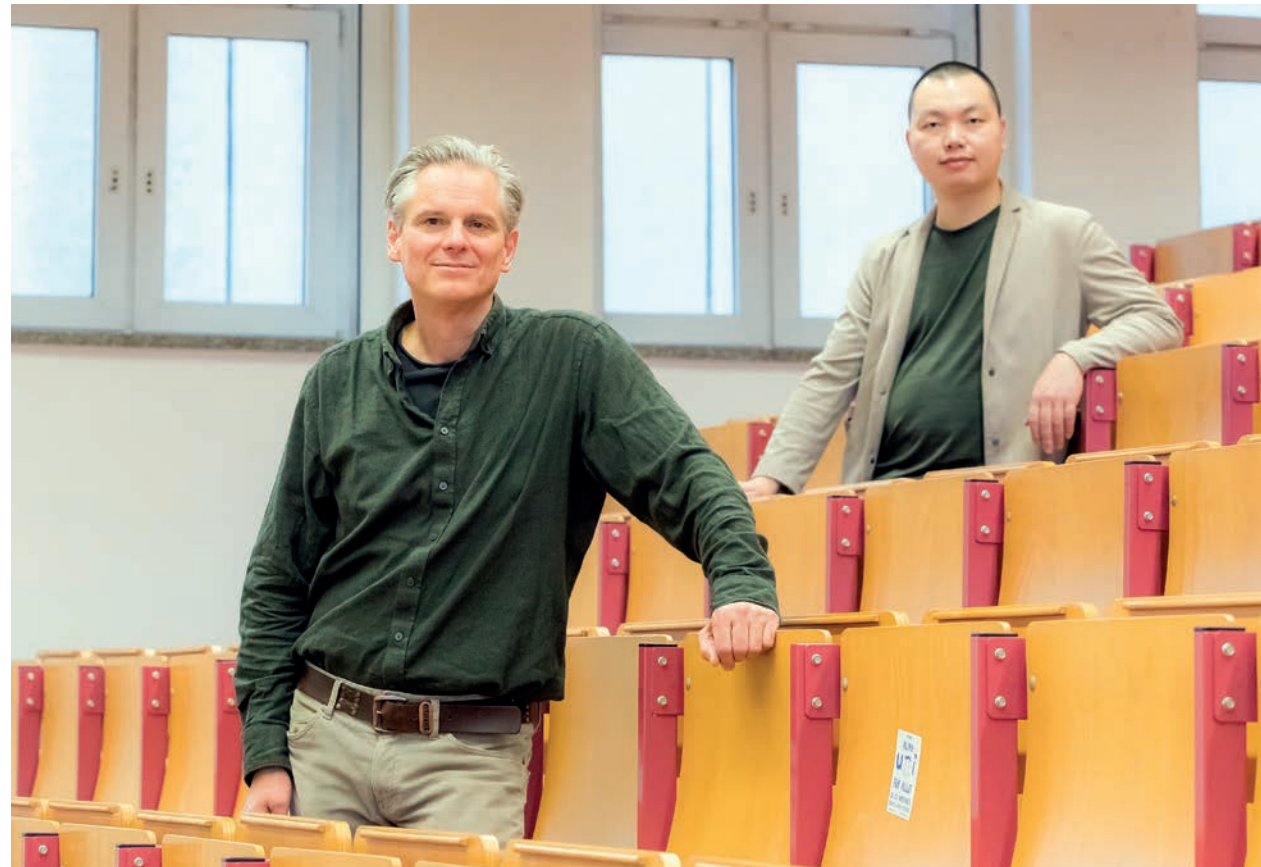
The optimisation of thermodynamic engines

Prof. Dr. Klaus Kroy
M.Sc. Phys. Constantin Huster, M.Sc. Phys. Zhuolin Ye

The performance of thermodynamic engines is usually described by two main quantities: output power and efficiency. Unfortunately, thermodynamic laws imply that they cannot be optimised simultaneously. The reason is that the largest efficiency corresponds to reversible and thus slow processes, leading to vanishingly small output power. Practical engines are therefore in general not designed to operate in the regimes of maximum efficiency or maximum power, but rather maximum efficiency at given power or vice versa. The latter received the attention of the theory of finite-time thermodynamics only recently, generalising results obtained previously for a variety of trade-off relations between power and efficiency. Essentially, by tuning the related system parameter, one can interpolate between a maximally powerful engine with efficiency at maximum power, and a reversible engine with maximum efficiency and null power.



Most of the idealised models are considered within the so-called low-dissipation assumption. In this setting, the total entropy change during isothermal branches of the working cycle of the engine is inversely proportional to the duration required for completing the isotherm. Noteworthy, the low-dissipation assumption fits quite well into at least two general realistic setups. On one hand, it can be interpreted as the first finite-time correction to the quasistatic limit. On the other hand, this setting exactly describes overdamped Brownian systems driven by special time-dependent protocols optimised for output power. Both situations were already investigated not only in theoretical studies, but also observed in experiments.

Our research mainly focus on the optimisation of lowdissipation refrigerators [1] and low-dissipation absorption refrigerators [2]. In these two papers, we derive exact expressions for the maximum efficiency at given power. These expressions allow us to obtain lower and upper bounds. They also imply that a slight decrease in power from its maximum value results in a large nonlinear increase in efficiency for a certain range of system parameters. Otherwise, the increase in efficiency is linear. This provides guidance on how to run the machine with the highest benefits.

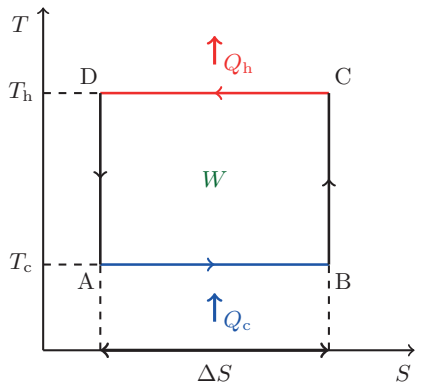


Fig. 1: Thermodynamic *T*-*S* (bath temperature-system entropy) diagram of the Carnot refrigeration cycle. The fridge uses the input work W to extract heat Q_c from the cold bath at temperature T_c during the cold isotherm (AB, blue). The used work and the extracted heat are then dumped as heat $Q_h = Q_c + W$ into the hot bath at temperature T_h during the hot isotherm (CD, red). The input work equals the enclosed area, $Q_c = T_c\Delta S$, and $Q_h = T_h\Delta S$ only if the cycle is performed reversibly. Otherwise, the work is larger and the extracted heat smaller, leading to a decreased efficiency (coefficient of performance) of the machine. The branches BC and DA (black) of the cycle are adiabats.

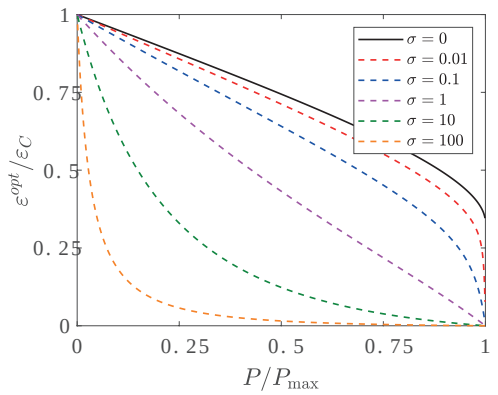


Fig. 2: The optimal efficiency, ε^{opt}, as a function of the cooling power, *P*, of the low-dissipation refrigerator for different values of the parameter σ, which measures the relative irreversibility of hot and colds isotherms.In the figure, ε_C and P_{max} denote maximum efficiency (reversible limit) and maximum cooling power, respectively. It is shown that ε^{opt} exhibits a fast nonlinear increase with power near the maximum power only for small values of σ. For large values of σ, the increase in efficiency is linear.

⇒ [1] *Maximum efficiency of lowdissipation refrigerators at arbitrary cooling power*
V. Holubec, Z. Ye / Phys. Rev. E (2020) **101** 052124

⇒ [2] *Maximum efficiency of absorption refrigerators at arbitrary cooling power*
Z. Ye , V. Holubec / Phys. Rev. E (2021) **103** 052125

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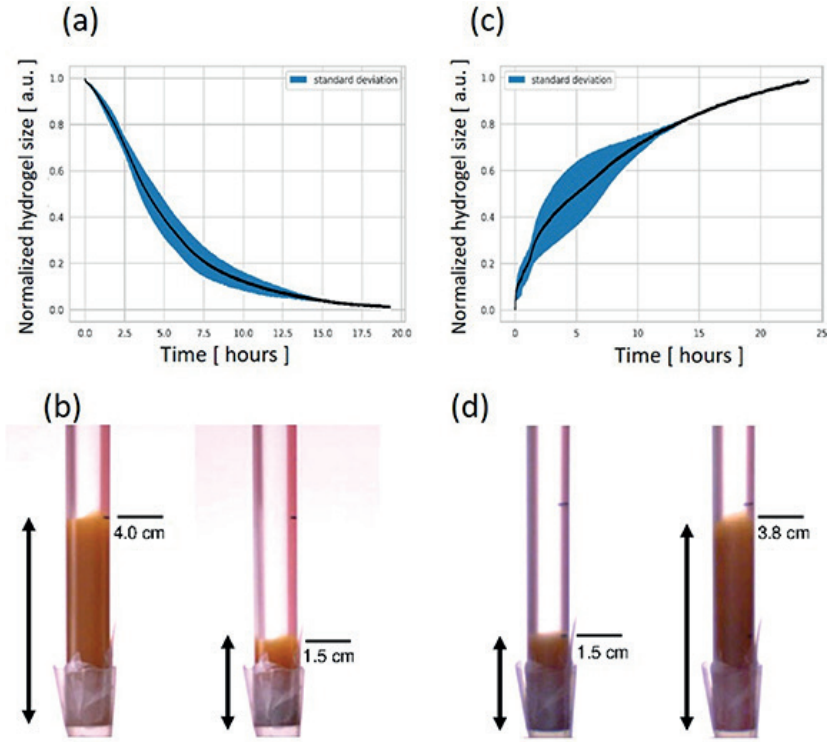
Cellular adhesion on tailored soft and hard materials

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

The surface physics research group investigates interactions of hard matter, ranging from nanoparticles to bulk materials, with soft matter, i.e. cells, proteins and hydrogels. In 2020, iron oxide nanoparticle based ferrogels with excellent stability and cytocompatibility were derived. Jauch et al. [1] show in detail that the magnetic nanoparticles do not induce any significant change of rheological characteristics of the hydrogels. In fact, storage and loss modulus as well as pore size of collagen with and without nanoparticles are similar, indicating that the network formation is not altered by the addition of nanoparticles. However, these ferrogels can be drastically deformed using an external magnetic field, see Fig. 1. Low concentrations of 0.5 mg/ml magnetic nanoparticles result in a compression of 62 % upon several hours at a magnetic field gradient of 0.32 T. By reversing the field gradient, the gel size could

be elongated to 95 % of its original size within 24 h. In addition, cytocompatibility of collagen gels stays unchanged with and without incorporated nanoparticles. Fibroblasts proliferate and migrate into the ferrogels, demonstrating a promising approach to design tailored biodegradable magnetic responsive systems.



⇑ Fig. 1: Deformation of collagen ferrogels under a magnetic field gradient of 0.32 T. Ferrogels can be cpompressed up to 62 % (see (a) and (b)) and elongated again to 95 % of their original size ((c) and (d)), adapted from [1]

⇒ [1] *Collagen–iron oxide nanoparticle based ferrogel: large reversible magnetostrains with potential for bioactuation*
P. Jauch, A. Weidner, S. Riedel, N. Wilharm, S. Dutz, S.G. Mayr / Multifunctional Materials (2020) **3**(3) 035001

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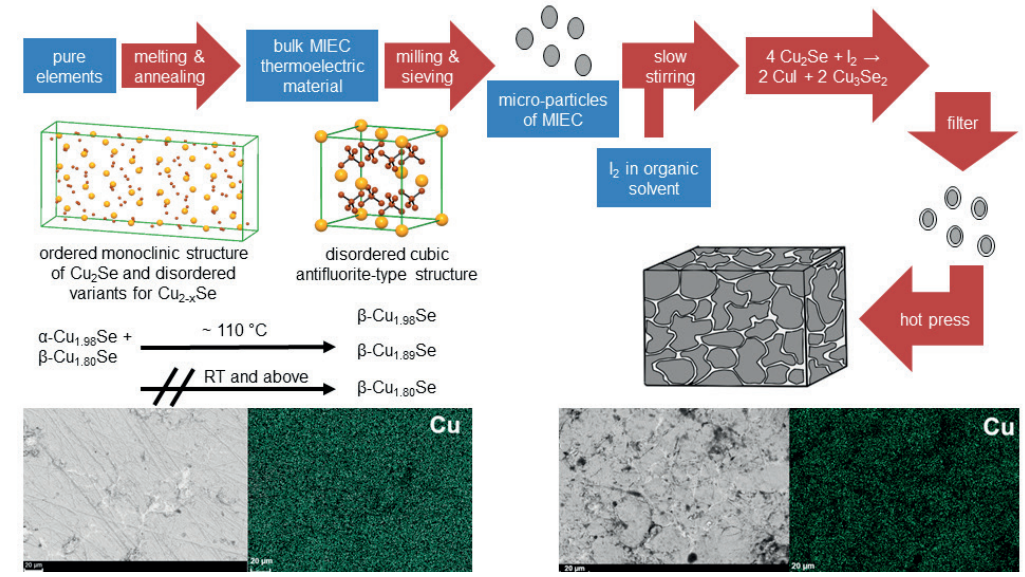
Stabilisation and optimisation of eco-friendly thermoelectric materials with mobile atoms

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

Thermoelectric materials make use of the Seebeck effect to harvest electrical energy at heat gradients. These materials have to meet several requirements to be considered for application: high electrical and low thermal conductivity, large absolute Seebeck effect as well as long-term stability under heat gradients and direct currents. Mixed ionic and electronic conductors (MIECs) have been studied in recent years because they feature high thermoelectric figures of merit *zT*. Copper chalcogenides are especially interesting due to the abundance and low toxicity of the elements they contain. However, atom mobility often involveds the serious drawback that they lead to decomposition under direct electrical current.

One objective of our research is to circumvent the critical voltage at which decomposition occurs by dividing the voltage applied on the MIECs by multiple parallel and serial connection in microstructured composites. Then, a current cannot flow only through MIECs as they are surrounded by a second phase and the local porential difference is small. With respect to second phases, e.g. graphite and CuI have been tested.

Tetrahedrite $Cu_{12}Sb_4S_{13}$ has attracted much attention, again due to its earth-abundant constituents and, in addition, because of very low thermal conductivity. As possible applications are limited by rather low thermoelectric performance, we aim at improving the transport properties of tetrahedrite, e.g. by substitution of antimony with rare earth elements.



⇑ Scheme depicting the synthesis of hierarchically structured copper chalcogenide – copper iodide composites, crystal structures of $Cu_{2-x}Se$ and SEM images as well as EDX maps of Cu_2Se/CuI (left) and Cu_2S/CuI (right) composites.

⇒ *Decomposition phenomena of $Zn_{13-\delta}Sb_{10}$ under working conditions of thermo electric generators and minimum current densities for electromigration*
M. Jakob, M. Grauer, P. Ziolkowski, O. Oeckler / ACS Appl. Energy Mater. (2020) **3** 2103–2109

⇒ *Characterisation and decomposition of the natural van der Waals $SnSb_2Te_4$ under compression*
J.A. Sans, R. Vilaplana, E.L. da Silva, C. Popescu, V.P. Cuenca-Gotor, A. Andrada-Chacón, J. Sánchez-Benitez, O. Gomis, A.L.J. Pereira, P. Rodríguez-Hernández, A. Muñoz, D. Daisenberger, B. García-Domene, A. Segura, D. Errandonea, R.S. Kumar, O. Oeckler, P. Urban, J. Contreras-García, F.J. Manjón / Inorg. Chem. (2020) **59** 9900–9918

⇒ *Hall-effect measurements and transport properties of heterostructures in the model system $NiTe_2$-$Sn_{12}Sb_2Te_{15}$*
C. Fraunhofer, S. Schwarzmüller, J.L. Gardiner, G.J. Snyder, O. Oeckler / Z. Anorg. Allg. Chem. (2020) **646** 1345–1351

⇒ *Lithium atom mobility in lithium germanium antimony tellurides elucidated by neutron diffraction and quasielastic neutron scattering*
S. Schwarzmüller, M. Hölzel, K. Fritsch, Z. Evenson, K. Habicht, O. Oeckler / J. Alloys Compd. (2020) **827** 154346

⇒ *A layered tin bismuth selenide with three different building blocks that account for an extremely large lattice parameter of 283 Å*
M. Nentwig, L. Eisenburger, F. Heinke, O. Oeckler / Chem. Eur. J. (2020) **26** 10676–10681

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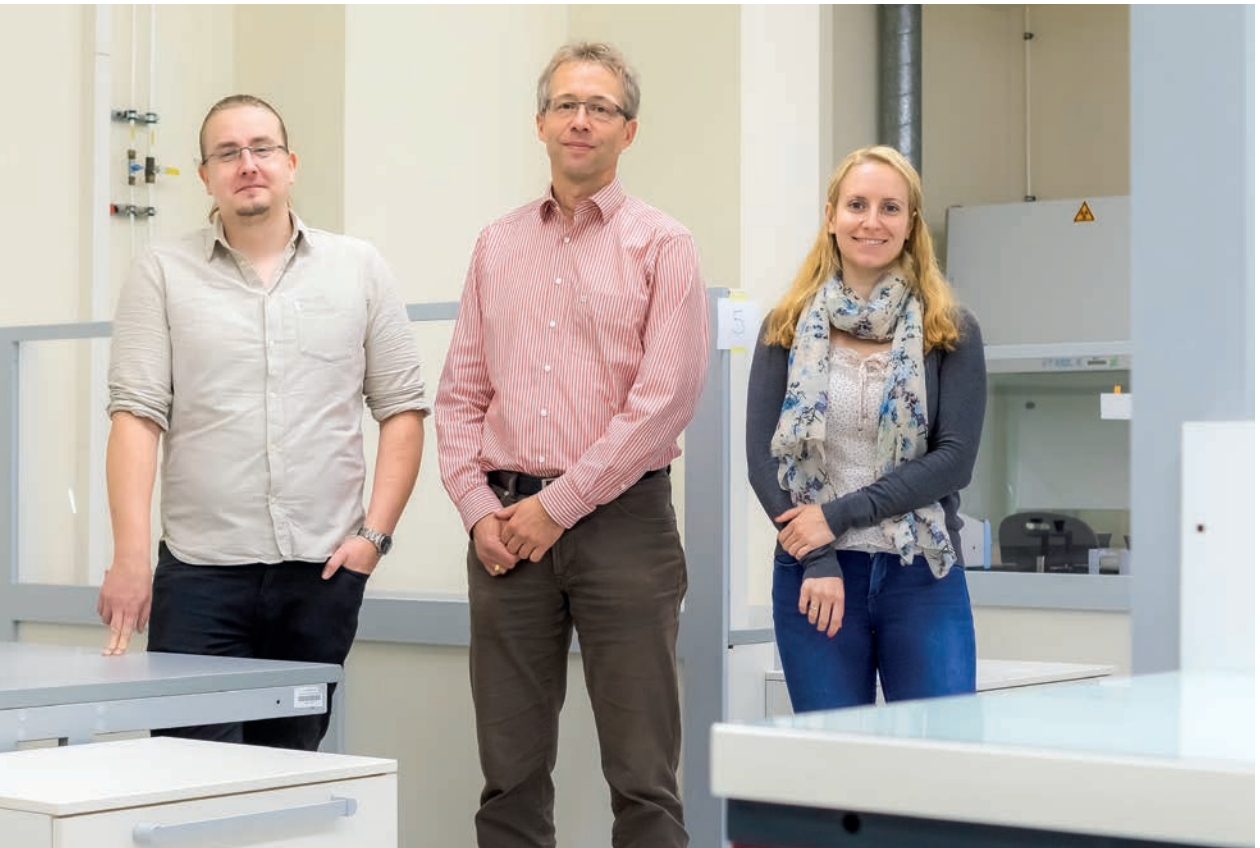
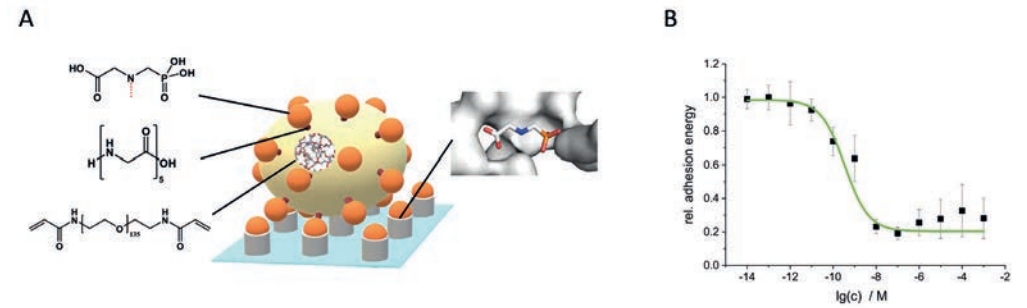
Soft colloidal probes as biomimetic sensors of low molecular weight analytes in aqueous solutions

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, reaching a detection limit of the 0.1 µg/l threshold for pesticide impurities in German tap water. 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. In this context three patent applications were filed for the SCP biosensing technology.





⇑ **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.

⇒ *Picomolar glyphosate sensitivity of an optical particle-based sensor utilising biomimetic*
D. Rettke, J. Doring, S. Martin, T. Venus, I. Estrela-Lopis, S. Schmidt, K. Ostermann, T. Pompe / Biosensors & Bioelectronics (2020) **165** 112262

⇒ *Verfahren zum Nachweis von hormonell aktiven Verbindungen, Kit und deren Verwendung*
T. Pompe, D. Rettke, F. Seufert, K. Ostermann, J. Döring, F. Seufert / Patent Anmeldenummer 10 2020 101 223.3 (2020)

⇒ *Verfahren und Kit zum Nachweis von Toxinen und Pathogenen*
L. Hannusch, G. Rödel, C. Dahmann, K. Ostermann, T. Pompe, D. Rettke / Patent Anmeldenummer 10 2020 124 279.4 (2020)

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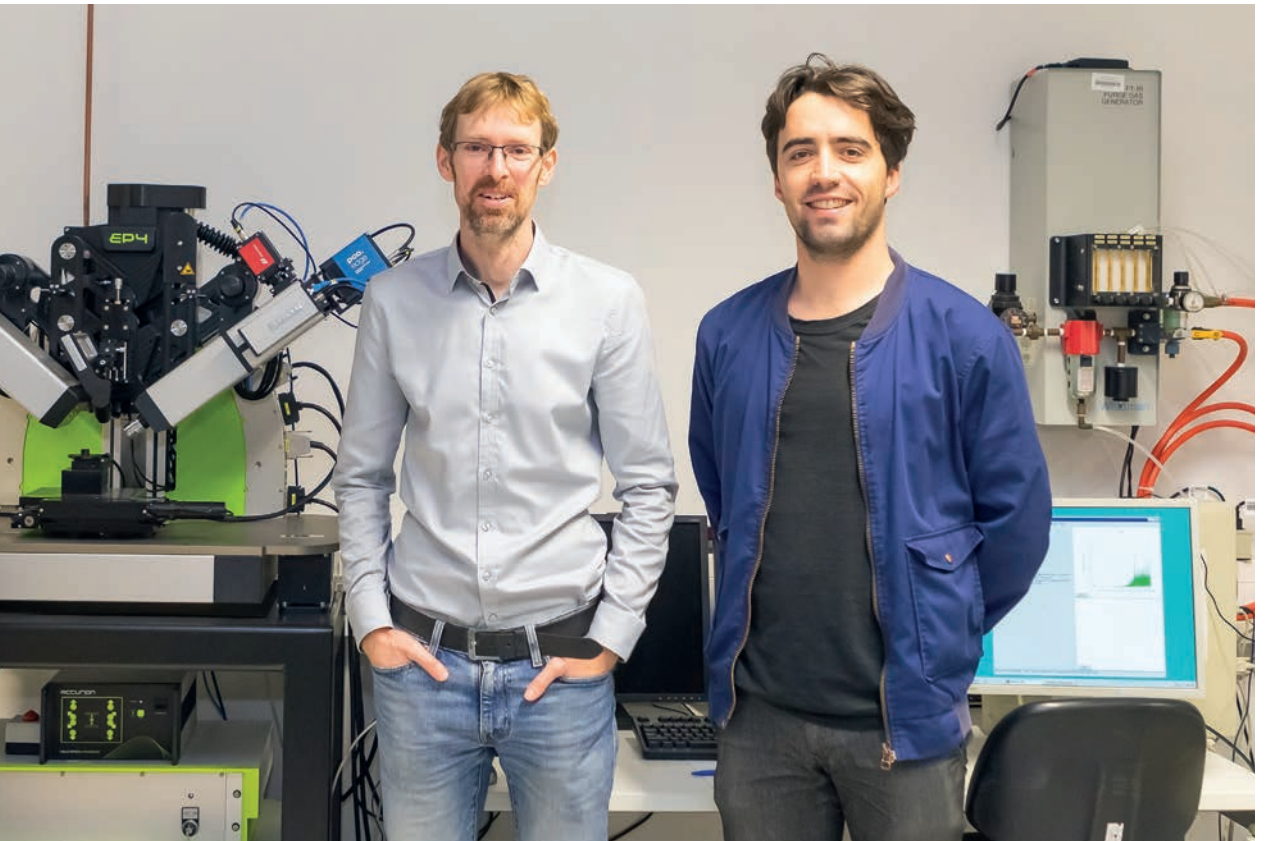
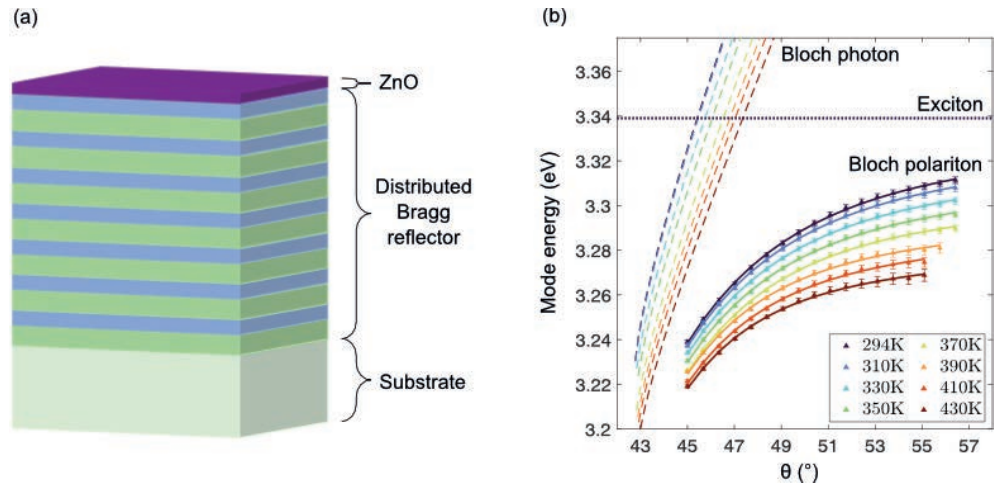
Bloch surface polaritons for long range propagation

Dr. Chris Sturm
M.Sc. Phys. Sebastian Henn

The strong coupling between two particles can lead to the formation of quasi-particles which inherit the properties of the composing particles. Of special interest are Bloch surface exciton-polaritons (polaritons) which are formed by the strong coupling between excitons and Bloch surface photons. In contrast to conventional exciton-polaritons in microcavities, the photonic part of the Bloch polaritons, i.e. the Bloch surface photons, exhibits a large in-plane momentum and cannot intrinsically couple to the surrounding environment, since they are related to surface evanescent waves. Thus, the corresponding polaritons can propagate over large distances. Furthermore, the Bloch surface photons and therewith the Bloch polaritons have a high surface sensitivity, which makes them interesting for sensing application and on-chip manipulation.



We realised such guided Bloch surface photons and polaritons in a ZnO-based structure (Fig. a). The properties of these particles were investigated numerically based on the transfer matrix approach as well as experimentally by using a prism coupler in Kretschmann-Raether configuration. In this structure we found a maximum coupling strength of about 96 meV, which can only be reached in conventional ZnO-based microcavities by using defect-free ZnO substrates as cavity material, which requires a high manufacturing effort. By means of numerical simulations we could show that the enhanced coupling strength can be attributed to the enhanced electric field strength of the surface polaritons in the active material, i.e., the ZnO layer, compared to conventional microcavities. Due to the large exciton binding energy of ZnO, which acts as active material in our structure, polaritons are stable well above room temperature and we were able to the prove the presence of the strong coupling regime up to 430 K (Fig. b). These results are promising for the realisation of devices based on polaritons with long range propagation at elevated temperatures.



(a) Schema of the structure for the realisation of the Bloch surface photons and polaritons. (b) Resonance energy of the Bloch-polaritons (symbols) as a function of incidence angle in the Kretschmann-Raether geometry for selected temperatures. The solid line represents the calculated energy. The energy of the uncoupled exciton and Bloch surface photons are shown as dotted and dashed lines, respectively.

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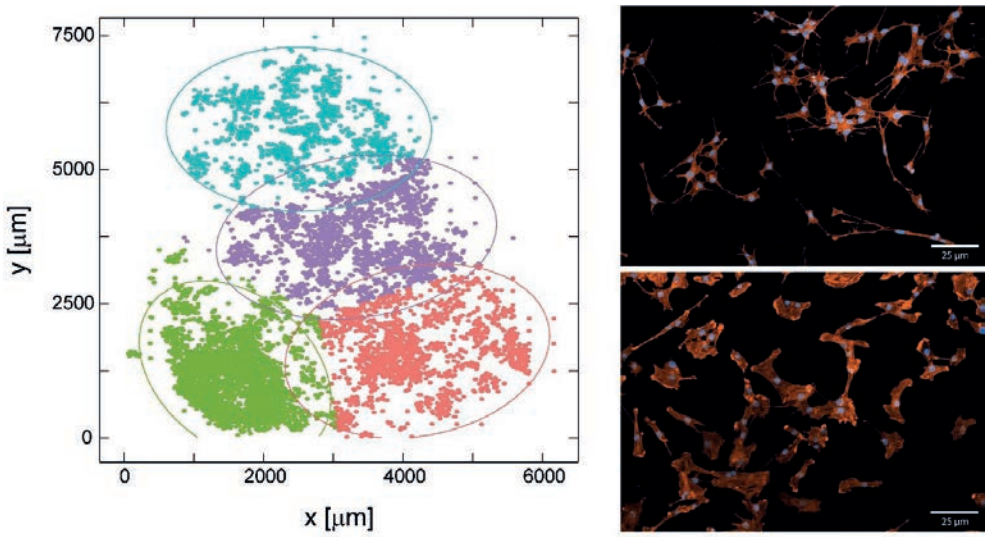
Cellular adhesion, proliferation and migration on artificial biomaterials

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

Many biomedical applications such as deep brain stimulation with electrodes for neurodegenerative diseases like Parkinson's disease rely on fine-tuned coupling of biomaterials and biological tissue. Cell survival, proliferation, adhesion, and biochemical function depend on surface topography and chemistry at the interface between electrode and biological matter. We investigate the interaction of neurons and glial cells with electrode materials such as titanium nitride (TiN) and TiN with a nanocolumnar surface patterning in contrast to gold and indium tin oxide substrates in our study [1]. We analysed cell organisation and network formation using fluorescence microscopy. Implementation of the radial autocorrelation function of the position of cells on biomaterial substrates combined with a K-means clustering algorithm allowed us to quantify cellular growth patterns and cell proliferation for different culture times. Glial cells turned out to form homogeneously distributed patterns on all substrate types. In contrast, the largest clusters of neuronal cells were found on nanocolumnar titanium nitride and cell proliferation was impaired on gold and indium tin oxide surfaces. Our study proves nanocolumnar titanium nitride as a potential candidate for bioactive material application in vitro and in vivo.



⇑ Result of application of K-means clustering algorithm on network of neurons grown on nanocolumnar titanium nitride. Fluorescence microscopy images of neurons (top) and glial cells (bottom). Actin fibers are orange and cell nuclei are coloured blue.

⇒ *Proliferation and cluster analysis of neurons and glial cell organisation on nanocolumnar TiN substrates*
A. Abend, C. Steele, S. Schmidt, R. Frank, H. Jahnke, M. Zink / Int. J. Mol. Sci. (2020) **21** 6249

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Experiences

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

Prof. Dr. Knut R. Asmis

I do not believe in numerology, but it is indeed BuildMoNa's thirteenth year, 2020, that will go into history as the year the coronavirus pandemic started. Who would have expected that a virus abbreviated with SARS-CoV-2 would change our lives so dramatically and, in many cases, irreversibly? Only now many of us start to realise, how vulnerable (with regard to many of life's different facets) our societies have become.

Also the graduate school BuildMoNa, which builds on in-person communication, was put to a stress test in 2020. To our all regret the ABC had to be cancelled at short notice (just ten days before it was planned to start), in the light of the developments regarding the Covid-19 pandemic and in response to the recommendation of our rectorate. Much of the regular (post)doctoral researcher-supervisor interactions had to be moved into the digital space and most classes were held online, instead of having them in the usual classroom environment. The BuildMoNa awards were also presented online. We all had to become experts using digital tools like Skype, Webex, BBB, Zoom and Mattermost, to just name a few, if we liked it or not.

Initially, I was very enthusiastic about digitalising work life, i.e., using teleconferencing for group meetings, attending online conferences and streaming my teaching program. I converted my office into an online studio with a headset and microphone, special lighting, multiple screens and a notepad as a drawing device. As initial frustrations with the universities band width problems went away, I tried to continuously improve my online teaching skills, which was quite frustrating at times. I missed my clickers from regular class but soon learned to efficiently incorporate queries in Zoom and BBB. However, at some point I realised, I was missing something more essential. Teaching online from (home-) office via Zoom, streaming directly from the classroom using BBB or giving a talk at a conference via Webex are great options to have, but they do not replace the excitement speaker feels, when he/she stands in-front of a crowded lecture hall, nervously looking into the attendees faces and sensing a curious interest for science as well as the soft anticipation for what one is about to say. While the annoying circumstances that a global pandemic brings with itself require us, out of respect for each other, to move many of our actions into the digital space currently, I'm feeling a stronger than before urge for face-to-face chats, conferences and classes. Let's work together to make this happen soon again, also so that graduate schools like BuildMoNa can operate at their best.

Prof. Dr. Knut R. Asmis

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

M.Sc. Chem. Max Grellmann

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. To make use of this training programme requires additional time but sometimes also provides a new interdisciplinary point of view on the own research.

Besides the educational part the participation in the modules helps the doctoral candidates 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. During this two-day conference invited speakers as well as the doctoral candidates of BuildMoNa, provide an insight in their field of research that 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. Chem. Max Grellmann

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	5							W					
Scientific symposium	R/E		SY											
Literature seminars	R/E			S		S		S		S		S		S
Guest lectures/colloquia	E		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			S	S	S	S			S	S	S	S	
					M		M				M		M	

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

Scientific and methods modules

Basic Concepts in Molecular Spectroscopy (2020-B4)

21 - 22 September 2020, online,
written exam, 2 credit points, yearly recurrence with modification, 19 participants

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

Responsible Scientist:
Prof. Dr. K. Asmis, Prof. Dr. F. Cichos, Prof. Dr. F. Kremer, Prof. Dr. K. Saalwächter

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

Quantum coherent structures: Non–Hermitian systems (2020-A3)

30 September 2020, online,
written exam, 2 credit points, bi-yearly recurrence with modification, 12 participants

The concept of a “closed” system is an idealisation. Every real system is open, i.e. at least some degree of coupling to the environment exists. The theoretical description thus requires non-Hermitian Hamiltonians or Liouvillians which have their intricacies, among them the occurrence of exceptional points (EPs). The module delivered an introduction to theoretical concepts and experimental realisations of exceptional points which possibly have applications in beyond-classical sensor sensitivities.

Responsible Scientists:
Prof. Dr. M. Grundmann, Prof. Dr. B. Rosenow

Contents:
⇒ The module contained introductory and more specialised lectures on exceptional points and non-Hermitian sy stems in general from theoretical and practical perspectives. The module was equally directed to theoretically and experimentally working students.

Scientific symposium

Chemical biology and biophysics of cancer (2020-A2)

22 - 24 September 2020, hybrid format,
written report, 2 credit points, yearly recurrence with modification, 11 participants

The BuildMoNa symposium was organised by the research group of Prof. Dr. J. Käs and dealt with 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. The speakers were:

⇒ Kristian Franze, University of Cambridge, United Kingdom
The mechano-chemical regulation of brain development and disease
⇒ Sandrine Etienne-Manneville, Institut Pasteur, France
Impact of microtubule acetylation on mechanosensitive migration
⇒ Tomasz Zielinski, Polish Academy of Sciences, Poland
Biomechanics of primary hippocampal neurons and SH-SY5Y cells in oxygen and glucose deprivation (OGD) model

⇒ Jens Januschke, University of Dundee, Great Britain
Dissecting asymmetric division of Drosophila neural stem cells by chemical genetics
⇒ Allen Ehrlicher, Mc Gill University, Canada
YAP mechanosensing in the nucleus
⇒ Kamran Hosseini, TU Dresden, Germany
EMT-induced cell-mechanical changes enhance mitotic Rounding strength
⇒ Jennifer M. Schwarz, Syracuse University, USA
How does the extracellular matrix affect the rigidity of an embedded spheroid?
⇒ Moumita Das, Rochester Institute of Technology, USA
Anomalous phase separation in co-cultures of cells with different mechanical properties
⇒ Geraldine O`Neill, The University of Sydney, Australia
Investigating the role of the biomechanical microenvironment in determining response to anti-brain cancer therapies
⇒ Emma van Bodegraven, Institut Pasteur, France
Intermediate filament heterogeneity and its role in the mechanics of glioblastoma invasion
⇒ Chase Broedersz, LMU Munich, Germany
Confined cell migration - a dynamical systems perspective
⇒ Mitchell Han, INM-Leibniz Institute for New Materials, Saarbrücken, Germany
Optoregulated force application to individual cellular receptors using molecular motors
⇒ Paul Janmey, University of Pennsylvania, USA
Viscoelastic properties of the isolated but metabolically intact nucleus
⇒ Sara Nizzero, Houston Methodist Hospital, USA
Physical targeting strategies for enhanced therapeutic efficacy: bridging physics and biology through rational design
⇒ Iman Elbalasy, Leipzig University, Germany
Elevation of keratin levels in reconstituted actin-keratin filament networks gradually increases their stress responsiveness
⇒ Alison E. Patteson, Syracuse University, USA
Control of cell shape by vimentin intermediate filaments
⇒ Michael Murrell, Yale University, USA
Traction-independent cellular flows in cell aggregates

Colloquia

Invited Speaker	Institution	Title	Date	Place
Dr. Nadine Utz	*German BioImaging Society for Microscopy and Image Analysis*	Microscopy data: challenges of research data management and first approaches	24 June 2020	*online*

Annual BuildMoNa Conference

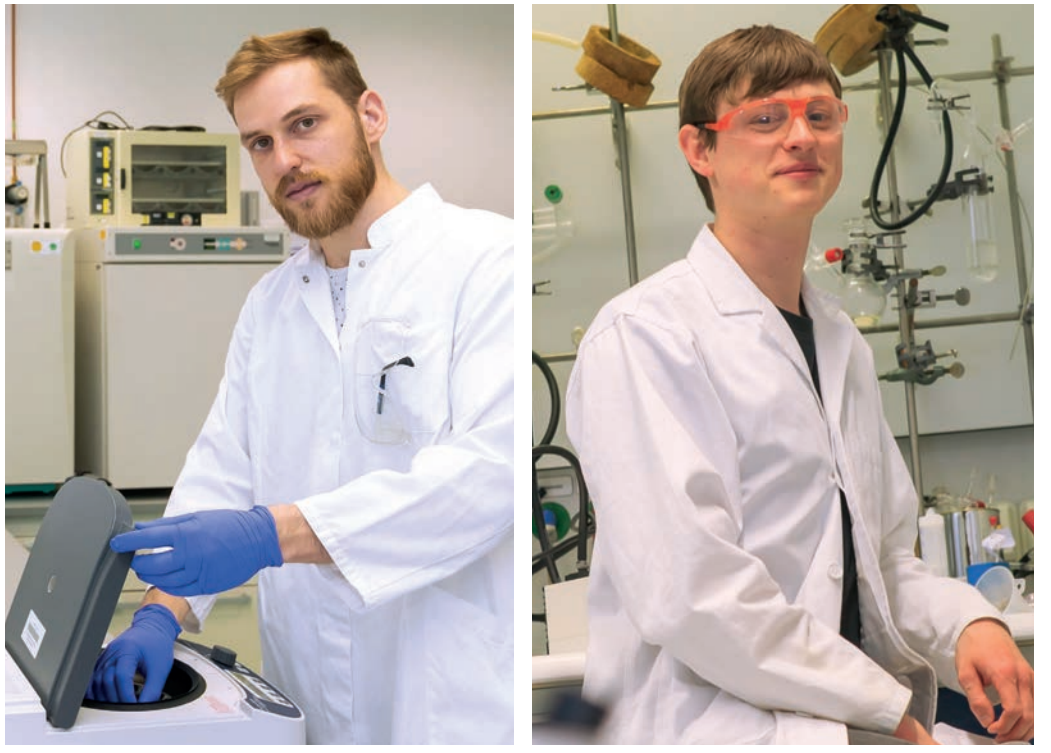
The annual conference of the Graduate School “Leipzig School of Natural Sciences – Building with Molecules and Nanoobjects” (BuildMoNa) had to be cancelled last-minute because of the Covid-19 pandemic situation.
The BuildMoNa Awards 2020 were given to doctoral candidates to recognise their outstanding scientific achievements. The Awards Ceremony was organised in a virtual format.

Martin Fränzl (Peter Debye Institute for Soft Matter Physics) received the first prize for his work on a new technique for the investigation of the amyloid formation as important factor in neurodegenerative diseases. For the first time, single amyloid fibril growth processes could be directly observed in solution. The work was published as:
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

⇑ Winner of the BuildMoNa Award 2020, Martin Fränzl (first prize).

Florian Scheffler (Peter Debye Institute for Soft Matter Physics) received the second prize for his work on the development of a hybrid drug carrier, combining micro- and nano-scale compartments, and the successful demonstration of its potential as carrier system with serum albumin as model drugs, published as:
A hybrid carrier system based on origami nanostructures and layer-by-layer microparticles
F. Scheffler, M. Brueckner, J. Ye, R. Seidel, U. Reibetanz / Advanced Functional Materials (2019) **29** 1808116

Peter Coburger (Institute of Inorganic Chemistry) received the third prize for demonstrating the extraordinary potential of carborane-substituted diphosphetanes to generate hemilabile tetradentate ligands for metal complexes in homogeneous catalysis or anionic ligands for stabilising highly unusual compounds, work published in:
Chem. Eur. J. (2019) **25** 11456 / Dalton Trans. (2019) **48** 9625 / Chem. Commun. (2019) **55** 3187



⇑ Winners of the BuildMoNa Awards 2020: Florian Scheffler (left), Peter Coburger (right).

Funding of doctoral candidates

DFG Deutsche Forschungsgemeinschaft

DAAD

GAČR
CZECH SCIENCE FOUNDATION

SAB
Sächsische AufbauBank

Europäische Union

Europa fördert Sachsen.
EFRE
Europäischer Fonds für regionale Entwicklung

Diese Maßnahme wird mitfinanziert durch Steuermittel auf der Grundlage des vom Sächsischen Landtag beschlossenen Haushaltes.

Europa fördert Sachsen
ESF
Europäischer Sozialfonds

HoME
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University of Applied Sciences

CHINA SCHOLARSHIP COUNCIL

SCIENCE WITHOUT BORDERS

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Funktionalität Oxidischer Grenzflächen
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