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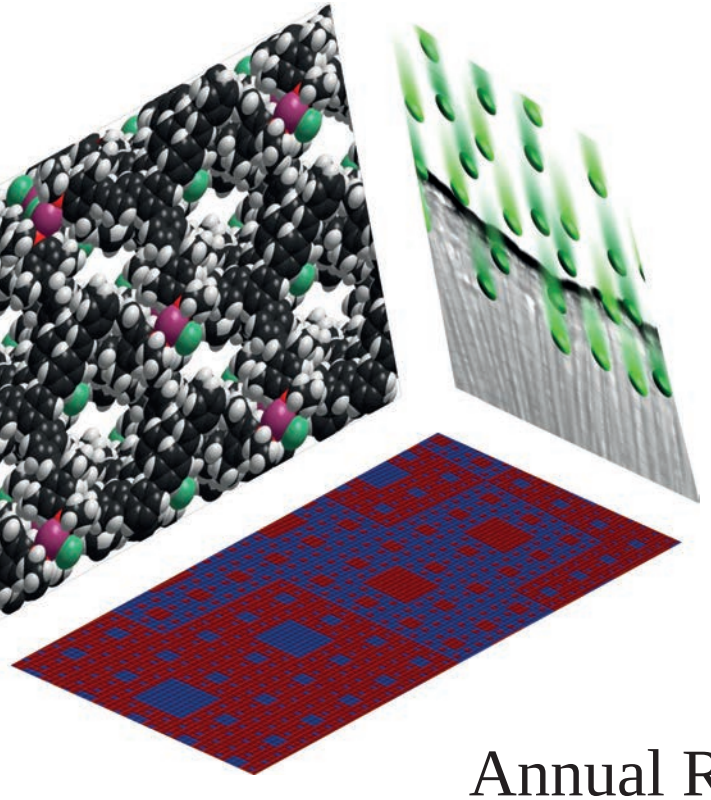
BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2021

Cover image:
⇒ *Left:* A supramolecular coordination complex in the nanometre scale formed by self-assembly of a ferrocene-based tetrakisphospholane ligand and gold(I). The nanosized molecules are stacked along the crystallographic [211] direction forming channels.
⇒ *Right:* Implantation of low-energy low-fluence carbon ions in titania nanotube scaffolds.
⇒ *Bottom:* Ising spin configuration constructed from superimposing 27^3 Menger sponges, with red (blue) corresponding to up (down) spins.

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Annual Report 2021

Founded as DFG Graduate School 185 in 2007

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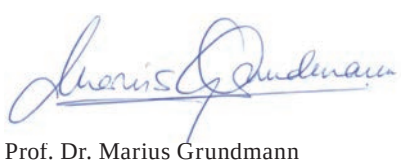
Preface
Prof. Dr. Marius Grundmann
Speaker of the Graduate School
Prof. Dr. Knut R. Asmis
Speaker of the Graduate School (beginning with October 2021)

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, 169 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.

In 2021, after the Covid-19 pandemic break, we were greatful to be able to organise the Annual BuildMoNa Conference again even though for the first time in an virtual format using the Zoom platform. The talks were given online, the poster session was held in breakout rooms and the prizes were awarded virtualy. Altough this was a great challenge for the organisers as well as for the participants, the conference was a success and the feedback positive. It can only be hoped that in the next period all the activities of the Graduate School will return to normal and the usual programme can be carried out to support excellent research and training of the doctoral researchers.



Prof. Dr. Marius Grundmann

Prof. Dr. Knut R. Asmis

Organisation and management

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M.Sc. Phys. Oliver Lahr

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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. Phys. Assem Afanah	Prof. Dr. B. Rosenow / Prof. Dr. K. Kroy / Prof. Dr. W. Janke	*Statistical mechanics of neural networks*
M.Sc. Phys. Gordei Anchutkin	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy / Prof. Dr. J. Meijer	*Dynamics of artificial active systems with delay*
M.Sc. Phys. Michael Sebastian Bar	Prof. Dr. M. Grundmann / Prof. Dr. habil. Michael Lorenz / PD Dr. habil. Holger von Wenckstern	*Electrical properties of CuI thin films and fabrication of CuI - based devices*
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. 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. Cornelia Clemens	Prof. Dr. T. Pompe / Prof. Dr. F. Cichos / Prof. Dr. K. Kroyr	*A biomimetic extracellular matrix model to reveal changes of invasive phenotypes of breast cancer cells at tissue interfaces*
M.Sc. Biochem. Anne Sophie Czerniak	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe / Prof. Dr. I. Coin	*Chemerin's structure and activity relationship*
M.Sc. Chem. Jan Dirks	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. B. Abel	*Immobilisation and applications of CyP450 proteins on surfaces*
M.Sc. Chem. Volker Eilrich	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis and applications of phosphorus-rich transition-metal phosphides*
M.Sc. Chem. Zeno Fickenscher	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting / Prof. Dr. K. Zeitler	*Investigation of heterobimetallic complexes in homogeneous catalysis*
M.Sc. Phys. Alexander Fischer	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Feedback controlled active particle assemblies*
M.Sc. 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*
B.Sc. Phys. Denis Gessert	Prof. Dr. W. Janke / Prof. Dr. F. Cichos / Prof. Dr. J. Vollmer	*High performance computing of structure formations*
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*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs	*Principles of mechanosensitivity and durotaxis in mammatian cells*
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. Ron Hildebrandt	Prof. Dr. M. Grundmann / Prof. Dr. C. Schnohr / Prof. Dr. C. Sturm	*Optical properties of copper iodide via Raman scattering*
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. Patrick Irmisch	Prof. Dr. R. Seidel / Prof. Dr. K. Kroy	*Target recognition by CRISPR-Cas enzymes*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
M.Sc. Chem. Dilara Issayeva	Prof. Dr. R. Gläser / Prof. Dr. B. Kersting / Dr. I. Titus	*Hydrogenation of CO_2 to methanol under dynamic reaction conditions: a novel concept for carbon capture and utilisation*
M.Sc. Phys. Tanja Jawinski	Prof. Dr. M. Grundmann / Prof. Dr. C. Schnohr / Dr. habil. H. von Wenckstern	*Preparation and analysis of intermediate band solar cells*
Dipl.-Math. Roger John	Prof. Dr. J. Meijer / Prof. Dr. B. Rosenow	*Coupling ^{13}C-superlattices to single nitrogen vacancy centres in diamond*
M.Sc. Chem. Aleksandr Kazimir	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler / Prof. 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. 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. Eng. Mabhoubeh Moslemi	Prof. Dr. O. Oeckler / Prof. Dr. H. Krautscheid / Prof. Dr. H. Kohlmann	*Influence on co-doping on the structures and transport properties of tetrahedrite compounds*

Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
M. Sc. Phys. Andreas Müller	Dr. C. Sturm / Prof. Dr. J. Meijer / Prof. Dr. F. Cichos	*Optical properties of CuI*
M. Sc. Phys. Jonas Naumann	Prof. Dr. M. Zink / Prof. Dr. J. Meijer / Prof. Dr. R. Seidel	*Biomechanics of the premature lung: from cell function under pressure to the development of artificial lung ECM*
M.Sc. Chem. Zahra Niavarani	Dr. A. Schulze / Prof. Dr. B. Abel / Prof. Dr. R. Gläser	*Development of molecularly imprinted membranes by electron beam irradiation*
M.Sc. Chem. Rafaella Precker	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. D. Huster	*MOFs as drug carriers for cancer therapy*
M.Sc. Chem. Ivana Predarska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. G. Kaluderovic / Prof. Dr. B. Kersting	*Development of novel dual-acting antitumour agents*
M.Sc. Chem. Kyzgaldak Ramazanova	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. K. Zeitler	*Synthesis of P-chiral bidentate phosphane ligands for applications in stereoselective catalysis*
M.Sc. 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. 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. Phys. Friedrich Schütte	Prof. Dr. J. Meijer / Prof. Dr. M. Zink / Prof. Dr. R. Seidel	*Mechanical properties in bio-derived collageneous systems*
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*

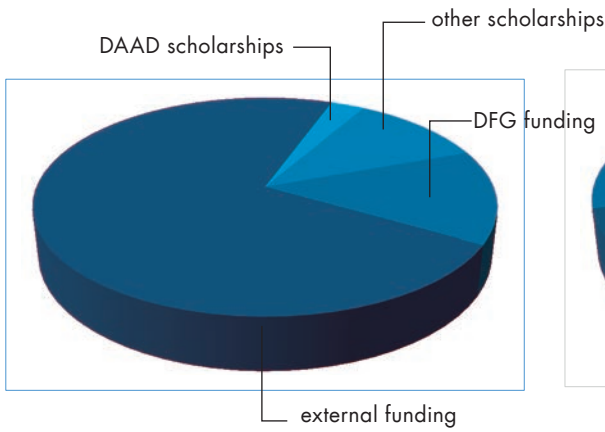
Title and Name	Thesis Advisory Committee	Working title of doctoral thesis
M.Sc. Phys. Nicola Söker	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Thermo-osmosis for manipulating microscopic liquid flow fields*
M.Sc. Chem. Lennart Staab	Prof. Dr. O. Oeckler/ Prof. Dr. H. Krautscheid / Dr. C. Benndorf	*Stability 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*
M.Sc. Chem. Lea Ueberham	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting / Prof. Dr. J. Pietzsch	*Development of carborane-based inhibitors for theranostic approaches*
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. 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. Eng. Jingjing Yu	Prof. Dr. M. Grundmann / Prof. Dr. M. Lorenz / Prof. Dr. H. Krautscheid	*Heteroepitaxial growth and microstructure of ultrawide bandgap germanate complex oxides thin films*

Alumni 2021

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Henrik Christiansen	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Nonequilibrium investigation of (bio-)physical systems*
Dr. rer. nat. Tobias Fischer	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe	*Identification of chemerin function*
Dr. rer. nat. Anna Hassa	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Deep UV photodetector arrays based on large bandgap oxides*
Dr. rer. nat. Oliver Herrfurth	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Femtosecond-time-resolved spectroscopic ellipsometry and its application to ZnO-based structures*
Dr. rer. nat. Lukas Trefflich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Fabrication and characterisation of carbon-nanodot-based planar microcavities*
Dr. rer. nat. Philipp Wolf	Prof. Dr. A. G. Beck-Sickinger / Prof. Dr. T. Pompe	*Selective drug uptake via peptide-mediated internalisation of the endothelin system*

Statistics

FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



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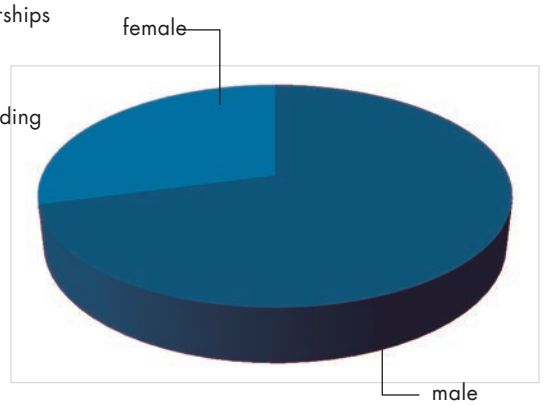

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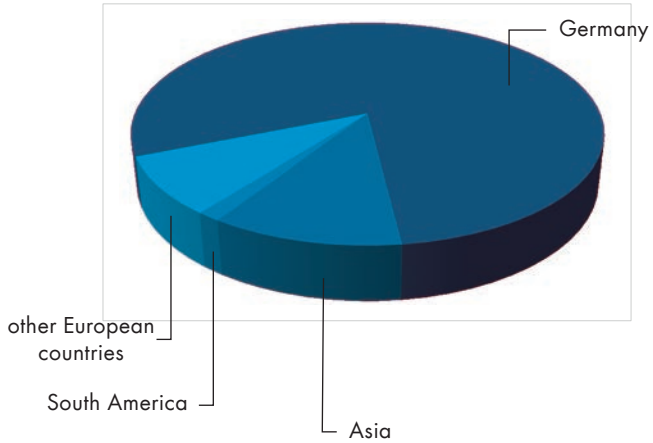


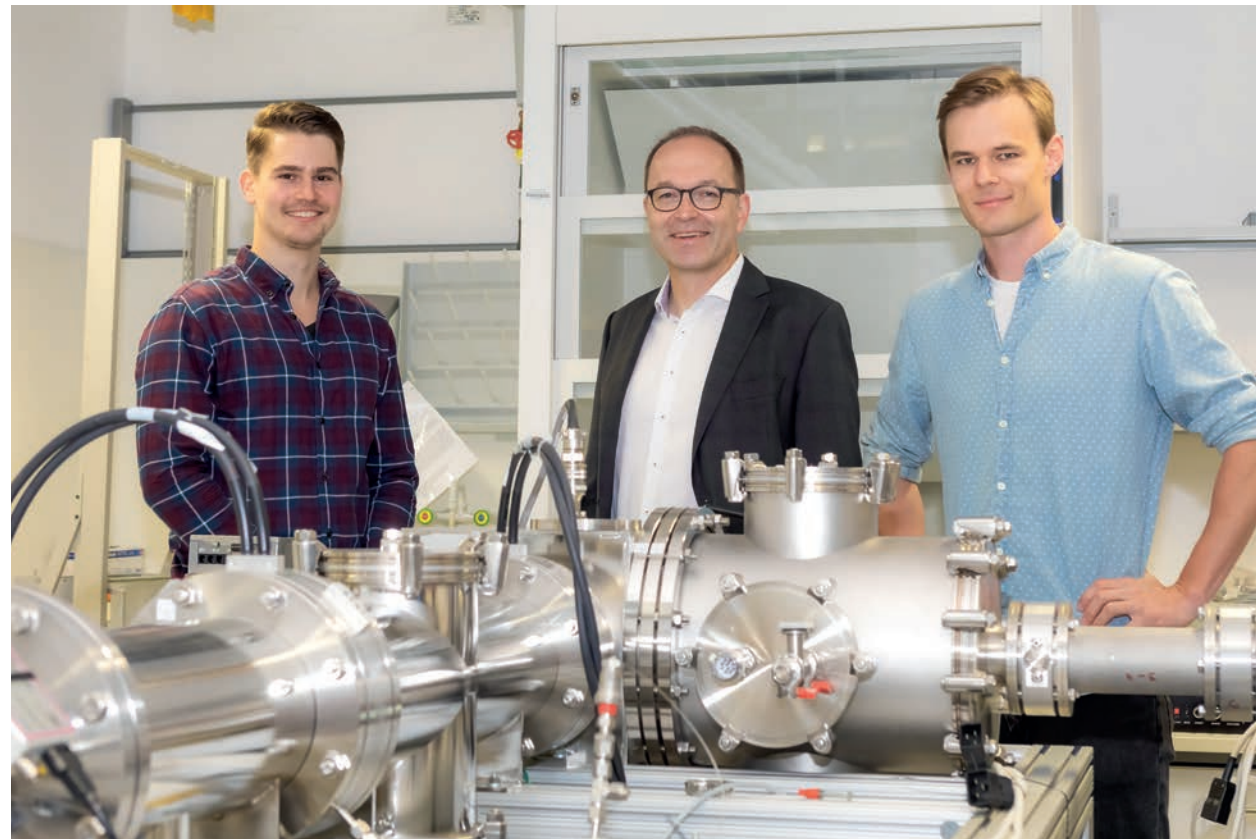
Bridging the gap between isolated nanoscale particles in the gas phase and condensed matter

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

The goal of the Asmis group is to bridge the information gap between the properties of small gas-phase clusters, heterogeneous nanoparticles and condensed matter in order to adress fundamental issues concerning heterogeneous catalysis, aerosol nucleation, ion solvation or the development of functional materials at the molecular level. To this end, cutting-edge mass spectrometric as well as laser and particle spectroscopic methods are being further developed in order to gain insight into the structure, reactivity and dynamics of clusters, NPs and ions in solution under precisely controllable conditions.

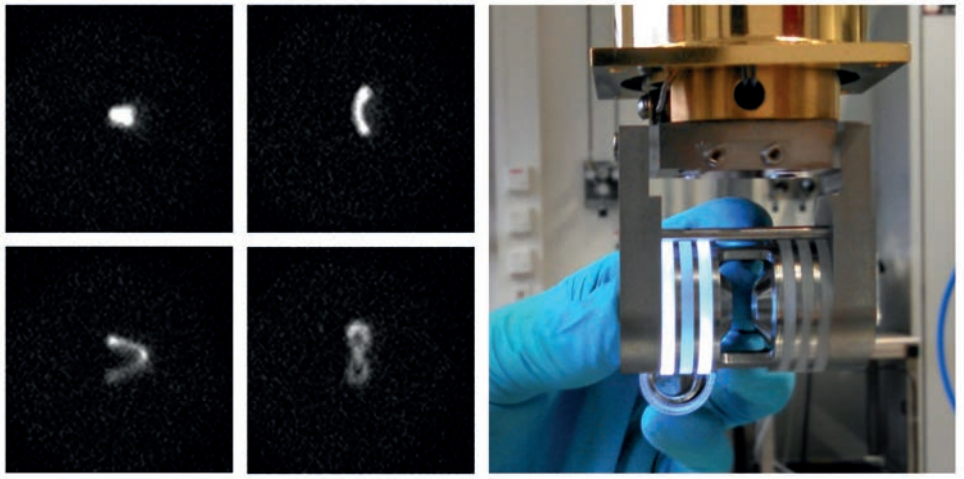
Single Nanoparticle Mass Spectrometry

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. For this



purpose, a novel NP mass spectrometer that allows to quasi-continuously and non-destructively monitor the absolute mass of a single NP is used. The heart of the instrument consists of a temperature-controllable (10-350 K) Paul-type ion trap that enables precisely controlled adsorption of inert gaseous compounds, e.g. N_2 or noble gases, onto the NP. Absorption of electromagnetic radiation from a tunable, quasi-continuous, supercontinuum laser (400 800 nm) is detected indirectly by monitoring the change in mass at low temperatures and thereby gain spectroscopic information about the electronic structure of NPs.

Gold NPs exhibit a surface plasmon resonance in the visible regime that is sensitive to the size, shape and surface of the NP. While measuring spectra of single 40 55 nm diameter Au NPs, Benjamin Hoffmann observed two unexpected effects: First, the plasmon resonance is red shifted by about 60 nm compared to the calculated value of pure Au NPs in vacuum and second, the plasmon resonance can be quenched in a stepwise fashion by heating the isolated NP with sufficiently high laser power. This behaviour can be modelled by assuming the formation of a refractive surface layer as a result of impurities in the vacuum chamber during trapping and heating the particle. The data thus suggest that the surface of the NPs can be chemically manipulated during the experiment to affect the spectral position and intensity of the plasmon resonance.



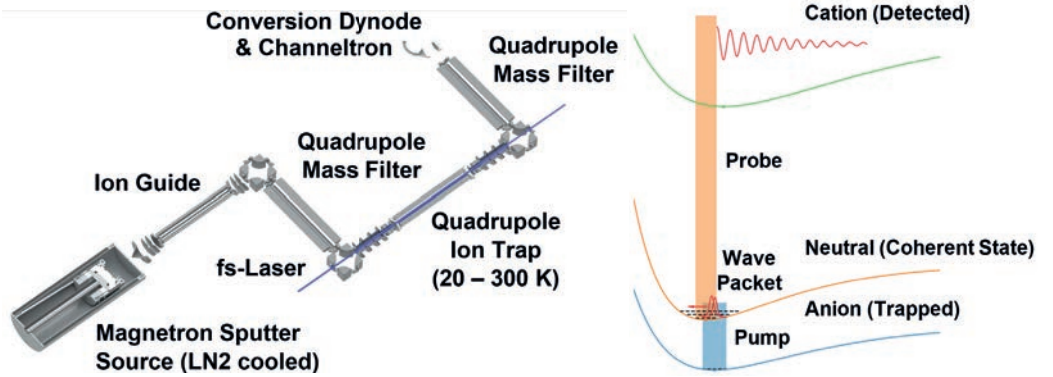
⇑ Characteristic oscillations of a trapped 100 nm particle in the ion trap (left) and image of the custom made quadrupole ion trap (right).

Lately, efforts are made to extend the method to the IR range, which would provide insight into 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 using electromagnetic fields as usual due to the lack of charge. This problem is overcome in femtosecond Negative-Neutral-Positive Spectroscopy (fs-NeNePo Spectroscopy). Here, mass-selected anions AB^- are photoionised by means of a fs pump laser pulse and transferred into the neutral charge state AB. The wave packet dynamics are interrogated after a variable time interval Δt by the fs probe laser pulse, which causes a photoionisation, that of the neutral cluster AB into the cationic state AB^+. The intensity of the mass-selected cation current is measured as a function of the delay time Δt and visualised 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. He investigated small silver clusters and observed wave packet dynamics on the electronic ground state of Ag_2 and Ag_4 in dependence of the ion trap temperature and the pump laser photon wavelength. By increasing the pump laser photon energy, wave packet dynamics on selectively chosen excited electronics state of these silver cluster species could also be observed. By comparison with results from quantum chemical calculations, geometric structures of the different electronic states of the neutral species can be identified. Currently, wave packet dynamics in Ce_2 and Ce_3 are studied to observe potential f-electron correlation effects.



⇑ Custom-built tandem mass spectrometer (left) and fs-NeNePo excitation scheme (right)..

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Chemical modification of peptides and proteins for drug design

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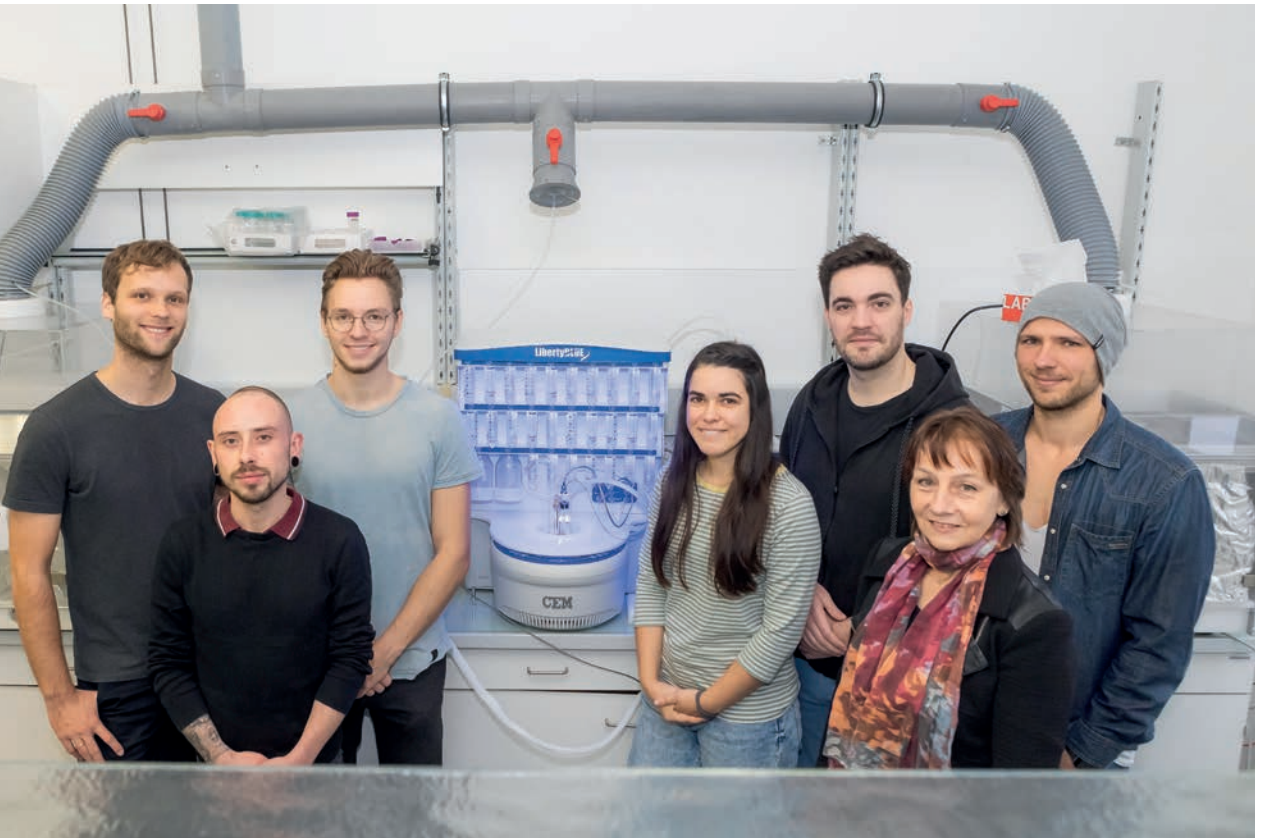
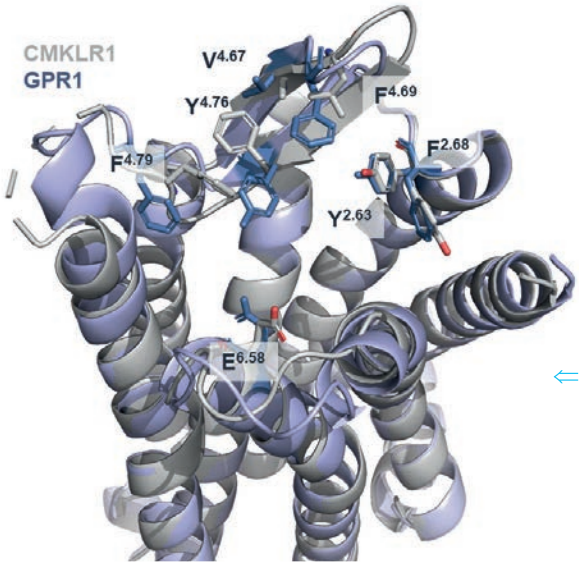
The synthesis and characterisation of chemically modified peptides and proteins to modulate their function is the common goal of the project. This includes proteins involved in tumor targeting, proteins for nanomedicine or biomaterial development. In this process, the peptides are synthesised by solid-phase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

In the summer of 2021, both Philipp Wolf and Tobias Fischer graduated with summa cum laude. Philipp Wolf left the group in July 2021 for a post doc position in the Faculty of Veterinary Medicine, Tobias Fischer stayed in the group with a postdoc position until February 2022 and then accepted a position in industry. No new members of the group joined BuildMoNa.



Tobias Fischer, Anne Czerniak and Kevin Kretschmer 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 worked on the modelling of chemerin receptors. Anne Czerniak works in the field of chemerin signalling. Kevin Kretschmer focused on the full length chemerin, managed to recombinantly express the protein and use native chemical ligation for modification. Three manuscripts in high impact journals (Cancer; Cell. Mol. Life Sci; J. Med. Chem.) have been published by the team, which demonstrates the excellent collaboration of them. These manuscripts describe the stabilisation of a small peptide ligand and its suitability as shuttle peptide as well as the identification of its binding mode at the GPR1 and CMKLR1. Moritz List takes up the concept of peptide-mediated shuttling, but focuses on methods to get the compounds out of the endosome. Receptor-mediated endocytosis usually transfers the constructs into the endosome. Moritz List efficiently applied and compared different endosomal escape strategies that are highly relevant for the overall concept.



⇐ Comparison of the binding pocket of the C-terminal chemerin peptide at the chemerin receptors CMKLR1 and GPR1.

The thesis of Philipp Wolf is devoted to the chemical modification of receptor proteins by peptide-templated ligation strategies. He applied the introduction of fluorophores to the endothelin-system and identified differences in the internalisation pathways by using small and selective peptides. Furthermore, he demonstrated the modification of GPCRs with peptide-nucleic acid, that leads to indirect and erasable labelling, and has been published in Nature Chem.

Jan Dirks investigates protein expression and chemical modification of enzymes. He worked on the engineering of BM3-P450 protein, a 112 kDa large member of the cytochrome family consisting of three domains. He succeeded in expression and the synthesis of photoactivatable linker to induce activity by light. Dennis Böhner

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. Most successful was the coating with antimicrobial peptides.

In addition to current members, several papers from former BuildMoNa-members have been published, including Sylvia Els-Heindl and Tristan Zellmann. Here, the papers from Sylvia Els-Heindl, in which we studied inverse agonists of the ghrelin receptor system have to be mentioned. As this manuscript includes radiolabeling and in vivo studies, it took more time until the data have been finalised and published in Oncotarget. A further manuscript, published in Science in 2021 describes an unusual signaling of Y2 receptors after inverse immobilisation. This is a nice combination of bio-materials and receptor signaling, as only the combination of both let to the identification of this event.

⇒ *Cyclic derivatives of the chemerin C-terminus as metabolically stable agonists at the chemokine-like receptor 1 for cancer treatment*
T. F. Fischer, A. S. Czerniak, T. Weiß, T. Zellmann, L. Zielke, S. Els-Heindl, A. G. Beck-Sickinger / Cancers (Basel) (2021) **13** 3788

⇒ *Ligand-binding and -scavenging of the chemerin receptor GPR1*
T. F. Fischer, A. S. Czerniak, T, Weiß, C. T. Schoeder, P. Wolf, O. Seitz, J. Meiler, A. G. Beck-Sickinger / Cell. Mol. Life Sci. (2021) **78** 6265

⇒ *The ring size of monocyclic ET-1 controls selectivity and signaling efficiency at both endothelin receptor subtypes*
P. Wolf, A. G. Beck-Sickinger / J. Pept. Sci. (2021) **27** e33256

⇒ *Development of a ghrelin receptor inverse agonist for positron emission tomography*
R. Bergmann, C. Chollet, S. Els-Heindl, M. Ullrich, N. Berndt, J. Pietzsch, D. Máthé, M. Bachmann, A. G. Beck-Sickinger / Oncotarget. (2021) **12** 450

⇒ *Cyclic analogues of the chemerin C-terminus mimic a loop conformation essential for activating the chemokine-like receptor 1*
T. F. Fischer, C. T. Schoeder, T. Zellmann, J. Stichel, J. Meiler, A. G. Beck-Sickinger / J. Med. Chem. (2021) **64** 3048

⇒ *Photoinduced receptor confinement drives ligand-independent GPCR signaling*
M. F. Sánchez, S. Els-Heindl, A. G. Beck-Sickinger, R. Wieneke, R. Tampé / Science (2021) **371** eabb7657

⇒ *Strategies for site-specific labeling of receptor proteins on the surfaces of living cells by using genetically encoded peptide tags*
P. Wolf, G. Gavins, A. G. Beck-Sickinger, O. Seitz / Chembiochem. (2021) **22** 1717

⇒ *Live cell PNA labelling enables erasable fluorescence imaging of membrane proteins*
G. C. Gavins, K. Gröger, M. D. Bartoschek, P. Wolf, A. G. Beck-Sickinger, S. Bultmann, O. Seitz / Nat. Chem. (2021) **13** 15

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Spontaneuous polarisation of active particles in activity landscapes

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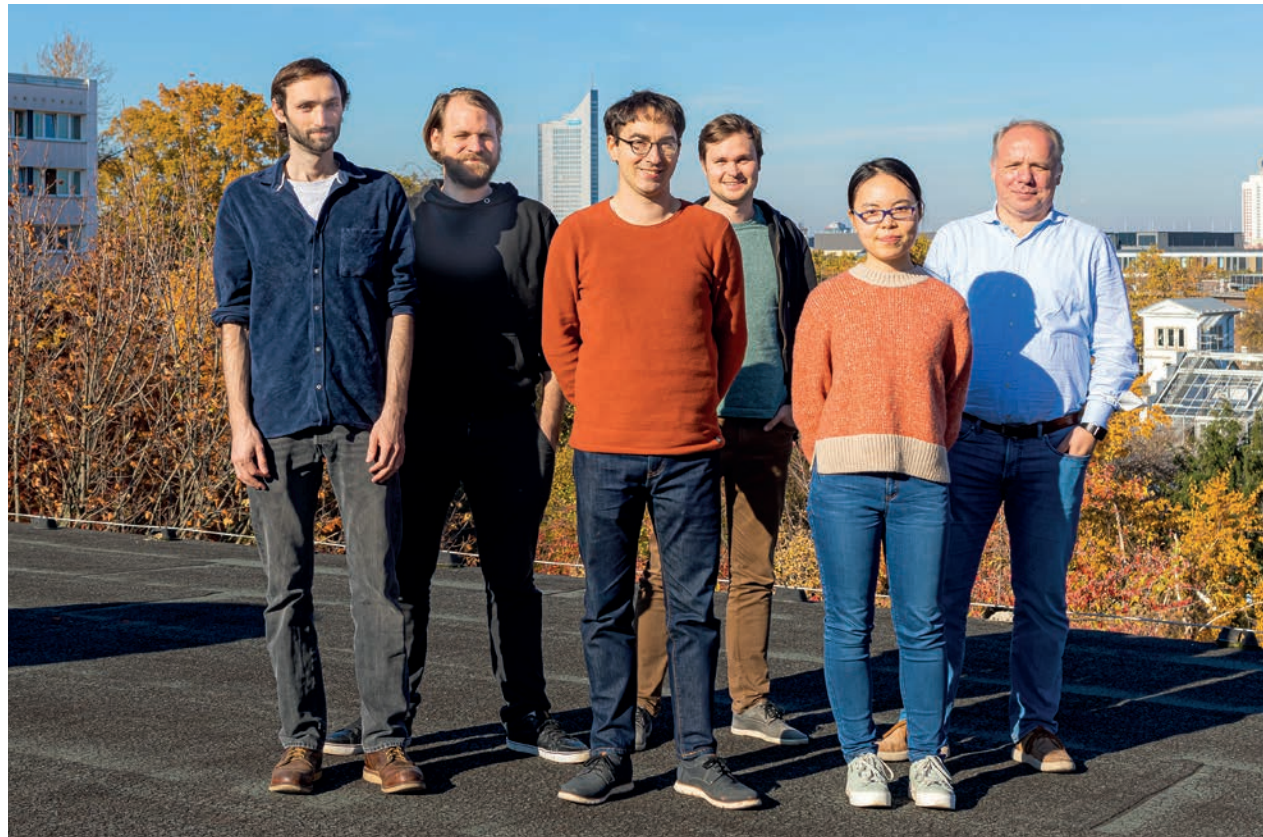
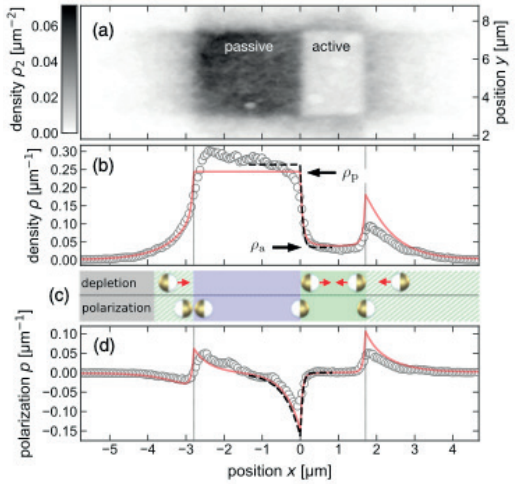
Motile active matter is unlike conventional matter powered from within. Its constituents convert local energy into motion and are therefore constantly out of equilibrium, while conventional matter is supplied with energy across its boundaries. Therefore, active matter can exhibit unusual material properties that would be strictly forbidden in conventional materials by symmetries implicit in the condition of thermal equilibrium. The non-equilibrium nature of active systems results in a plethora of emergent phenomena that are observed in living matter being the largest class of active matter systems. In recent years, researchers have developed different types of synthetic active particles, which mimic some basic properties of living active particles. They break the symmetry of low-Reynolds number hydrodynamics by a shape asymmetry or asymmetric energy conversion to propel along their symmetry axis.

We explore how fundamental concepts such as detailed balance transfer to these



non-equilibrium systems. We have therefore developed a sophisticated technique that allows us to confine active particles in virtual containers by feedback control actuation of the particles called photon-nudging. In these arenas, we can carry out experiments without physical wall interactions to explore fundamental physical phenomena. One of those is the behaviour of active particles at boundaries between regions of different activities. We find that active particles densities scale inversely with the activity (particle speed) such that a density difference appears between regions of different activity. Yet the bulk densities do not create a bulk active pressure. Yet, particles exhibit a spontaneous polarisation at the boundary without any external force providing an orientation. Nevertheless, this polarisation can be linked to what is known as the active particle pressure, which is commonly thought as the pressure induced on a boundary due to the active propulsion of the particles. Our work on the appearing polarisation has been published in Physical Review Letters [2].



⇐ Fig. 1: Density of trajectory points (top, middle) of an active particle with different speeds (left right) and polarisation (bottom).

⇒ [1] *Fully steerable symmetric thermoplasmonic microswimmers*
M. Fränzl, S. Muiños-Landin, V. Holubec, F. Cichos / ACS Nano (2021) **15** 3434

⇒ [2] *How activity landscapes polarise microswimmers without alignment forces*
N.A. Söker, S. Auschra, V. Holubec, K. Kroy, F. Cichos / Phys. Rev. Lett. (2021) **126** 228001

⇒ [3] *Polarisation-density patterns of active particles in motility gradients*
S. Auschra, V. Holubec, N.A. Söker, F. Cichos, K. Kroy / Phys. Rev. E (2021) **103** 062601

⇒ [4] *Towards measuring the Maxwell–Boltzmann distribution of a single heated particle*
X. Su, A. Fischer, F. Cichos / Front. Phys. (2021) **9** 669459

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Nanostructured materials for sustainable catalytic applications

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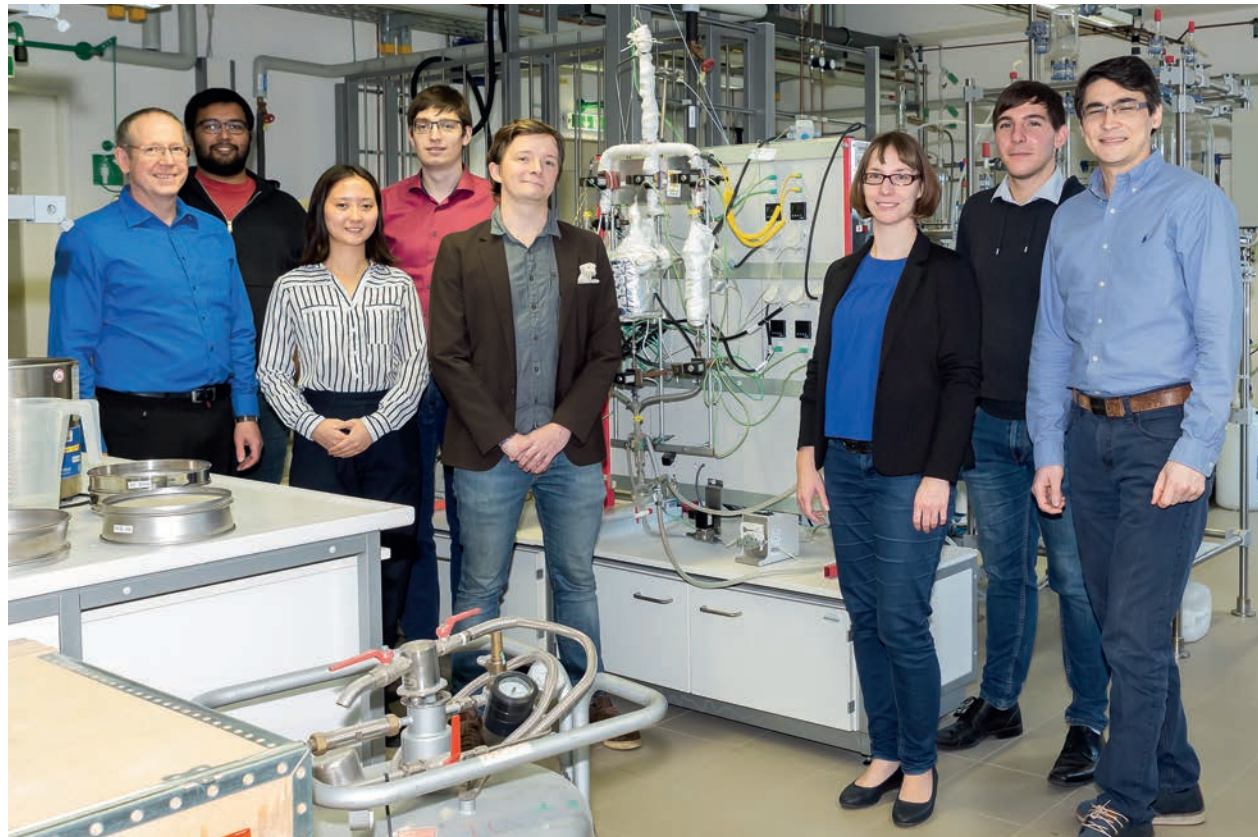
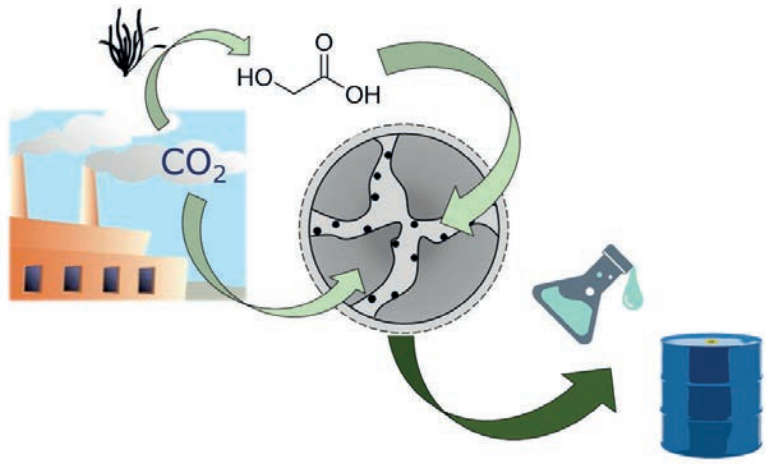
A major focus of our group is to tailor the properties of solid nanoporous catalysts for various applications, including CO_2 utilisation and biomass utilisation. Recently, we investigated the role of support materials for the selective hydrogenation of algae-derived glycolic acid (GA) to ethylene glycol (EG), an industrially demanded polymer precursor. Our group identified TiO_2- and ZrO_2-supported Ru catalysts as the most active metal-support combinations for the selective conversion of GA to EG in the aqueous phase. These catalysts exhibit favorable metal-support interactions, which enhance the reduction of Ru nanoparticles in the catalyst.

Prior to its chemical conversion, CO_2 must be captured from point sources or ambient air. Our group uses porous mesoporous silica surface-functionalised with amines, which chemisorb CO_2 in the form of carbamates even at low atmospheric CO_2 concentrations. In a collaboration with group pf Prof. Matysik, we recently



found that MAS NMR can be used for the quantitative investigation of CO_2 capture on porous solids. For CO_2 utilisation, our group investigates Ni-containing monolithic catalysts based on Al_2O_3 and ZrO_2, both with a hierarchical meso-/macropore system for CO_2 hydrogenation to methane. In particular, Ni/Al_2O_3 methanation catalysts were treated under artificial coking conditions to study the presence and location of carbon deposits forming during CO_2 hydrogenation reactions.



⇑ Schematic representation of the CO_2 utilisation and biomass conversion strategies using nanoporous solid catalysts investigated in the Gläser group.

⇒ *Selective hydrogenation of glycolic acid to renewable ethylene glycol over supported ruthenium catalyst*
F. M. Harth, M. Goepel, R. Gläser / ChemCatChem (2021) **14** e202101275

⇒ *Flow MAS NMR for in situ monitoring of carbon dioxide capture and hydrogenation using nanoporous solids*
M. Wenzel, M. A. Zaheer, D. Issayeva, D. Poppitz, J. Matysik, R. Gläser / J. Phys. Chem. C (2021) **125** 10219

⇒ *Hard X-ray nanotomography for 3D analysis of coking in nickel-based catalysts*
S. Weber, D. Batey, S. Cipiccia, M. Stehle, K. L. Abel, R. Gläser, T. L. Sheppard / Angew. Chem. Int. Ed. (2021) **60** 21772

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Thin film electronics from amorphous oxide and halogen semiconductors

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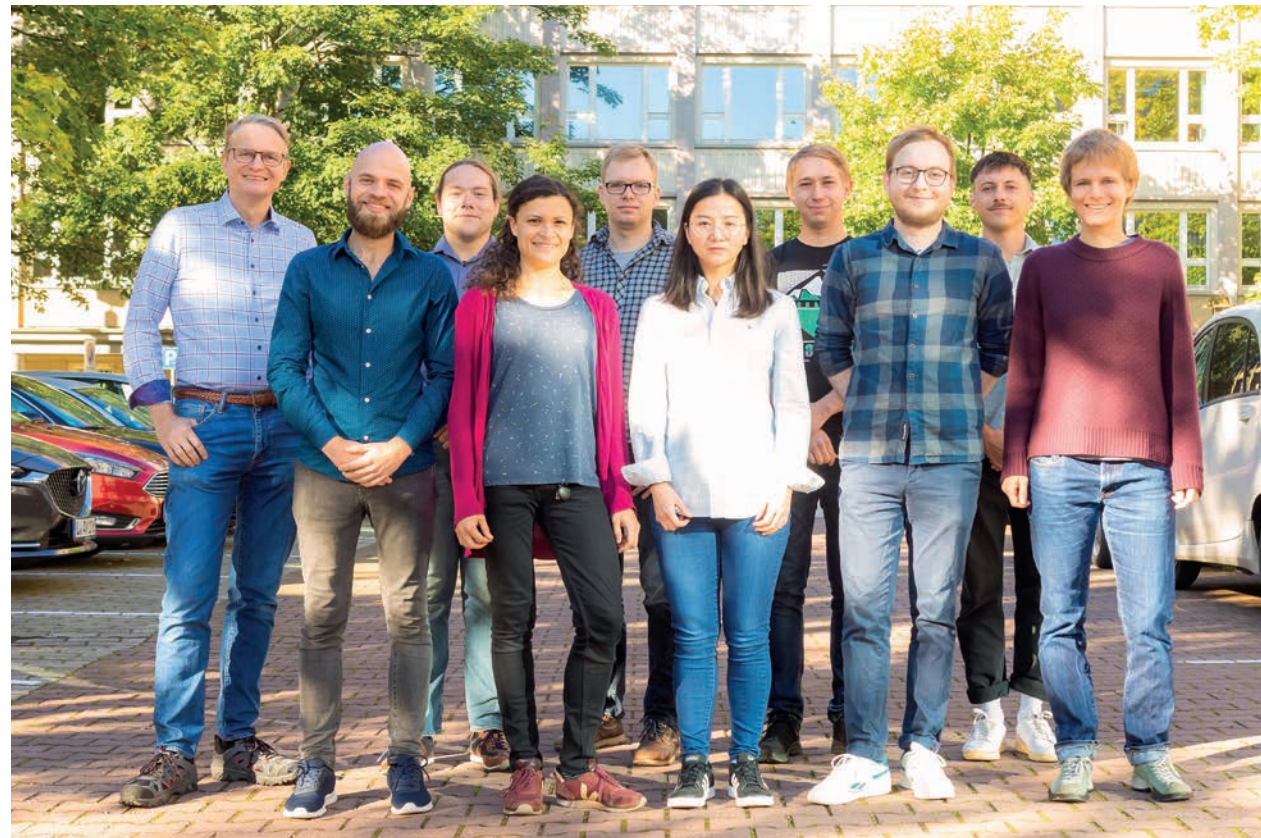
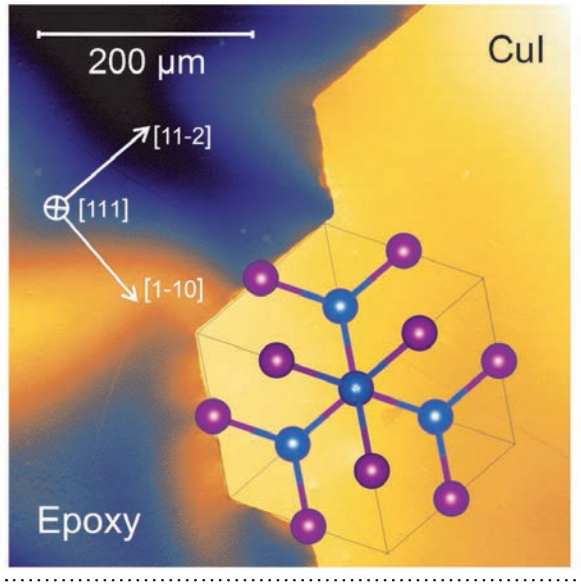
Amorphous semiconductors have rapidly gained in importance in recent years. They can be used to build transistors that function on glass as a substrate and are thus important for displays. Polymer substrate also allows the production of devices that are flexible and thus bendable. Indium gallium zinc 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 characterizing the world's best field effect transistors (FET's) and inverters from this material. 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. As special features, the devices are characterised by having extremely steep characteristics and their properties are very close to the thermodynamic limit. This has been achieved by optimizing 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 in detail and found to allow the control of the charge carrier density, however, for the price of reduced electron mobility [R1, R2]. Also, pure zinc-nitride has been studied in detail together with colleagues in France [R3]. Flexible devices from ZTO were investigated in [R4], allowing for small bending radii.



⇐ Fig. 1: Optical image of single-crystalline CuI thin film fabricated using pulsed laser deposition (PLD). The film has been lift-off and redeposited on a carrier. Adapted from [R5].

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 Unit ("Forschungsgruppe") 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 songle-crystalline CuI thin films (Fig. 1) using both pulsed laser deposition (PLD) [R5]. This will be the basis for fabricating p-type transparent FET's and subsequently complementary-type inverters. An important piece of the puzzle is doping and the control of charge carrier density; here, oxygen and selenium were investigated successfully [R6, R7]. In [R8, R9] the optical properties, in particular the carrier and recombination dynamics were investigated.

⇒ [R1] *Analysis of an extended percolation-based random band-edge model applied to the amorphous oxide semiconductors: multi-anionic zinc oxynitride, multi-cationic zinc tin oxide and multinary zinc magnesium oxynitride*
A. Welk, A. Reinhardt, D. Splith, H. von Wenckstern, M. Grundmann, O. Herrfurth / Phys. Rev. Appl. (2022) **17** 024007:1

⇒ [R2] *Tuning material properties of amorphous zinc oxynitride thin films by magnesium cationic substitution*
A. Welk, A. Reinhardt, O. Herrfurth, T. Schultz, H. von Wenckstern, N. Koch, M. Grundmann / APL Mater. (2021) **9** 021120:1

⇒ [R3] *Epitaxial Zn_3N_2 thin films by molecular beam epitaxy: Structural, electrical and optical properties*
P. John, M. A. 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

⇒ [R4] *Mechanical stress stability of amorphous zinc tin oxide thin-film transistors*
O. Lahr, M. Steudel, H. von Wenckstern, M. Grundmann / Front. Electron. (2021) **2** 797308:1

⇒ [R5] *Suppression of rotational domains of CuI employing sodium halide buffer layers*
P. Storm, K. Karimova, M. S. Bar, S. Selle, H. von Wenckstern, M. Grundmann, M. Lorenz / ACS Appl. Mater. Interfaces (2022) **14** 12350

⇒ [R6] *Evidence for oxygen being a dominant shallow acceptor in p-type CuI*
P. Storm, S. Gierth, S. Selle, M. S. Bar, H. von Wenckstern, M. Grundmann, M. Lorenz / APL Mater.(2021) **9** 051101:1

⇒ [R7] *P-type doping and alloying of CuI thin films with selenium*
P. Storm, M. S. Bar, S. Selle, H. von Wenckstern, M. Grundmann, M. Lorenz / Phys. Status Solidi RRL (2021) **15** 202100214:1

⇒ [R8] *Dynamics of exciton-polariton emission in CuI*
E. Krüger, M. S. Bar, S. Blaurock, L. Trefflich, R. Hildebrandt, A. Müller, O. Herrfurth, G. Benndorf, H. von Wenckstern, H. Krautscheid, M. Grundmann, C. Sturm / APL Mater. (2021) **9** 121102:1

⇒ [R9] *Hot-phonon effects in photo-excited wide-bandgap semiconductors*
O. Herrfurth, E. Krüger, S. Blaurock, H. Krautscheid, M. Grundmann / J. Phys.: Condens. Matter (2021) **33** 205701:1

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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 applications (M. Milewski, A. Sherstiuk). A new approach includes carborane-based phosphine ligands (J. Schulz, M. Milewski).

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 (Fig. 1), S. Baweja, K. Ramazanova).

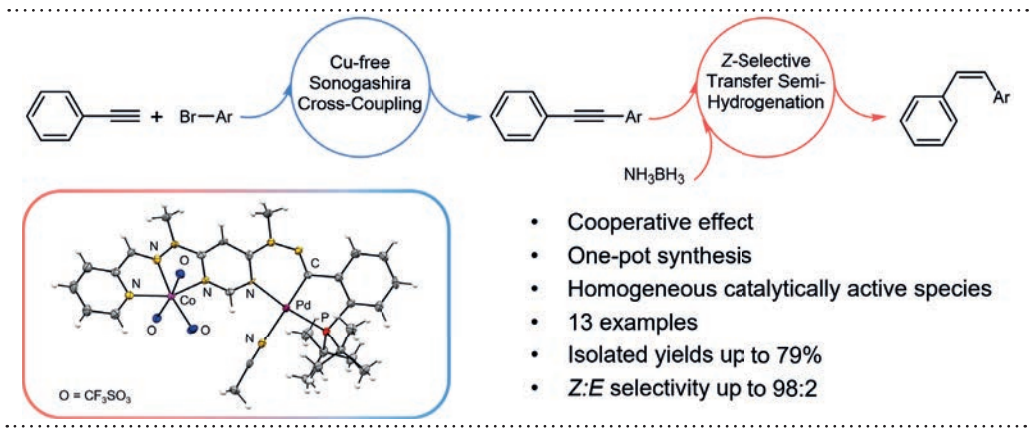


Fig. 1: The heterobimetallic Pd^{II}/Co^{II} complex is a suitable precatalyst for sequential Sonogashira coupling-alkyne semi-hydrogenation reactions to form Z-aryl alkenes in a one-pot fashion, demonstrating a cooperative effect. This generally applicable reaction could also be used for the synthesis of biologically active combretastatin A-4.

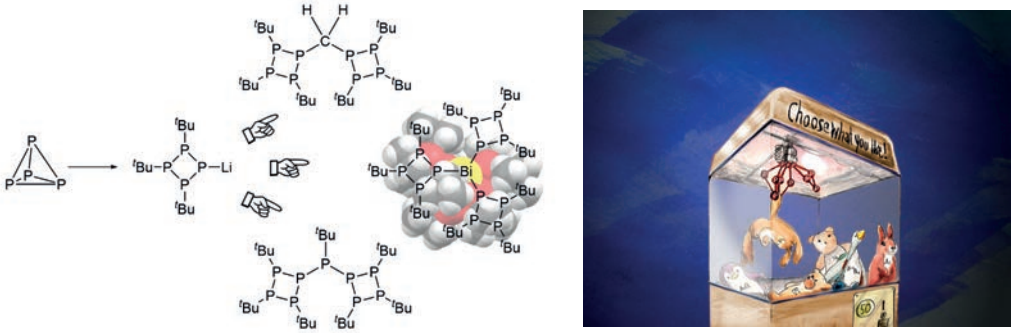


Fig. 2: P_4 activation enables the facile synthesis of novel oligo- and pnictaphosphanes, among these the first examples of molecules containing a tri-coordinated group 15 element with an EP_3 substructure (design on the right: Dr. Christoph Selg, Leipzig University).

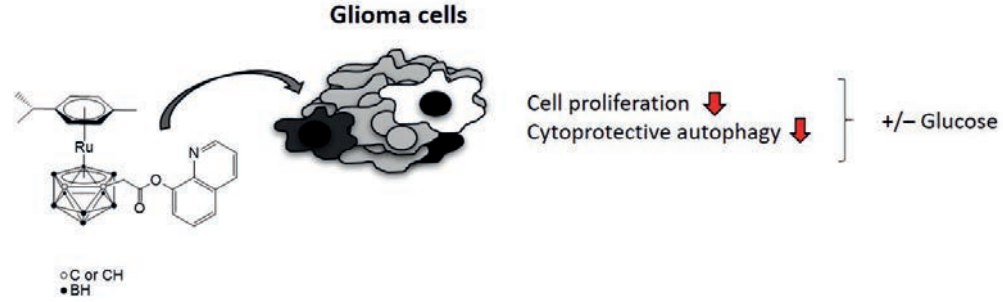
From Molecules to Novel Materials

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 phosphorus-based polymers are strained phosphorus-based rings (V. Eilrich) or phosphole derivatives showing aggregation-induced emission (AIE) properties (N. König).

Molecular precursors: Binary metal phosphides MPx 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. 2).

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) or other enzyme inhibitors (S. Braun, P. Stockmann, L. Ueberham) or for boron neutron capture therapy (BNCT) as conjugates with tumour-targeting entities.
Chemotherapy using platinum-based anti-tumour agents, such as cisplatin, is often associated with strong side effects and is further limited by resistance of tumour cells. Therefore, specific MOFs with large cavities are being studied for targeted drug delivery (R. Precker). Furthermore, to increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. COX inhibitors (I. Predarska), tamoxifen (A. Kazimir)). A new approach utilises the nido cluster $[C_2B_9H_{11}]^{2-}$ (also called dicarbollide, which is isolobal to cyclopentadienide) as ligand in metal complexes that exhibit anticancer properties (A. Kazimir) (Fig. 3).



⇑ Fig. 3: Gliomas and glioblastomas are very aggressive forms of brain tumours, prone to the development of a multitude of resistance mechanisms to therapeutic treatments, including cytoprotective autophagy. We have shown that the combination of a ruthenacarborane derivative with 8-hydroxyquinoline linked via an ester bond was able to significantly affect cellular viability in glioma U251 cells via inhibition of the autophagic machinery, making it a very attractive candidate for evading the known resistances of brain tumours to chloroquine-based therapies.

⇒ *Cyclooligophosphanes and their coordination chemistry*
V. J. Eilrich, E. Hey-Hawkins / Coord. Chem. Rev. (2021) **437** 213749

⇒ *Reductive rearrangement of a 1-phospha-2-azanorbornene*
P. Wonneberger, N. König, M. B. Sárosi, E. Hey-Hawkins / Chem. Eur. J. (2021) **27** 7847

⇒ *Preparing (metalla)carboranes for nanomedicine*
M. Gozzi, B. Schwarze, E. Hey-Hawkins / ChemMedChem (2021) **16** 1533

⇒ *Modulation of γ-secretase activity by a carborane-based flurbiprofen analogue*
S. Saretz, G. Basset, L. Useini, M. Laube, J. Pietsch, D. Drača, D. Maksimović-Ivanić, J. Trambauer, H. Steiner, E. Hey-Hawkins / Molecules (2021) **26** 2843

⇒ *Palladium goes first: A neutral asymmetric heteroditopic N,P ligand forming Pd-3d heterobimetallic complexes*
R. Clauss, A. Kazimir, A. Straube, E. Hey-Hawkins / Inorg. Chem. (2021) **60** 8722

⇒ *Synthesis of a carborane-substituted bis(phosphanido) cobaltate(I), ligand substitution, and unusual P_4 fragmentation*
P. Coburger, J. Leitl, D. J. Scott, G. Hierlmeier, I. Shenderovich, E. Hey-Hawkins, R. Wolf / Chem. Sci. (2021) **12** 11225

⇒ *Hafnium oxide-based nanoplatform for combined chemoradiotherapy*
A. A. Sherstiuk, S. A. Tsymbal, A. F. Fakhardo, V. N. Morozov, E. F. Krivoshapkina, E. Hey-Hawkins, P. V. Krivoshapkin / ACS Biomater. Sci. Eng. (2021) **7** 5633

⇒ *Ruthenacarborane and quinoline: A promising combination for the treatment of brain tumors*
D. Drača, M. Marković, M. Gozzi, S. Mijatović, D. Maksimović-Ivanić, E. Hey-Hawkins / Molecules (2021) **26** 3801

⇒ *Selective formation of a supramolecular coordination complex in the nanometre scale with a ferrocene-based phospholane ligand*
R. Hoy, T. Grell, P. Lönnecke, E. Hey-Hawkins / Chem. Commun. (2021) **57** 9200

⇒ *Facile synthesis of cyclo-($P_4^{t}Bu_3$)-containing oligo- and pnictaphosphanes*
V. J. Eilrich, T. Grell, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2021) **50** 14144

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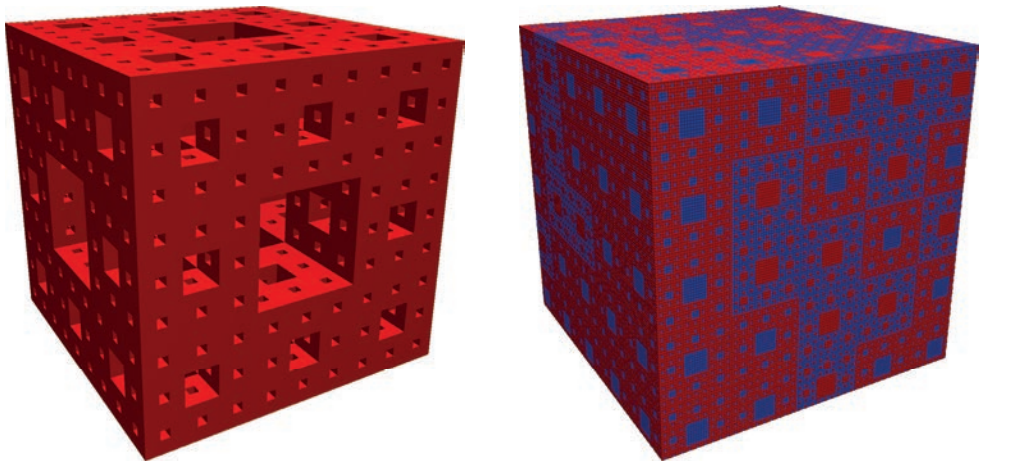
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
M.Sc. Phys. Denis Gessert, 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 system to a 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 verified with MC simulations a long-standing theoretical prediction for the growth law of the ordered structures and, moreover, for the first time also determined their aging characteristics. Recently he has generalised these considerations to the persistence properties of a quench to zero temperature. The main goal of such studies is to elucidate the dynamic scaling laws governing the kinetics of complex physical systems. Along another line of research he generalised the population annealing method first proposed and applied for MC simulations to MD studies and demonstrated its efficiency by simulations of the optiate peptide Met-enkephalin.



⇑ Left: third iteration of a Menger sponge of size 27^3. Right: 128^3 Ising spin configuration constructed from superimposing 27^3 Menger sponges, with red (blue) corresponding to up (down) spins.

(iii) Denis Gessert also investigates coarsening and aging properties of spin systems, thereby currently focusing on the particularly intriguing zero-temperature quench in the prototypical threedimensional Ising model with nonconserved order parameter. Quite astonishingly, in this setup, the value of the coarsening growth exponent has been elusive for the last 40 years. Whereas early work reported values close to 1/3, recent numerical studies suggested that the theoretically expected value of 1/2 might be approached asymptotically. To shed further light on this problem, he developed sophisticated computer codes on graphics processing units (GPUs) and simulated significantly larger systems with more than 8 billion spins. As a surprising discovery he instead observed a growth exponent greater than 1/2 and, performing an analog study based on so-called Menger sponges, convincingly argued that this superdiffusive behaviour can be qualitatively understood by the fractal sponge-like domain structure of the emerging spin pattern.

⇒ *Zero-temperature coarsening in the 2D long-range Ising model*
H. Christiansen, S. Majumder, W. Janke / Physical Review E (2021) **103** 052122-1

⇒ *Knots are generic stable phases in semiflexible polymers*
S. Majumder, M. Marenz, S. Paul, W. Janke / Macromolecules (2021) **52** 5321

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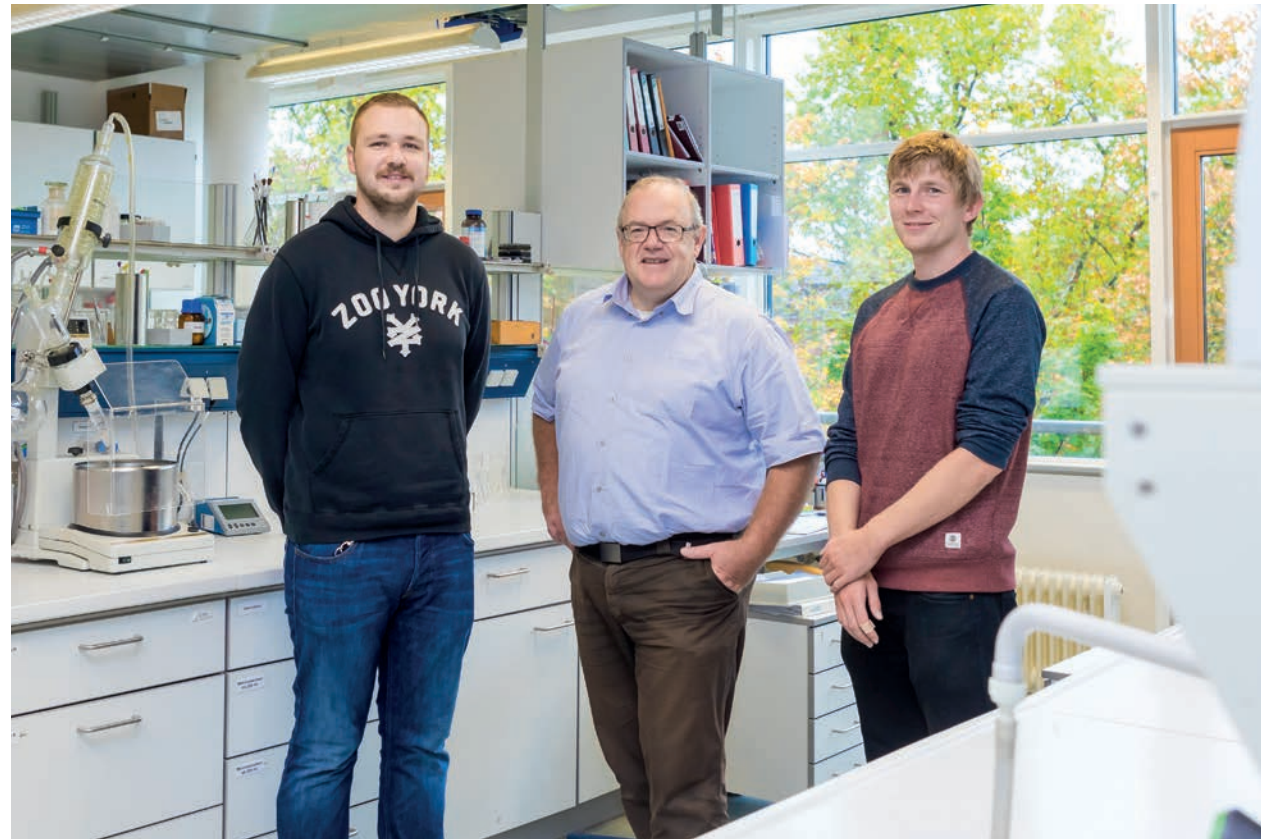
Coordination compounds in supramolecular chemistry and materials chemistry

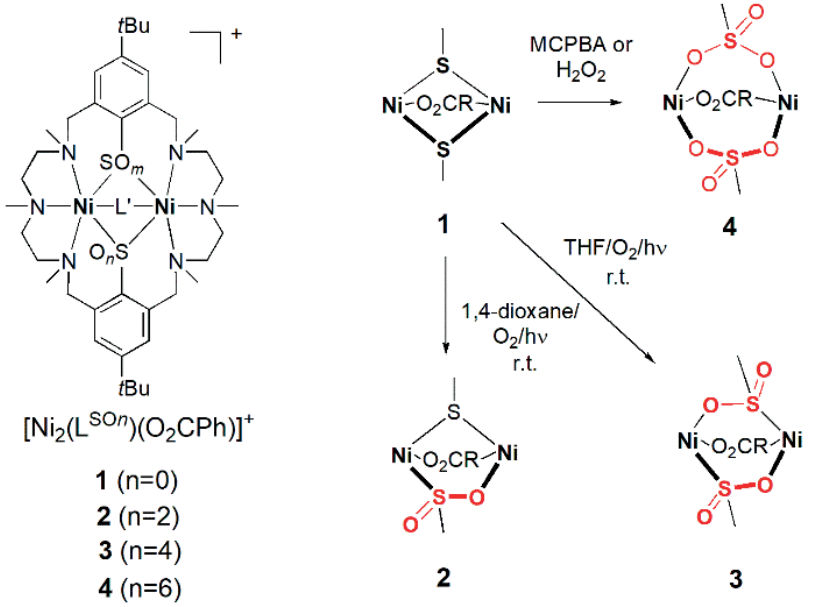
Prof. Dr. Berthold Kersting
M.Sc. Chem. Peter Hahn

The research of our group dealt again mainly with the coordination chemistry of macrocyclic compounds based on calix[4]arene and thiophenolate head units capable of forming discrete stable complexes with d- and f-block metals. The spectroscopic and magnetic properties of the synthesised complexes and their reactivity features were again studied by a range of methods including UV/vis, IR and luminescence spectroscopy, SQUID magnetometry and X-ray crystallography. The compounds are of interest for sensing and signaling applications. Some compounds are also of relevance in bioinorganic chemistry.

The oxygenation of metal thiolate complexes is of general interest concerning the deactivation of metallocysteinate enzymes and to the metabolism of cysteine.



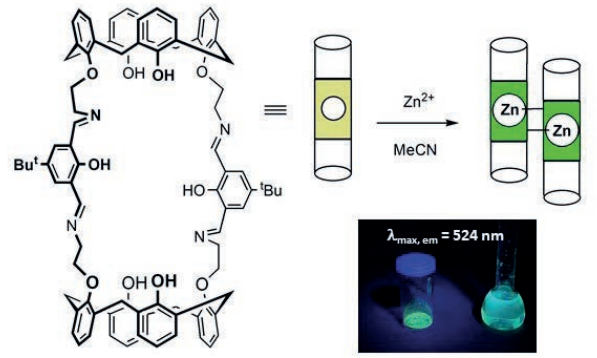
Thus, the S-oxygenation of thiophenolate bridges by ethereal hydroperoxides was studied. $[Ni^{II}_2L(PhCO_2)]^+$ (**1**, Fig. 1) is readily S-oxygenated with ether/O_2 at r.t. in the presence of daylight. The oxygenation was found to depend strongly on the choice of the ether. Uptake of two oxygen atoms occurs in dioxane to give a mixed thiolate/sulfinate complex $[Ni^{II}_2LSO_2(PhCO_2)]^+$ (**2**), which exhibits the rare five-membered Ni($\mu_{1,1}$-S)($\mu_{1,2}$-OS)Ni core. In THF, four oxygen atoms are taken up to



⇑ Fig. 1: S-oxygenation reactions of compound **1** with various oxidants[1].

from a bis-sulfinate species $[Ni^{II}_2LSO_4(PhCO_2)]^+$ (3). The oxygenation reactions proceed without complex disintegration and invariably provide $\mu_{1,2}$-bridging sulfinates as established by various spectroscopic methods, X-ray crystallography, and accompanying density functional calculations. The oxygenation of the sulfur atoms has also a strong impact on the electronic structures of the Ni complexes. The monosulfinate complex 2 has an S = 2 ground state that results from moderate ferromagnetic exchange coupling interactions (J = +15.7 cm^{-1}, H = $-2JS_1S_2$), while an antiferromagnetic exchange interaction in 3 shows the presence of a ground state with spin S = 0 (J = – 0.56 cm^{-1}).

Another study was undertaken to investigate the luminescence properties of Zn^{2+} supported by hybrid bis(iminomethyl)phenol/calix[4]arene macrocycles. The macrocyclic calix[4]arene ligand H_2L comprises two non-fluorescent 2,6-bis-(iminomethyl)phenolate chromophores, which show a chelation-enhanced fluorescence enhancement upon Zn^{2+} ion complexation. Macrocyclic [ZnL] complexes aggregate in the absence of external coligands via intermolecular Zn-N bonds to give dimeric $[ZnL]_2$ structures comprising two five-coordinated Zn^{2+} ions. The absorption and emission wavelengths are bathochromically shifted upon going from the liquid ($\lambda_{max,abs}$ (CH_2Cl_2) = 404 nm, $\lambda_{max,em}$ (CH_2Cl_2) = 484 nm) to the solid state ($\lambda_{max,abs}$= 424 nm (4 wt%, $BaSO_4$ pellet), $\lambda_{max,em}$ = 524 nm (neat solid)). Insights into the electronic nature of the UV-vis transitions were obtained with time-dependent density functional theory (TD-DFT) calculations for a truncated model complex.



⇐ Fig. 2: Structure of a macrocyclic ligand containing calix[4]arene and bisiminomethyl-phenol head units. The Zn^{2+}-complex dimerizes in solution and the solid state to give a bright-green fluorescent $[Zn_2L_2]$ complex [2].

⇒ *Etheral hydroperoxides: Powerful reagents for S-oxygenation of bridging thiophenolate functions*
M. Börner, D. Fuhrmann, J. Klose, H. Krautscheid, B. Kersting / Inorg. Chem. (2021) **60** 13517

⇒ *Green-emissive Zn^{2+} complex supported by a macrocyclic Schiff-base/calix[4]arene-ligand: Crystallographic and spectroscopic characterisation*
S. Ullmann, M. Börner, A. Kahnt, B. Abel, B. Kersting / Eur. J. Inorg. Chem. (2021) **36** 36911

⇒ *Synthesis and characterisation of luminescent $[Cr^{III}_2(L)(\mu\text{-carboxylato})]^{3+}$ complexes with high-spin S = 3 ground states (L = N_6S_2 donor ligand)*
M. Börner, J. Klose, M. E. Gutierrez Suburu, C. A. Strassert, F. Yang, K. Y. Monakhov, B. Abel, B. Kersting / Chem. Eur. J. (2021) **27** 14899

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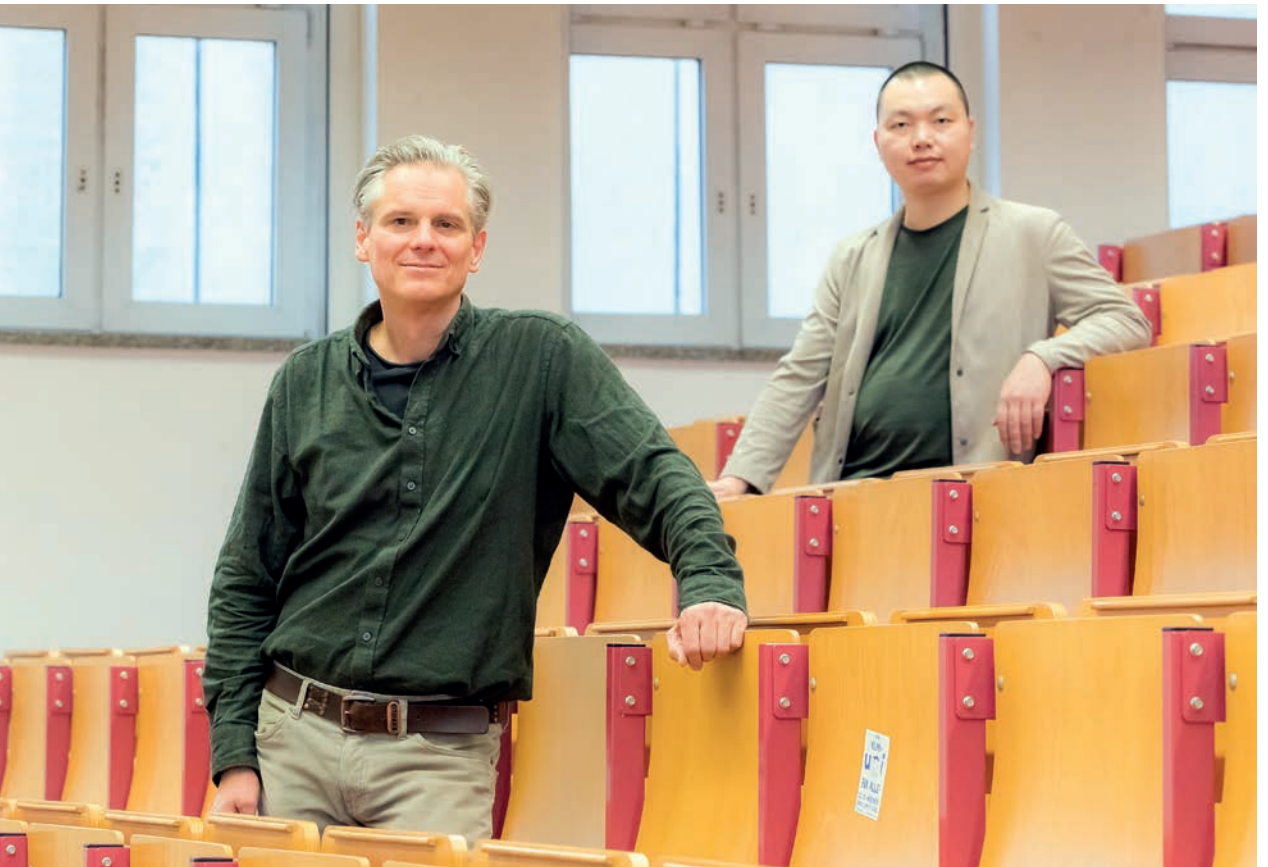
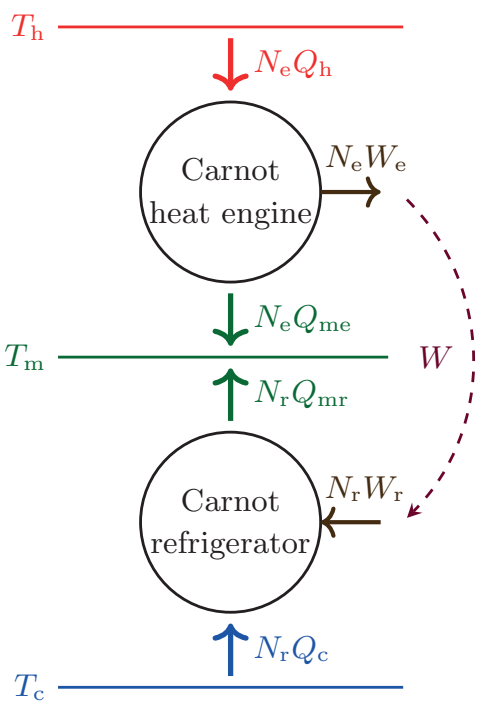
Maximum efficiency of absorption refrigerators at arbitrary cooling power

Prof. Dr. Klaus Kroy
M.Sc. Phys. Zhuolin Ye

The performance of heat engines, transforming heat to work, or refrigerators and heat pumps, displacing heat against a temperature gradient, is determined by two main quantities: output power and efficiency. Unfortunately, thermodynamic laws imply that they cannot be optimised simultaneously. This is because largest efficiencies correspond to reversible and thus slow processes, leading to output powers which are at best negligible fractions of the maximum power.

The implication for engineers, whose natural task is to develop designs that deliver a desired (fixed) power as cheap as possible, is that their devices in general do not operate in the regimes of maximum efficiency or maximum power, which were both thoroughly investigated theoretically in the past, but rather in the regime with maximum efficiency corresponding to the given power (MEGP). The latter received the attention of the theory of finite-time thermodynamic processes only recently, generalizing results obtained previously for a variety of trade-off relations between power and efficiency. Essentially, one can interpolate using the MEGP between a maximally powerful engine with efficiency at maximum power, and a reversible engine with maximum efficiency and null power.





⇐ Fig. 1: Sketch of the Carnot absorption refrigerator (CAR) composed of internal Carnot heat engine and Carnot refriger-ator. The overall CAR system communicates with three heat reservoirs at temperatures $T_h > T_m > T_c$. Both the internal engine and refrigerator use as their heat sink the reservoir at the intermediate temperature T_m. The engine in addition communicates with the hot bath at T_h and the refrigerator with the cold bath at T_c. MEGP for such CAR follows from the MEGPs for the internal heat engine and refrigerator.

As shown in Fig. 1, we consider absorption refrigerators consisting of simultaneously operating Carnot-type (internal) heat engine and refrigerator [1]. We show how the MEGP for this general model follows from the MEGPs for the internal heat engine and refrigerator. To derive explicit results, we consider absorption refrigerators consisting of low-dissipation (LD) heat engines and refrigerators, for which expressions for MEGPs are known. The obtained MEGP represents a loose upper bound for efficiency of real-world absorption refrigerators, which recently experienced a renewed interest of physicists due to their potential to recycle waste heat in microscopic (quantum) devices. It also implies that a slight decrease in power of the absorption refrigerator from its maximum value results in a large nonli-near increase in efficiency observed in heat engines whenever the ratio of maximum powers of the internal engine and the refrigerator does not diverge.

Otherwise, the increase in efficiency is linear as observed in LD refrigerators. Thus, in all practical situations, the efficiency of LD absorption refrigerators significantly increases when their cooling power is slightly decreased from its maximum.

⇒ [1] *Maximum efficiency of low-dissipation refrigerators at arbitrary cooling power* V. Holubec, Z. Ye / Phys. Rev. E (2021) **103** 052125

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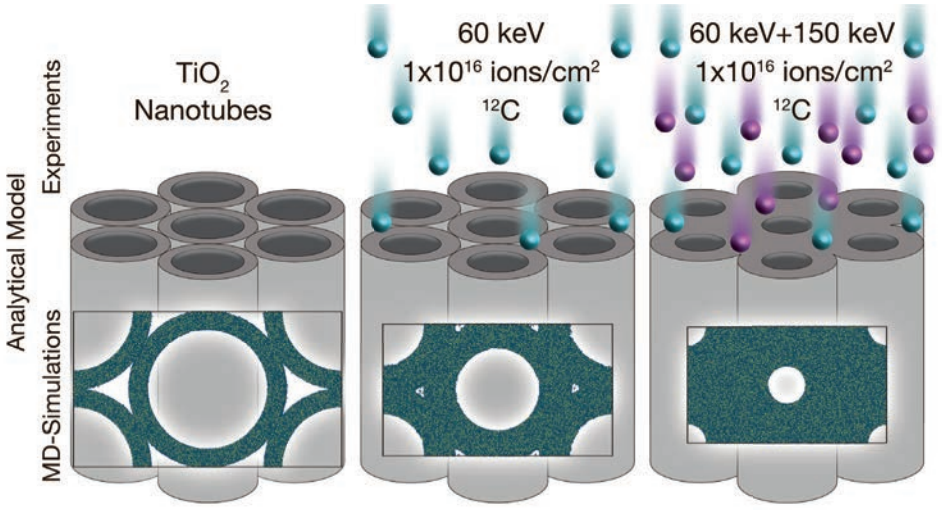
Carbon implanted TiO_2 nanotube arrays and agarose hydrogels for biomedical applications

Prof. Dr. Stefan G. Mayr
M. Sc. Phys. Catharina Krömmelbein, M.Sc. Phys. Astrid Kupferer, M.Sc. Phys. Friedrich Schütte

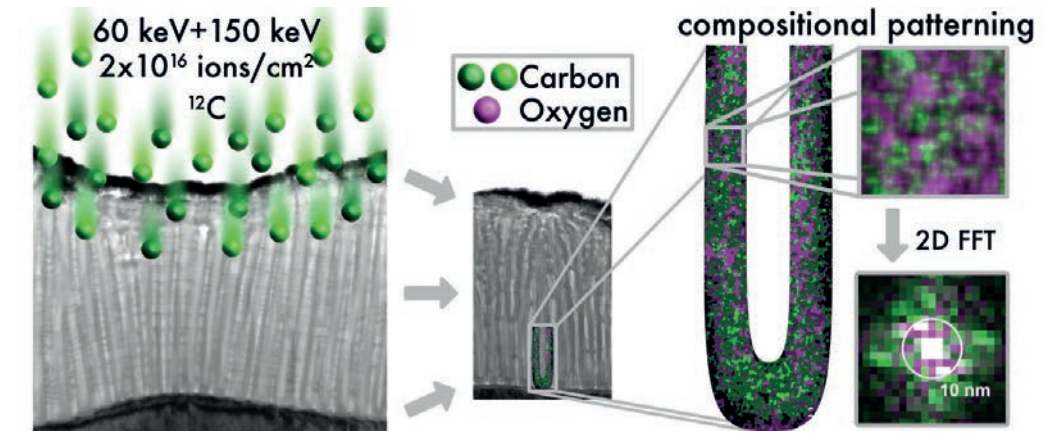
BuildMoNa related research within the surface physics group involves two different projects to develop and optimise biomedical applications. The first project concentrates on the improvement of TiO_2 nanotube (NT) arrays, which serve as a unique platform for long term tissue culture. The hexagonal titania NTs arrangement can be fine-tuned to meet the high demands of sensitive, adult primary tissues. As a post-process treatment, ion implantation is shown to be a versatile tool to change both surface morphology and chemical composition of titania NTs. In detail, Kupferer et al. [1] show that an irradiation-induced viscous material flow causes the NTs to shrink in diameter and height. In their study, they combine experimental work

with an analytical model and molecular dynamics simulations to demonstrate that pore shrinkage is driven by surface stress that is released upon carbon implantation, see Fig. 1. In fact, these effects also appear for neon implantation, as depicted in reference [2]. In addition, Kupferer et al. [3] reveal an interplay of phenomenological effects within the tubular structure upon carbon implantation, as depicted in Fig. 2: atoms are sputtered on the inner NT surfaces and again readsorb deeper within the structures due to the incoming ion flux. This results in a plastic deformation of the NT array. Also, the ion irradiation-induced amorphisation counteracts the beginning crystal growth due to increased temperatures in the collision cascades. Further, this gives rise to an experimentally observed compositional patterning governed by enthalpic (and, also, entropic) reasons, as presented in molecular dynamics calculations. In conclusion, these results show that ion implantation enables tailoring of the titania NT characteristics for various applications. approach to design tailored biodegradable magnetic responsive systems.



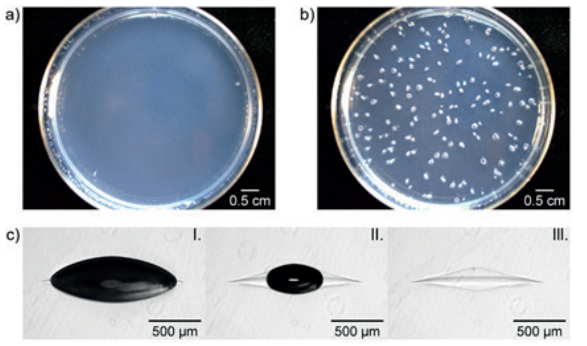
⇑ Fig. 1: Schematic representation and molecular dynamics simulations of titania nanotube pore shrinkage upon carbon ion implantation (adapted from [1]).

Second project focuses on sterilisation and improvement of an affinity chromatography-based cell separation technique in an industrial cooperation with Cell.copedia GmbH, Leipzig. Within this application, granular agarose hydrogels are used to effectively isolate target cells which is important for cancer immunotherapy. Fast and powerful 10 MeV electron irradiation is employed to sterilise the biomedical product. Thereby, electron beam treatment is used to adjust the physical properties of agarose hydrogels to obtain optimal results in the cell isolation application. In response to the high-energy electron irradiation, agarose hydrogels can react either with the formation of additional crosslinks or with the cleavage of agarose polymer chains directly effecting the material's stiffness. In this study, Krömmelbein et al. describe that polymer chain scission is the dominating process for electron

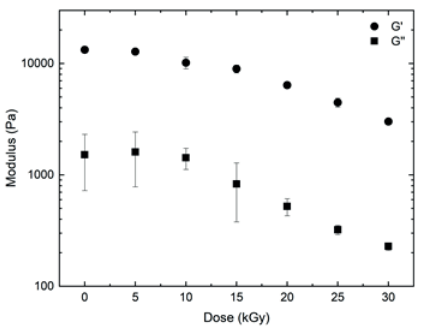


⇑ Fig. 2: Implantation of low-energy low-fluence carbon ions in titania nanotube scaffolds results in a decrease of array height, a plastic deformation of the nanotubes and a compositional patterning of oxygen-rich and carbon-deficient as well as oxygen-deficient and carbon-rich domains.

beam treated agarose hydrogels resulting in a material softening [5], see Fig. 3 and Fig. 4. Based on investigations regarding the mechanical, structural, and chemical properties of electron beam treated agarose hydrogels, a radiolysis mechanism was proposed. Overall, this study provides an overview of the material properties of electron beam treated agarose hydrogels in the sterilisation relevant dose range to characterise and modify the material changes critical for cell isolation applications.



⇑ Fig. 3: Gas cavity formation in 1 wt.% agarose hydrogels after high-energy electron irradiation with a) 10 kGy and b) 30 kGy. c) shows phase contrast images of a characteristic gas cavity in a 1 wt.% agarose hydrogel directly after irradiation with 10 kGy (i), 24 hours after irradiation (ii) and 48 hours after irradiation (iii). The formed gas was determined as CO_2 and CO in trace amounts (from [2]).



⇑ Fig. 4: Storage G' and loss modulus G'' of 1 wt.% agarose hydrogels in dependence on the applied electron dose determined by rheology measurements (from [2]).

⇒ [1] *Tailoring morphology in titania nanotube arrays by implantation: experiments and modelling on designed pore size - and beyond*
A. Kupferer, S. Mändl, S. G. Mayr / Materials Research Letters (2021) **9**:11 483

⇒ [2] *Carbon and neon ion bombardment induced smoothing and surface relaxation of titania nanotubes*
A. Kupferer, M. Mensing, J. Lehnert, S. Mändl, S. G. Mayr / Nanomaterials (2021) **11**(9) 2458

⇒ [3] *Compositional patterning in carbon implanted titania nanotubess*
A. Kupferer, A. Holm, A. Lotnyk, S. Mändl, S. G. Mayr / Advanced Functional Materials (2021) **31**(35), 2104250

⇒ [4] *Fibroblast response to nanocolumnar TiO_2 structures grown by oblique angle sputter deposition*
U. Kapprell, S. Friebe, S. Grüner, C. Grüner, A. Kupferer, B. Rauschenbach, S. G. Mayr / Advanced Materials Interfaces (2021) **8**(17), 2100646

⇒ [5] *Impact of high-energy electron irradiation on mechanical, structural and chemical properties of agarose hydrogels*
C. Krömmelbein, M. Mütze, R. Konieczny, N. Schönherr, J. Griebel, W. Gerdes, S. G. Mayr, S. Riedel / Carbohydrate Polymers (2021) **263** 117970

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Influence of doping on the structures and transport properties of tetrahedrite compounds

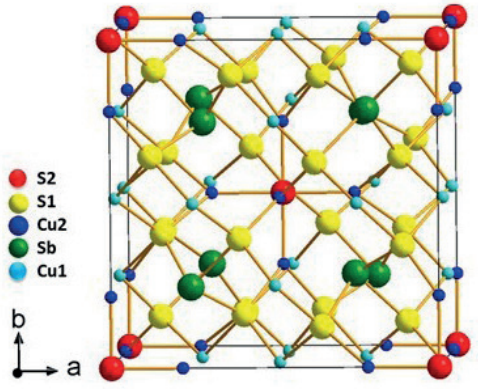
Prof. Dr. Oliver Oeckler
M.Sc. Chem. Christina Fraunhofer, M.Sc. Chem. Mahboubeh Moslemi,
M.Sc. Chem. Lennart Staab

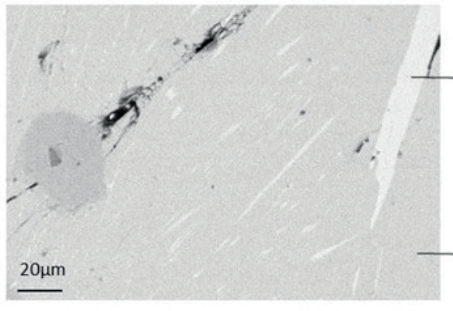
Thermoelectric materials have drawn a lot of attention due to their ability to convert waste heat into electricity. Tetrahedrite materials derived from $Cu_{12}Sb_4S_{13}$ are intriguing as they consist only of abundant and non-toxic elements. However, their application is limited by rather low thermoelectric performance. High efficiency of energy conversion requires a high Seebeck coefficient, high electrical conductivity, and low thermal conductivity. Therefore, we studied the effects of substituting Sb with rare earth elements with respect to microstructures and thermoelectric properties of $Cu_{12}Sb_4S_{13}$. The incorporation of rare earth elements may enhance ther-

mopower by local distortions, localised magnetic moments, and the formation of 4f-electron "resonant" states near the Fermi level.

The synthesised materials consist of two tetrahedrite phases, copper-poor and copper-rich, as well as famatinite (Cu_3SbS_4), and a minor side phase composed of copper, rare earth elements, and sulfur. The two tetrahedrite phases present at low temperatures form a single tetrahedrite phase at temperatures above ~100 °C. Famatinite as well as the side phase are stable at higher temperatures. Homogeneous samples with nominal compositions $Cu_{12}Sb_{4-x}RE_xS_{13}$ (RE = rare earth element) can thus not be obtained, but the heterostructures obtained may have interesting properties. Further substitution experiments will aim at replacing part of the SbIII by a group 13 element such as Ga or In. Aliovalent substitution may be possible with e.g. Sn.

With respect to abundance and low toxicity, copper chalcogenides are also interesting thermoelectric materials. However, Cu atom mobility leads to decomposition under direct electrical current at a critical voltage specific to each material. An approach to increasing the critical voltage involves dividing the applied voltage by separating grains of the chalcogenide with graphite or CuI. However, this strongly affects transport properties and the corresponding heterostructures require targeted optimisation.





Element	S	Cu	Nd
Atomic%	50.4	25.6	24.0

Element	S	Cu	Sb
Atomic%	44.7	40.8	14.5

⇑ Crystal structure of tetrahedrite $Cu_{12}S_{b4}S_{13}$ and SEM image of a sample with the nominal composition $Cu_{12}Sb_{3.75}Nd_{0.25}S_{13}$ as well as EDX maps of the main phase with tetrahedrite (gray areas), and $CuNdS_2$ as a side phase.

⇒ *Anomalous Raman modes in tellurides*
F. J. Manjón, S. Gallego-Parra, P. Rodríguez-Hernández, A. Munoz, C. Drasar, V. Muñoz-Sanjosé, & O. Oeckler / J. Mater. Chem. C (2021) **9** 6277

⇒ *Ceramic composites based on $Ca_3Co_{4-x}O_{9+\delta}$ and $La_2NiO_{4+\delta}$ with enhanced thermoelectric properties*
R. Hinterding, Z. Zhao, M. Wolf, M. Jakob, O. Oeckler, A. Feldhoff / Open Ceramics (2021) **6** 100103

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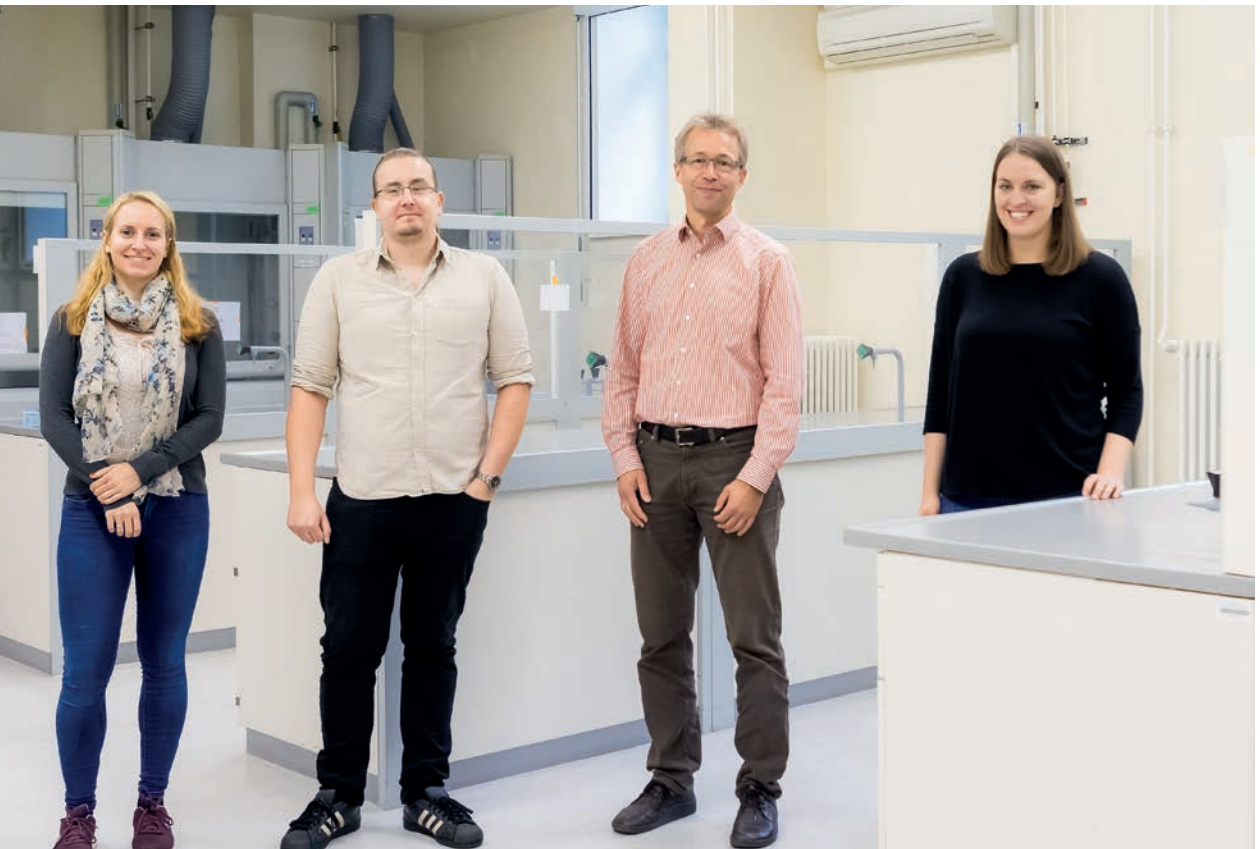
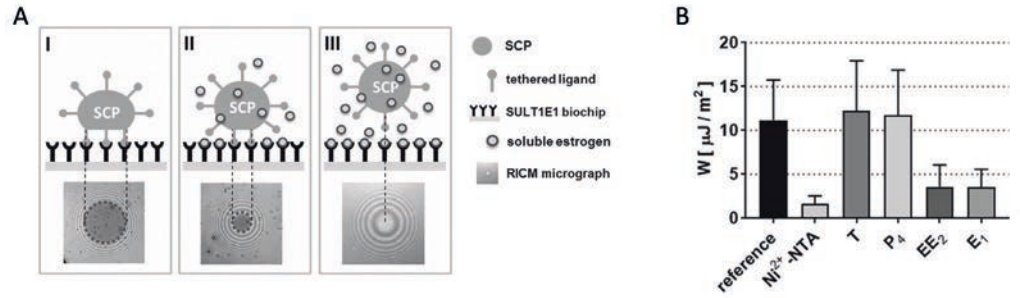
Biomaterials engineering for applications as biomimetic cell culture scaffolds and highly sensitive and specific biosensors in environmental monitoring

Prof. Dr. Tilo Pompe
M.Sc. Biochem. Cornelia Clemens, M.Sc. Biochem. David Rettke,
M.Sc. Biochem. 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 are developed, as already shown for the detection of the controversially discussed herbicide glyphosate in the pM range. In a new publication we now demonstrated the detection of a full class of estrogenic compounds known to be active in the estrogen pathway in animals and humans. Furthermore, the SCP principle is currently used to develop a sulfonamide antibiotics biosensor using dihydropteroate synthase as the capture site on the chip surface. Other technological options are investigated, too, in order to establish a platform to be commercialised. In this context three patent applications were filed for the SCP biosensing technology.



⇑ **Estrogen sensor based on soft colloidal probes.** (**A**) Scheme of the biosensor principle with site-specific coupling of the sulfotransferase SULT1E1 to the biochip surface and estradiol 17β-D-glucuronide (E217G) to the (polyethylene glycol)-SCP. (**B**) Proof of concept for the specific detection of estrogens with strong adhesion of the reference to the surface (absence of competitors) and diminished adhesion in presence of the estrogens ethinylestradiol (EE2) and estrone (E1) but no effect in the presence of testosterone (T) or progesterone (P4).

⇒ *Biomimetic estrogen sensor based on soft colloidal probes*
D. Rettke, F. Seufert, J. Döring, K. Ostermann, D. Wilms, S. Schmidt, T. Pompe / Biosensors & Bioelectronics (2021) **192** 113506

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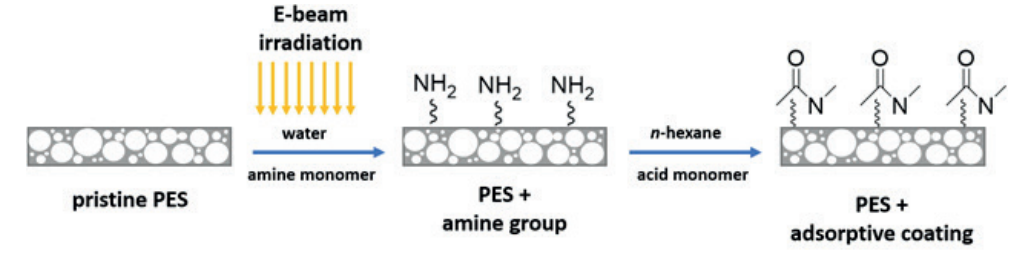
Surfaces of porous membrane filters

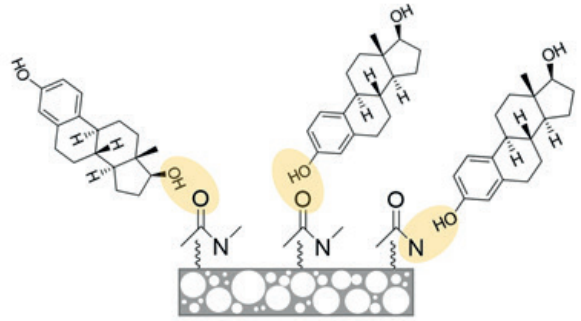
Dr. Agnes Schulze
M.Sc. Chem. Zahra Niavarani

Humans and aquatic life are frequently exposed to substances through water that cause endocrine disruption, which has become a serious environmental and health problem worldwide. In this study, the removal of 17β-estradiol (E2) in water was investigated using adsorbent membranes. The polyethersulfone membranes were functionalised with amide groups using electron beam irradiation to produce a hydrophilic surface coating.

The modified membranes showed high E2 adsorption capacity. Interestingly, modification of the membrane surface by alkyl and aromatic amide functionalities resulted in comparable E2 adsorption properties. Thus, it can be concluded that hydrophobic interactions were not significantly involved in the adsorption process.

Rather, it can be assumed that the successful formation of hydrogen bonds between E2 and the amide groups is responsible for the high adsorption capacities of the modified membranes toward E2. The modified membranes additionally exhibited higher water permeation than the untreated PES membranes. The pore structure, on the other hand, was not changed, indicating a very thin or even monomolecular layer of amide modification. Evaluation of the synthesis conditions on the modified membranes revealed that the addition of toluene had the strongest effect on the adsorber capacity of the PES membranes (0.82 $g \cdot cm^{-2}$), which can probably be explained by swelling of the membrane during the modification reaction.





⇑ Polyethersulfone membranes were functionalised with amide groups to efficiently adsorb 17β-estradiol from water. It is assumed that hydrogen bonds play an important role for adsorption and hydrophobic interactions can be neglected.

⇒ *Estradiol removal by adsorptive coating of a microfiltration membrane*
Z. Niavarani, D. Breite, A. Prager, B. Abel, A. Schulze / Membranes (2021) **11** 99

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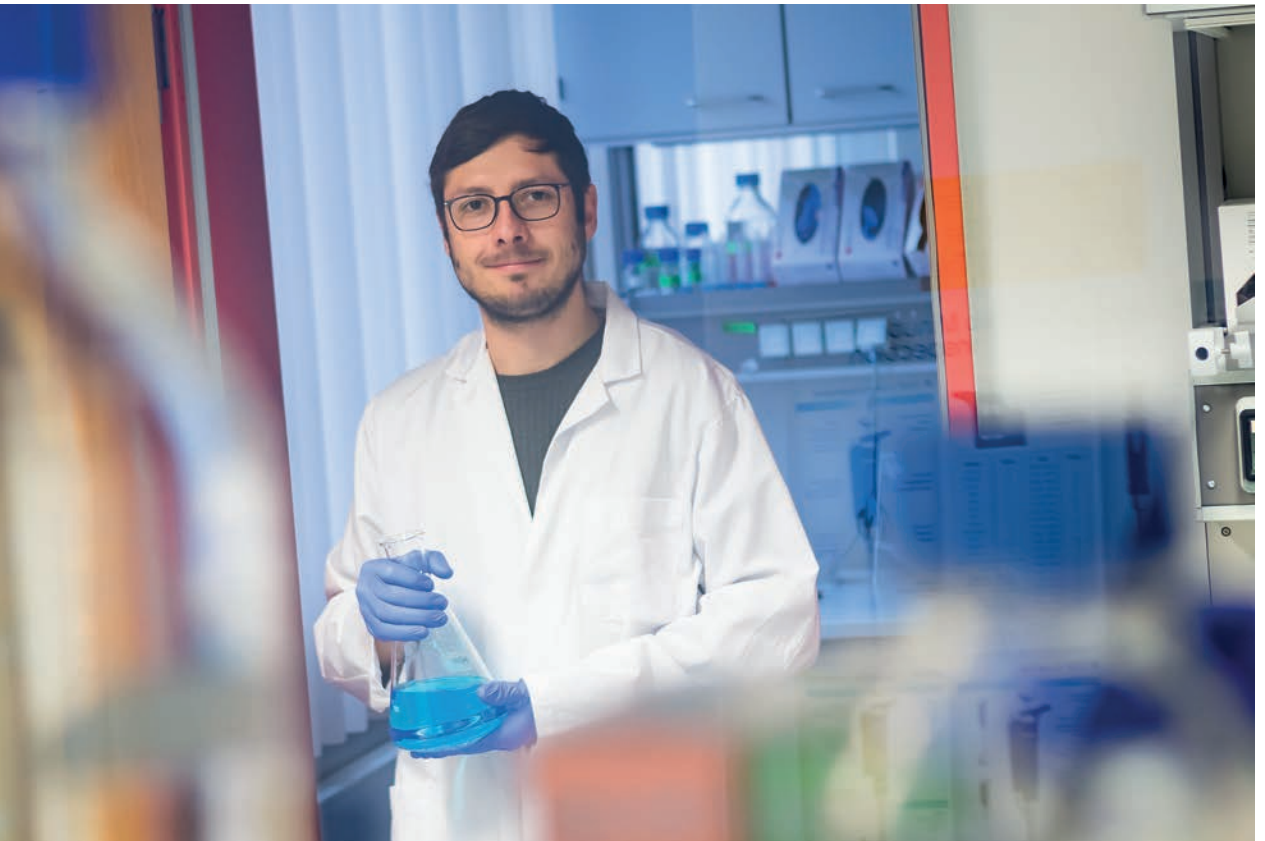
Phone: +49 341 235-2400

Modeling target recognition by CRISPR-Cas enzymes

Prof. Dr. Ralf Seidel
M.Sc. Phys. Patrick Irmisch

CRISPR-Cas systems are part of the immune system in most archaea and many bacteria, which achieve adaptable and heritable resistance against viruses by integrating short DNA sequences of former invaders into their genome. By transcription of these sequences, short RNAs (crRNAs) are produced. These are integrated by the CRISPR effector complexes that would destroy any invader DNA with a corresponding sequence. By altering the crRNA sequence, the effector complexes can be flexibly reprogrammed to target any desired DNA sequence which makes them promising for genome engineering.

One interesting feature of these target recognition proteins is that they are highly specific, but tolerate targets with a significant number of mismatches. This is suggested to be beneficial for the system to adapt to slightly mutated target sequences.



While this is desirable in nature, it is highly problematic in genome engineering, since this could lead to off-targeting (recognition of wrong sequences). Therefore, we try to understand the mechanics behind target recognition using single molecule measurement techniques (see Figure 1) combined with kinetic modelling.
Beyond the target recognition of CRISPR-Cas Enzymes, we also investigate DNA-based toehold-mediated strand-displacement reactions. These reactions rely on simple and programmable interactions between purified nucleic acid strands and allow to design dynamic DNA-based reaction systems, whereby functionality is incorporated via sequence design. Here, we combine bulk fluorescence assays with biophysical modelling to make kinetic predictions of strand-displacement reaction networks.

Interestingly, CRISPR-Cas effector complexes and strand displacement share the common feature that nucleobase-pairing and -displacement govern the reaction progress. Our modelling provides mechanistic insights into the underlying biophysical principles and can be used as helpful tools for the rational design of strand displacement systems.

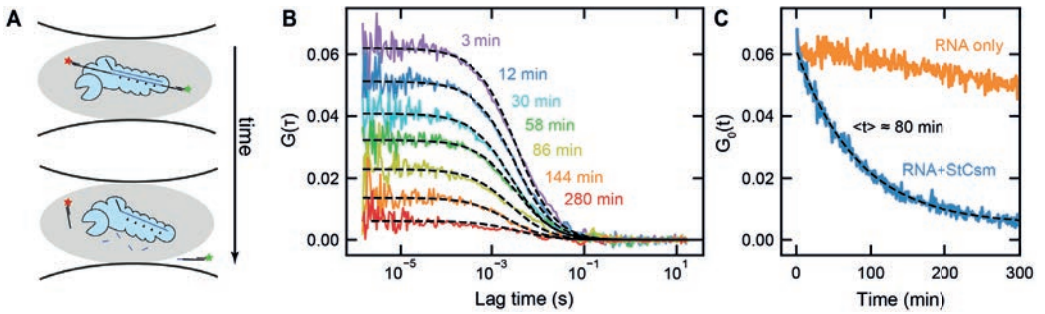


Fig. 1: Fluorescence cross-correlation spectroscopy reveals RNA retention timescale. (A) Scheme of the Type III CRISPR-Cas StCsm complex diffusing through the confocal excitation volume. Intact target RNA enables the measurement of a cross correlation between green (ATTO-532) and red (ATTO-647N) fluorophore emission. Reaction initiation leads to cleavage and consecutive release of the target RNA, resulting in a spatial separation of the dyes. (B) Fluorescence cross correlation curves depending on the lag time measured for the activating RNA target calculated over periods of one minute at different timepoints (coloured solid lines) together with fits to a simple 3-dimensional diffusion model (dashed solid lines). (C) Cross-correlation amplitude depending on time for activating target RNA only (solid orange line) and in presence of StCsm (blue solid line). The approximate timescale of 80 minutes for RNA end release was obtained from an exponential fit (solid dashed line) to the experimental data..

⇒ *A quantitative model for the dynamics of target recognition and off-target rejection by the CRISPR-Cas Cascade complex*
M. Rutkauskas, I. Songailiene, P. Irmisch, F. E. Kemmerich, T. Sinkunas, V. Siksnys, R. Seidel / bioRxiv, (2022)

⇒ *Dissipative control over the toehold-mediated DNA strand displacement reaction*
E. Del Grosso, P. Irmisch, S. Gentile, L. J. Prins, R. Seidel, F. Ricci / Angew. Chem. Int. Ed. (2022)

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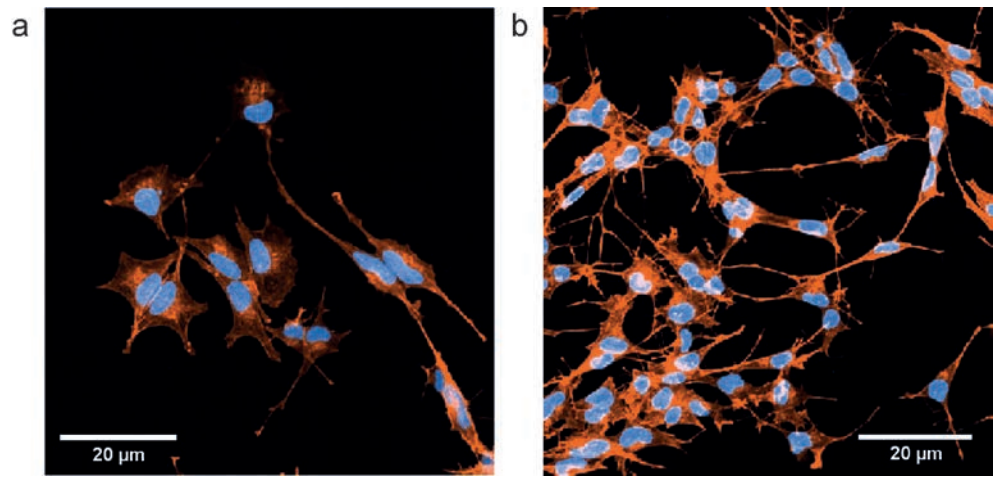
From neuroelectrodes to the premature lung: how physics can help to improve medical therapy

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

From a physics point of view, living cells and tissues can be considered as viscoelastic materials which comprise complex elastic properties. During elastic deformation, Young's moduli often highly depend on deformation rate and – in contrast to "dead" condensed materials – cells can actively adapt their behaviour and function to the surrounding environment. Thus, during any medical therapy in which implants and other invasive treatments are used, interaction of cells and tissues with the employed biomaterial should be consider. Within an interdisciplinary project, we investigated the interaction of neurons and glial cells with nanocolumnar TiN substrates – a potential biomaterial for multielectrode arrays (MEA) due to improved electronic properties such as a lowered self-impedance. Combining single-cell force-spectroscopy in combination with a quantification of cell spreading behaviour for longer adhesion times, we showed that nanocolumnar TiN exhibited improved biocompatibility features compared to conventional MEA materials.

In another PhD project, we focused on the mechanical properties of the premature lung. Many very preterm infants require mechanical ventilation as life-saving therapy. However, prolonged ventilation and related mechanical load may cause pulmonary diseases such as bronchopulmonary dysplasia – also seen e.g., in COVID-19 pneumonia patients. Why mechanical stress occurring during ventilation can result in lung failure, still remains unclear. We studies differences in fetal and adult lung mechanical properties under tension and compression at different loading rates as occurring during normal breathing and mechanical ventilation, respectively. Furthermore, experiments with a pressure-adjustable Ussing-chamber demonstrated that cellular ion channel activity important for gas exchange in the lung is hampered. Thus, pressure induced cellular dysfunction might explain clinical observations of ventilation-related side-effects.



⇑ (a) Fluorescence image of SH-SY5Y cells (neurons) grown on indium tin oxide (ITO) substrate for 3 days. Actin fibers are shown in orange and cell nuclei in blue; (b) Same as in (a) for cells cultured on nanocolumnar TiN.

⇒ *Adhesion of neurons and glial cells with nanocolumnar TiN films for brain-machine interfaces*
A. Abend, C. Steele, H.-G. Jahnke, M. Zink / Int. Journal of Molecular Sciences (2021) 22 8588

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Experiences

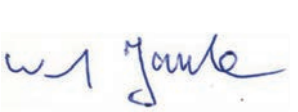
BuildMoNa's fourteenth year – a principal investigator's view

Prof. Dr. Wolfhardt Janke

Starting in 2007 with full funding by the German Excellence Initiative, BuildMoNa has grown steadily and now as a "teenager" is fully integrated as a Graduate School into the Research Academy Leipzig. Since I have had the pleasure to participate in the BuildMoNa activities from the very beginning, I can overview its development with many "ups" and few "downs" fairly well. While some of the organisational structures have been adapted over the past 14 years, the main spirit of BuildMoNa has survived all changes: the fruitful combination of physical, chemical and bio-chemical natural sciences under one unifying umbrella. For the doctoral candidates – and also the PIs – this opens enriching and often stimulating views on similar problems from different perspectives. The regular participation of the doctoral candidates in topical modules provides excellent opportunities to get into contact with the basics in fields they would have otherwise probably not even thought of. And the PIs, who teach or organise these modules, get a worthwhile incentive to think about the really important aspects of their research work with broader impact. Also the Annual BuildMoNa Conferences ("ABC") in spring transport this "ABC" of BuildMoNa: external and internal speakers communicate recent new developments in all three disciplines, supplemented by poster sessions where the doctoral candidates present and discuss their latest results with their fellows and the PIs. The ABCs and particularly the barbecue parties in Summer provide a perfect forum for (not only scientific) contacts with colleagues from other faculties. Such events across disciplines could have been also initiated by other means, but without BuildMoNa it is very unlikely that this would have had happen. This integrating function is in my view the most important aspect of BuildMoNa.

The initial talk of the doctoral candidates presenting an outline of their planned thesis work, the personal development plan and the assignment of a co-supervisor, which are required for admission to BuildMoNa, help in structuring the 3-4 years until the final PhD thesis defense and force the doctoral candidates – and also the PIs – to reflect on what they are doing on a day-by-day basis. While the involved administrative overhead is at times considered as a burden, the overall gain of these structuring measures clearly overcompensates this.

The years 2020 and 2021 were heavily affected by the Covid-19 pandemic, preventing most of the important and well established face-to-face activities of BuildMoNa. Let's hope that we can soon return to the normal mode which made BuildMoNa so successful.



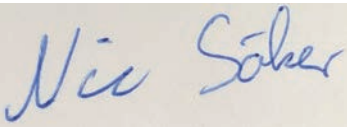
Prof. Dr. Wolfhardt Janke

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

M.Sc. Phys. Nicola Andreas Söker

The year 2021 was very exciting for me as my daughter was born early in the year. With these new and demanding responsibilities it took some time to find again a productive scientific workflow. Later that year I enjoyed taking a scientific module that was organised by the Graduate School BuildMoNa. It felt more of going back to a known habit and brought me back to the bench of a lecture hall. The online format of the lecture due to the pandemic situation was damping this feeling only a little. A variety of international speakers presented a broad view on the scientific topic. It is very likely that some of the methods I learned about in this module will soon find their way into my current project which is not the case too often. One learns about topics outside the scope of his/her own research and bursts the so called "bubble" that is set up around a doctoral candidate and the corresponding working group. From experience I can say that other modules followed a similar scheme of having various international speakers invited as well as lab tours. This is a strength of the graduate school and the chance it offers: translating knowledge that goes beyond the subject across eager doctoral candidates to gain more insight that can eventually be used for their own projects and therefore expand their expertise.

As I had to manage my new (family) responsibilities I may had not had the time to notice all the chances for social activities around the graduate school and there might have been less due to the ongoing pandemic situation. Creating spaces where people can get into contact scientifically and socially should in my eyes always be a priority.



M.Sc. Phys. Nicola Andreas Söker

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			Month (March to February)											
	Type	Min. CP	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	5		S	S	S	S			S	S	S	S	
					M		M				M		M	

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

Scientific and methods modules

Basic Concepts in Molecular Spectroscopy (2021-B4)

04 - 05 November 2021,
written exam, 2 credit points, yearly recurrence with modification, 9 participants

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

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

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

Chemical Biology and Biophysics of Cancer (2021-A2)

30 August - 01 September 2021, hybrid,
written report, 2 credit points, yearly recurrence with modification, 20 participants

This module discussed how physics, chemistry, biochemistry, molecular and materials science can provide a new perspective on oncology. Molecular biology shows the complexity and ambiguity that arises from the variability of tumours. Nevertheless, some biochemical and biophysical changes are universal to solid tumour progression and may provide both, novel diagnostic as well as therapeutic concepts. The state of the art in diagnostics and therapeutics was discussed to identify the current needs.

Responsible Scientist:
Prof. Dr. J. Käs

Lecturers:
X. Trepat, Institute for Bioengineering of Catalonia, Barcelona, Spain; M. Lütolf, EPFL, Lausanne, Switzerland; T. Brandstätter, Ludwig-Maximilians-University Munich, Germany; Y. Mao, University College London, GB; J. Würfel, University of Basel, Switzerland; M. Doyley, University of Rochester, USA; J. Huston III, Mayo Clinic, USA; J. Guo, Charité, Germany; F. Sauer, Leipzig University, Germany; A. Melzer, Leipzig University, Germany; L. Zhu, Peking Union Medical College Hospital, China; J. Rheinlaender, University Tübingen, Germany; R. Barr, Northeast Ohio Medical University, USA; I. Andreu, Universidad de Navarra, Spain; T. Fuhs, Leipzig University, Germany; O. Chaudhuri, Stanford University, USA; C. Monzel, Heinrich-Heine University Düsseldorf, Germany; C. Clemens, Leipzig University, Germany; T. Phillips, King´s College London, GB; O. Campàs, TU Dresden, Germany; E. Fischer-Friedrich, TU Dresden, Germany; D. Böhringer, Friedrich Alexander University Erlangen-Nuremberg, Germany; S. Köster, University of Göttingen, Germany; M. Lekka, Institute of Nuclear Physics, Polish Academy of Sciences, Poland; F. Lautenschläger, Saarland University, Germany; A. Loneker, University of Pennsylvania, USA; J. Ivaska, Turku University, Finland; L. Munn, Harvard Medical School, USA; P. Janmey, University of Pennsylvania, USA; A. Abend, Leipzig University, Germany; M. Guo, Massachusetts Institute of Technology, USA

Contents:
⇒ Biomechanics (biopolymers, networks, rheology, cytoskeleton, cell shape)
⇒ Models of tumour growth (finite element-based models, differential adhesion hypothesis, glass-like behaviour)
⇒ Forces, motion, adhesion (cell motility, assembly, molecular motors)

⇒ Tumour progression (tumour growth and homeostasis, uncontrolled proliferation, invasion and metastasis, tumour induced alterations of the stroma, vascular system and immune system, role of chemical cues as well as active and passive forces in triggering cell division and apoptosis)
⇒ Diagnostics and screening (imaging [CT, MRI/MRE], tumour markers, histology, tumour staging)
⇒ Personalised medicine and better tumour staging (single cell analysis, high throughput and content, genetic networks, tumour specificmtracers and their application by PET-imaging or fMRI-scanning, tumour cell biomechanics and adhesion)
⇒ Therapy (surgery, radiation, chemotherapy [antineoplastic drugs, cytostatic molecules, protein kinase inhibitors])
⇒ Targeted tumour therapy (specific and unspecific shuttles, specific expression of cell surface proteins, internalisation of biomolecules into tumour cells, linkers for controlled release, etc.)
⇒ Relapse (selective pressure and resistant tumour cells, dormant cancer cells, cancer stem cells)

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

Complex Nanostructures: Halide-based Functional Materials (2021-T3)

30 September - 01 October 2021, hybrid format,
written report, 2 credit points, bi-yearly recurrence with modification, 17 participants

The module gave an overview of the international and current developments in the research area of halogen-based functional materials. Manifold application potentials arise from such materials, e.g. in the fields of thin film electronics or solar power conversion.

Responsible Scientist:
Prof. Dr. M. Grundmann

Lecturers:
H. Hosono, Tokyo Institute of Technology, Yokohama, Japan; S. Botti, Friedrich-Schiller-Universität Jena, Germany; M Nakamura, RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan; A. Crovetto, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; C. Yang, East China Normal University, Shanghai, China; T. Unold, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; T. Mazur, AGH University of Science and Technology, Kraków, Poland

Contents:
⇒ The lectures in the module covered topical developments in the field of functional compound materials, in particular semiconductors, containing halogen elements
⇒ Two foci are copper iodide (CuI) and related materials as well as perovskites
⇒ Besides physical principles and material science and fabrication aspects, device applications were discussed.

From Molecules to Materials: Photocatalysis (2021-T4)

09 September, online,
written report, 2 credit points, bi-yearly recurrence with modification, 19 participants

This module linked molecular sciences and materials science. Starting with basic concepts it teaches how photocatalysis can be applied as versatile synthetic tool in various fields, incl. (asymmetric) organic synthesis, and ligand design. Furthermore, the development of new molecular (incl. biobased), immobilised and heterogeneous catalysts was described. Insights into photocatalyst characterisation, implementation in multi-catalytic transformations and mechanistic understanding was provided.

Responsible Scientist:
Prof. Dr. E. Hey-Hawkins, Prof. Dr. K. Zeitler

Lecturers:
B. König, Regensburg University; C. Nevado, Zürich University; R. Wolf, Regensburg University; B. Lotsch, LMU München& MPI for Solid State Sesearch Stuttgart; J. Strunk, Likat, Rostock; J. Weigand, TU Dresden; T. Hyster, Cornell University

Contents:
⇒ Photocatalysts based on “hard” (synthetic molecules, crystalline “soft” nanostructures, covalent organic frameworks (COFs), immobilised catalysts) building blocks for the application in synthesis, including combinations with “soft” (enzymes, biomolecules) co-catalysts.
⇒ Properties of these materials (optical, redox and photocatalytic properties); applications (photocatalysis, immobilised catalysts, (solar) energy conversion and storage; theoretical and mechanistic aspects.

Methods:
⇒ Synthesis, immobilisation techniques, characterisation, photocatalytic studies

Deep Learning/Machine Learning (2021-T7)

16 - 17 September 2021, online,
written exam, 2 credit points, bi-yearly recurrence with modification, 20 participants

The course aimed at two aspects of machine learning. The first goal was an introduction to statistical mechanics of learning, which aimed at describing the typical learning behaviour of neural networks, discussion of the generalisation performance of strongly overparametrised neural networks. Information field theoretic description of ultrawide neuralnetworks. The second aim was to give an introduction to machine learning techniques and its applications in natural sciences. It included fields of image recognition, time series analysis and reinforcement learning with examples and applications of neural networks in fluid mechanics.

Responsible Scientist:
Prof. Dr. F. Cichos, Prof. Dr. B. Rosenow

Lecturers:
P. Sollich, Göttingen University, Germany; G. Volpe, Gothenburg University, Sweden; K. Gustavsson, Gothenburg University, Sweden; P. Sollich, Göttingen University, Germany; Z. Ringel, Hebrew University, Israel; S. Brunton, Washington University, USA; F. Cichos, Leipzig University, Germany; B. Rosenow, Leipzig University, Germany

Contents:
⇒ Introduction to machine learning and deep learning techniques
⇒ Deep learning statistical physics: mapping of ultrawide neural networks to Gaussian processes, description of neural networks with the help of functional integrals
⇒ Machine learning applications: image segmentation, tracking and feature extraction with convolutional neural networks
⇒ Time series analysis with recurrent neural networks
⇒ Applications of reinforcement learning in physics
⇒ Machine learning for fluid mechanics

Methods:
⇒ Theoretical methods of modern statistical mechanics
⇒ Image processing methods
⇒ Time series analysis
⇒ Programming

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Dmitry Budker	*Helmholtz Institute Mainz and Johannes Gutenberg University*	Extreme NMR - zero field, single spins and dark matter	26 October 2021	*Universität Leipzig, Faculty of Physics and Earth Sciences*

Annual BuildMoNa Conference

The annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nanoobjects" (BuildMoNa) was held online on 8 and 9 March 2021. The poster session took place via Zoom using breakout rooms. The following guest speakers gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Claudia Schnohr, Leipzig University
Atomic-scale structure of complex semiconductors

⇒ Prof. Dr. Tanja Gulder, Leipzig University
Combining the best of both worlds: Bioinspired methods for directed halogenations

⇒ Prof. Dr. Christian Hackenberger, Humboldt Universität zu Berlin and Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP)
The power of chemoselectivity: Functional protein-conjugates for intra- and extracellular targeting

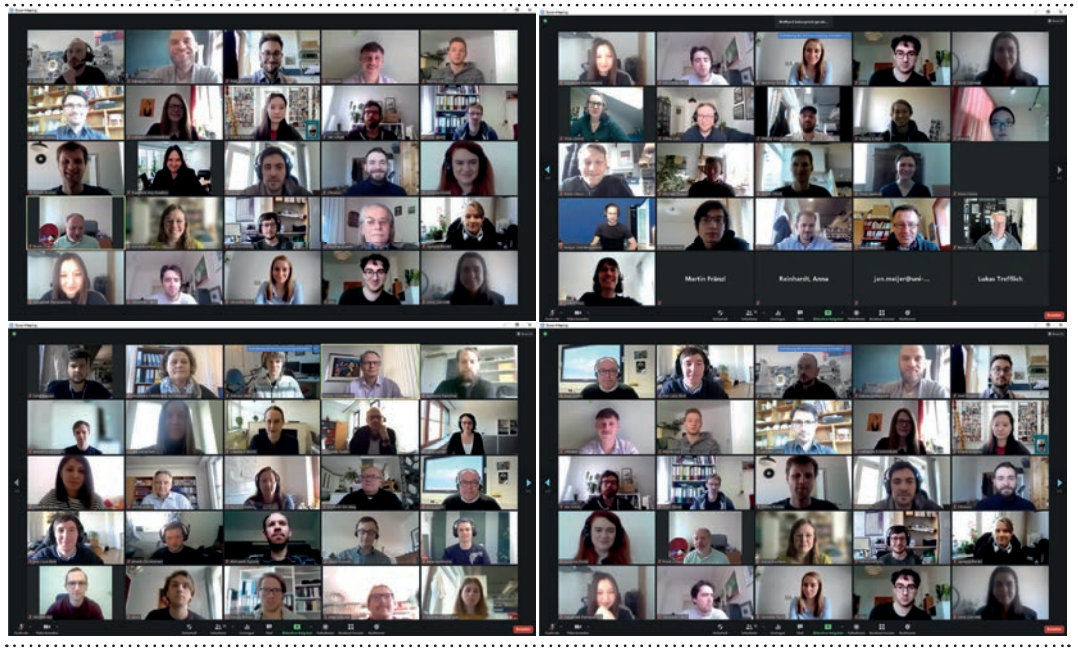
⇒ Prof. Dr. Regine von Klitzing, TU Darmstadt
Swelling behaviour and mechanical properties of multiresponsive polymer coatings

⇒ Dr. Agnes Schulze, Leibniz Institute for Surface Engineering (IOM)
Surface engineering of polymer membranes for use in water treatment

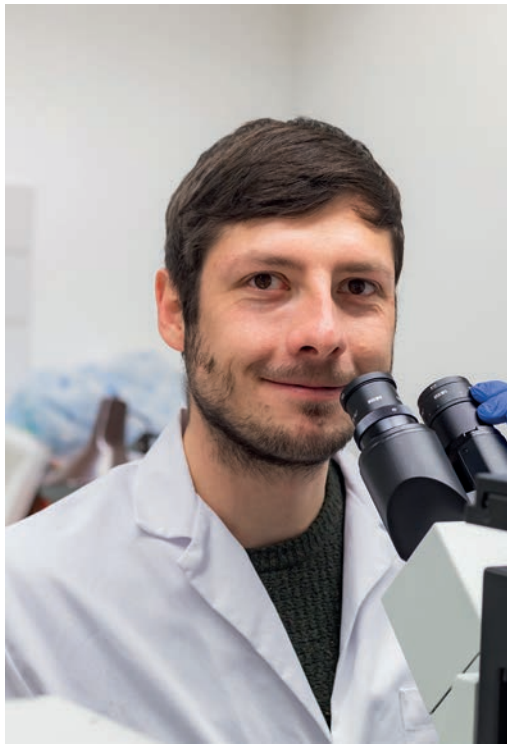
The BuildMoNa Awards 2021 were given to doctoral candidates to recognise their outstanding scientific achievements. The Awards Ceremony was organised in a virtual format.

Patrick Irmisch (Peter Debye Institute for Soft Matter Physics) received the first prize for his work on establishing a simple and easily applicable model framework, which allows quantitative prediction of the kinetics of DNA-strand displacement reactions in the presence of mismatches, using a minimal set of parameters. The work was published as: *Modeling DNA-strand displacement reactions in the presence of base-pair mismatches* P. Irmisch, T. E. Ouldridge, R. Seidel / J. Am. Chem. Soc. (2020) **142** 11451

Benjamin Hoffmann (Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry) received the second prize for his work on electronic excitation spectra of individual nanoparticles in the gas phase obtained by single nanoparticle action spectroscopy, published as: *Electronic action spectroscopy on single nanoparticles in the gas phase* T. K. Esser, B. Hoffmann, J. L. Anderson, K. R. Asmis / J. Phys. Chem. Lett. (2020) **11** 6051.



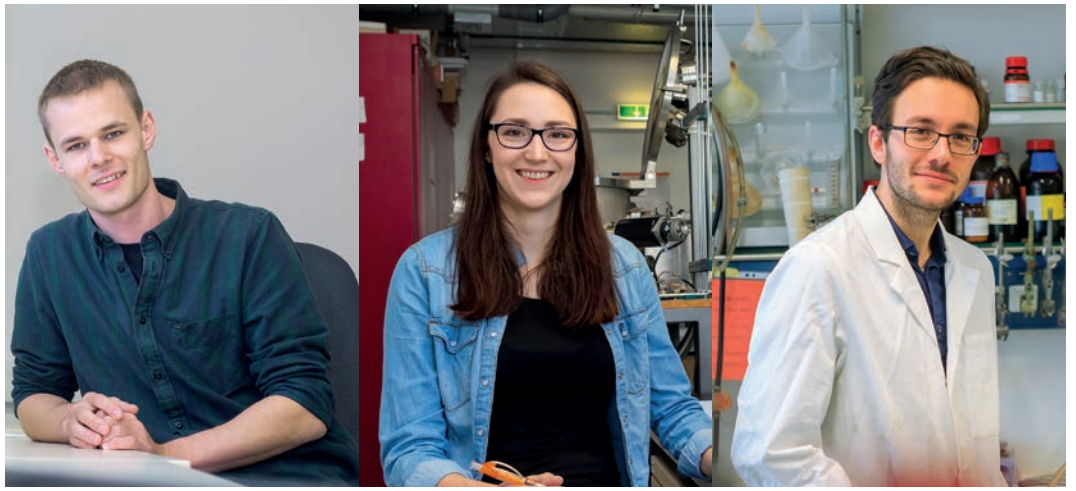
⇑ Annual BuildMoNa Conference 2021.



⇑ Winner of the BuildMoNa Award 2021, Patrick Irmisch (first prize).

Axel Straube (Institute of Inorganic Chemistry) received the third prize for his work on the coordination behaviour and application in redox-switchable catalysis of C3-symmetric tris(ferrocenyl)arene-based tris-phosphane, work published in: Chem. Eur. J. (2020) **26** 5758 / Chem. Sci. (2020) **11** 10657 / Dalton Trans. (2020) **49** 16667.

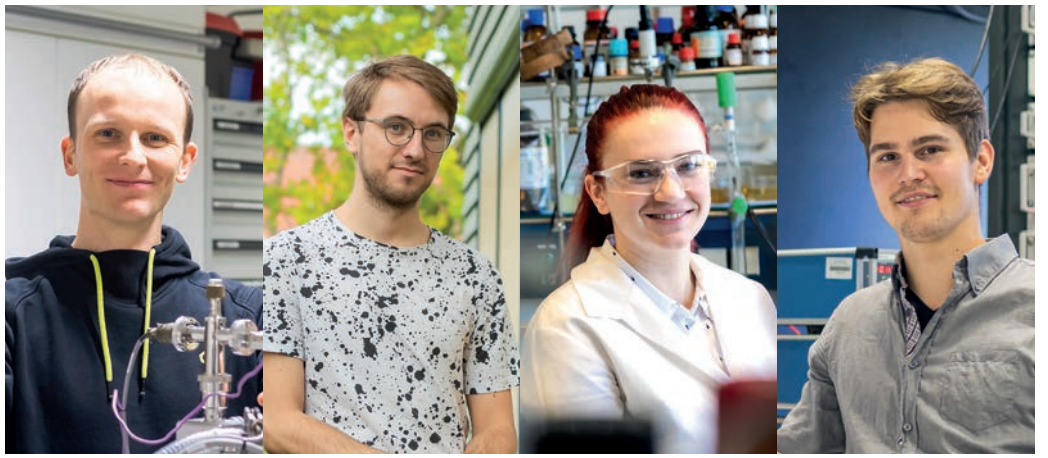
Anna Hassa (Felix Bloch Institute for Solid State Physics) received also the third prize for her work on on the metastable, orthorhombic k-phase of the (Al,Ga)2O3 alloy system. She proved that the long thought hexagonal phase is actually orthorhombic and provides more favorable layer properties than films from the thermodynamic ground state phase. The work published as: *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.



⇑ Winners of the BuildMoNa Awards 2021: Benjamin Hoffmann, Anna Hassa and Axel Straube (from left to right).

16 doctoral candidates presented their scientific results with short talks. Presentations covered partly the research profile of the graduate school: development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. For the 10 participants of the Presentation Workshop held by Dr. Frank Lorenz in a virtual format this was the opportunity to directly apply their newly acquired knowledge in that area. Their talks were recorded and critically discussed afterwards.

At the end of the workshop a jury selected the best presentations given by the doctoral candidates. The first prize was awarded to Liridona Useini for her presentation “Synthesis of carboranyl analogues of the non-steroidal anti-inflammatory drug mefenamic acid” and to Max Grellmann for his presentation “Femtosecond pump-probe spectroscopy on small cerium clusters (Ce n ≤ 10)”. The second prize was awarded to Oliver Herrfurth for his presentation “Ring-structure formation of hot carriers in ZnO studied with time-resolved imaging ellipsometry” and to Zeno Fickenscher for his talk “Synergistic catalysis in heterobimetallic complexes for homogeneous carbon dioxide hydrogenation“.



⇑ Winners of the presentation awards at the Annual BuildMoNa Conference: Oliver Herrfurth, Zeno Fickenscher, Liridona Useini and Max Grellmann (from left to right).

Funding of doctoral candidates

DFG Deutsche Forschungsgemeinschaft

DAAD Deutscher Akademischer Austauschdienst German Academic Exchange Service

IOM Leibniz Institute of Surface Engineering

SAB Sächsische AufbauBank

Europäische Union

Europa fördert Sachsen. EFRE Europäischer Fonds für regionale Entwicklung

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Europa fördert Sachsen. ESF Europäischer Sozialfonds

HoME Hochschule Merseburg University of Applied Sciences

China Scholarship Council

SACHSEN SMWK Sächsisches Staatsministerium für Wissenschaft und Kunst

Alexander von Humboldt Stiftung / Foundation

FEM POWER

Heinrich Böll Stiftung

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