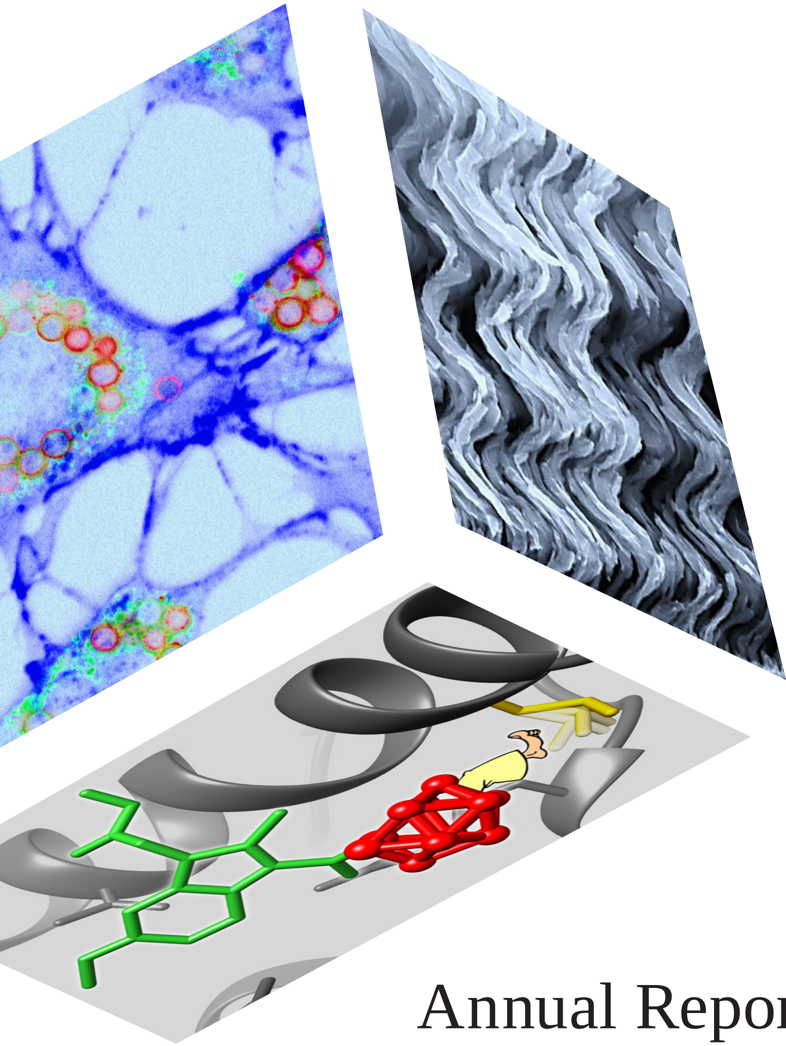
UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2015

UNIVERSITÄT LEIPZIG

Cover image:
⇒ *Left:* Confocal Laser Scanning Microscopy image of 3T3-CD4-CXCR4 cells in interaction with antibody-functionalised SiO_2-microcarriers (d=5µm) after 24h of co-incubation
⇒ *Right:* Cromium nanospirals produced by Glancing Angle Deposition
⇒ *Bottom:* Selective COX-2 inhibitor based on a *nido*-dicarbaborate derivative

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Annual Report 2015

Founded as DFG Graduate School 185 in 2007

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Leipzig school of natural sciences – the eighth year of building with molecules and nano-objects

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

The Graduate School BuildMoNa focuses on interdisciplinary education of young scientists based on excellent research. The materials research concept is based on a “bottom-up” approach. Progressive building blocks, such as nano-objects, smart molecules, polymeric scaffolds, peptides and active proteins, will be combined — preferentially by self-organisation — to create fundamentally new classes of materials that are inspired by active, adaptive living matter, and which are environmentally friendly, highly efficient, low-cost devices serving multifunctional purposes for a steadily more diversified modern society. The paradigm shift from uniform bulk materials towards nanostructured multifunctional materials that emerge from combinations of smart molecules, proteins and nano-objects is essential for future knowledge transfer from fundamental to applied sciences.

Since the establishment of the Graduate School in 2007, the number of doctoral candidates has continuously grown. At the end of 2015, 63 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 116 young scientists have already finished their doctoral studies. In 2015, 4 doctoral candidates were awarded a DAAD-GSSP scholarship, and 85 doctoral candidates were funded by third-party grants. Additionally, 4 doctoral candidates were funded by doctoral positions provided by the European Social Fund (ESF) of the European Union and the Free State of Saxony.

The Graduate School provides a well-structured training programme including multi-disciplinary scientific training and a transferable skills programme in cooperation with the Research Academy Leipzig. The scientific training programme consists of introductory modules to bridge interdisciplinary gaps, thematic modules and advanced modules linked to ongoing research and technological applications. Each year, one of the advanced modules is organised as an international minisymposium. In 2015, the minisymposium “Quantum coherent structures: Unconventional conductivity” was organised by the research groups of Prof. Marius Grundmann and Prof. Bernd Rosenow and brought together researchers that are concerned with the investigation of the macroscopic coherent quantum states such as superfluids, superconductors or Bose-Einstein condensates. Science-related events included the third Annual BuildMoNa Conference, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School.

Although the funding by the DFG within the German Excellence Initiative expired in October 2014, BuildMoNa will for now be continued with financial support from other sources as a class at the Research Academy Leipzig until October 2017.

Prof. Dr. Evamarie Hey-Hawkins

Organisation and management

The Graduate School BuildMoNa is a class of the *Research Academy Leipzig* within the Graduate Centre Mathematics / Computer Science and Natural Sciences, its director being Prof. Dr. M. Droste. BuildMoNa is represented within the Research Academy by Prof. Dr. Dr. h.c. E. Hey-Hawkins as Research Academy Board member and by André Heber as representative of the doctoral candidates.

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

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

The Speaker of the Graduate School is head of the Steering Committee as well as the external representative of BuildMoNa.

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

The BuildMoNa Office consists of one professional scientific manager (half-time position) and one multilingual secretary (part-time position), who support the Steering Committee. They coordinate the doctoral training activities and ensure information and 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.

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Dr. Alexandra Hildebrand

Multilingual Secretary
Isabel Holzke

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Deputy
M.Sc. Phys. Martin Glaser

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Prof. Dr. Frank Cichos
Prof. Dr. Daniel Huster
Prof. Dr. Frank-Dieter Kopinke
Prof. Dr. Harald Krautscheid
Prof. Dr. Felix Otto

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Faculty of Biosciences, Pharmacy and Psychology
M.Sc. Chem. Michael Ansorge

Faculty of Chemistry and Mineralogy
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M.Sc. Chem. Ulrike Junghans

Faculty of Physics and Earth Sciences
M.Sc. Phys. André Heber
M.Sc. Phys. Martin Glaser

Leibniz Institute of Surface Modification
M.Sc. Phys. Alina Bischoff

Institute of Medical Physics and Biophysics
Dipl.-Phys. Martin Göse

Helmholtz Centre for Environmental Research
M.Sc. Yuting Guo

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Anup Kumar Adhikari	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis and reactivity of phosphorus-rich compounds*
M.Sc. Phys. Uta Allenstein	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Dynamic mechanical cell manipulation and characterisation using magnetostrain*
M.Sc. Chem. Michael Ansorge	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	*Biomimetic signalling gradients in reconstituted extracellular matrices*
M.Sc. Phys. Francis Bern	Prof. Dr. P. Esquinazi / Prof. Dr. B. Kersting	*Coupling phenomena in multilayerd oxide nanostructures*
M.Sc. Phys. Alina Bischoff	Prof. Dr. S. Mayr / Prof. Dr. M. Grundmann	*Mechanical characterisation and training of ferromagnetic iron-palladium shape memory alloy thin films*
M.Sc. Chem. Eng. Paul Cosmin Boar	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phosphorus-based metallacycles for applications in catalysis*
M.Ed. Math./Phys. Johannes Bock	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Computer simulations of semiflexible polymers in disordered media*
M.Sc. Phys. Michael Bonholzer	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Magneto-tunnel junctions with oxidic contacts*
Dipl.-Phys. Marco Braun	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Gold nanoparticle based thermophoretic nanofluids*
Dipl.-Phys. Jörg Buchwald	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Mechanical properties of surfaces at nanoscale*
Dipl.-Phys. Jakob Tómas Bullerjahn	Prof. Dr. K. Kroy / Prof. Dr. B. Abel	*How a polymer breaks a bond*
M.Sc. Chem. Antonio Buzharevski	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Synthesis, characterisation and evaluation of biologically active carborane derivatives of nonsteroidal anti-inflammatory drugs (NSAIDs) that are known COX inhibitors to improve COX-2 selectivity and reduce side effects*
M.Sc. Chem. Milos Erak	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. T. Pompe	*Synthesis of difficult and long peptide sequences, modifications and activity testing*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Gianmaria Falasco	Prof. Dr. K. Kroy / Prof. Dr. F. Cichos	*Non-equilibrium dynamics of heated and self-propelled nanoparticles*
M.Sc. Phys. Annemarie Finzel	Prof. Dr. B. Rauschenbach / Prof. Dr. B. Abel	*Ion-beam assisted deposition of gallium nitride films*
M.Sc. Chem. Jan-Patrick Fischer	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification and characterisation of therapeuticaly relevant peptide hormones*
Dipl.-Phys. Niklas Fricke	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Polymer conformations in disordered environments*
M.Sc. Phys. Nataliya Georgieva	Prof. Dr. J. Haase / Prof. Dr. B. Rosenow	*Magnetic resonance of topological insulators*
M.Sc. Chem. Anika Gladytz	Prof. Dr. B. Abel / Prof. Dr. A.G. Beck-Sickinger	*Nanospectroscopy near chemical and biological interfaces*
M.Sc. Chem. Thomas Gladytz	Prof. Dr. B. Abel / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Tracing chirality, reactivity and structures in space and time of smart molecules and materials near interfaces by XUVI soft X-ray photoelectron emission and absorption spectroscopy*
M.Sc. Phys. Martin Glaser	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	*Investigation of actin structures*
M.Sc. Chem. Florian Glasneck	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Novel calix[4]arene derivatives and their complexation behaviour towards f-elements*
M.Sc. Phys. Tom Golde	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Actin related contractile structures*
Dipl.-Phys. Martin-Patrick Göse	Prof. Dr. D. Huster / Prof. Dr. T. Pompe	*Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake*
M.Sc. Chem. Marta Gozzi	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Nido-carbaborate complexes as cytotoxic agents*
M.Sc. Chem. Toni Grell	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Preparation of phosphorus-rich metal phosphides on the basis of oligophosphanide complexes*
M.Sc. Chem. Yuting Guo	Prof. Dr. H. Harms / Prof. Dr. F.-D. Kopinke	*Nanoparticle interactions with microorganisms on the molecular level*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Principles of mechanosensitivity and durotaxis in mammalian cells*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. André Heber	Prof. Dr. F. Cichos / Prof. Dr. M. Grundmann	*Spatially resolved investigations of thermal transport in micro- and nanostructures*
Dipl.-Phys. Marcel Hennes	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Synthesis and characterisation of magnetic core-shell nanoparticles*
M.Sc. Chem. Reinhard Hoy	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phospholane-based coordination cages for application in homogeneous catalysis*
M.Sc. Chem. Astrid Jäschke	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Synthetic approaches towards novel calix[4]arene based f-metal receptors*
Dipl.-Phys. Alexander Janot	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Quantum condensates-coherence, fluctuations and disorder*
Dipl.-Pharm. Cathleen Jendrny	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Design and development of peptides for therapeutic application*
M.Sc. Chem. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Heterogeneously catalysed liquid phase oxidation of hydrocarbons over metal-organic frameworks*
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. Phys. Robert Karsthof	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Transparent photovoltaic cells*
M.Sc. Chem. Karolin Kobalz	Prof. Dr. H. Krautscheid / Prof. Dr. B. Kersting	*1,2,4-triazolyl ligands for the synthesis of porous coordination polymers*
Dipl.-Phys. Jonas Kohlrautz	Prof. Dr. J. Haase / Prof. Dr. P. Esquinazi	*Magnetic resonance under extreme conditions*
Dipl.-Phys. Andrea Kramer	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	*How temperature affects cell mechanics*
M.Sc. Chem. Robert Kuhnert	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranes as phenyl mimetics in biologically active substances*
Dipl.-Phys. Anja Landgraf	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Magneto-mechanical characterisation and training of single crystalline FePd films for the purpose of designing a thin film membrane pump*
Dipl.-Phys. Marc Lämmel	Prof. Dr. K. Kroy / Prof. Dr. W. Janke	*Stiff biopolymer solutions and networks*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Fritz Lehnert	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Ion-aided synthesis and investigation of nanoporous materials*
M.Sc. Phys. Susann Liedtke	Prof. Dr. B. Rauschenbach / Prof. Dr. J. Meijer	*Sculptered metal films*
Dipl.-Chem. Ing. Felix Link	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Diesel exhaust catalyst deactivation by biofuel-originated poisons and hydrothermal treatment*
M.Sc. Phys. Jürgen Lippoldt	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Stochastic analysis of plasma membrane fluctuations of neuronal growth cones*
Dipl.-Phys. Martin Marenz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Development of a coarse-graining procedure for polymer adsorption*
M.Sc. Chem. Michael Marx	Prof. Dr. R. Gläser / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Modifying metal nanoparticles by oxidative extraction into supercritical solution*
M.Sc. Chem. Georgia Mhanna	Prof. Dr. R. Gläser / Prof. Dr. A.G. Beck-Sickinger	*Hexagonal mesoporous silicates for immobilisation of multi-enzyme conjugates*
M.Sc. Phys. Tom Michalsky	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Light-matter interaction in systems of reduced dimensionality*
M.Sc. Phys. Erik Morawetz	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	*Optical deformability and tumour aggressiveness*
Dipl.-Phys. Andreas Müller	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	*Peptide friction in cell adhesion*
M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Metal-organic frameworks with chiral binaphthalene-based linkers*
M.Sc. Phys. Marcus Purfürst	Prof. Dr. R. Gläser / Prof. Dr. M. Grundmann	*Influence of soot loading on the catalytic behaviour of diesel particulate filters – experiment and modelling*
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Spin polarisation investigations on exciton-polaritons and their condensates*
M.Sc. Phys. Stefanie Riedel	Prof. Dr. S. Mayr / Prof. Dr. A. Käs	*Radiation assisted modification of gelatin and collagen for biomedical applications*
M.Sc. Chem. Stefan Saretz	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranes for medical applications*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Marina Sarmanova	Prof. Dr. B. Rauschenbach / Prof. Dr. S. Mayr	*Measurements with nanometer resolution of mechanical properties of thin layers and structured surfaces by the contact resonance atomic force microscopy*
M.Sc. Phys. Philipp Schierz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Investigation of polymer aggregation by computer simulations*
M.Sc. Phys. Peter Schlupp	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Growth and optimisation of amorphous p- and n-type oxide semiconductors for electronic device applications*
M.Sc. Chem. Andy Schmied	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Phosphorus-based nano-frames*
Dipl.-Biol. Ria Anne-Rose Schönauer	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of peptide analogues*
M.Sc. Phys. Daniel Thomas Splith	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Investigation and optimisation of ß-Ga_2O_3 thin films and their application for electronic devices*
M.Sc. Chem. Axel Straube	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Multi-ferrocene-based phosphorus ligands for homogeneous catalysis*
M.Sc. Phys. Xinxing Sun	Prof. Dr. B. Rauschenbach / Prof. Dr. S. Mayr	*Phase change materials*
Dipl.-Phys. Martin Thunert	Prof. Dr. M. Grundmann / Prof. Dr. B. Rosenow	*Bose-Einstein-condensation and superfluids of exciton-polaritons in ZnO-based microresonators*
M.Sc. Phys. Martin Treffkorn	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Theoretical analysis of nanostructures for topological quantum computing*
M.Sc. Chem. Steve Ullmann	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Extraction of rare earths by means of preorganised calixarene*
M.Sc. Phys. Marcel Wille	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Whispering gallery modes: influence of the resonator shape on lasing properties*
B.Sc. Eng. Emilia Wisotzki	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Interaction of nanoparticles and polymers with biological matter for mechanical coupling*
M.Sc. Biochem. Dennis Worm	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Synthesis and biochemical evaluation of carbaborane - modified peptide ligands*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Nanosc. Muhammad Ayman Zaheer	Prof. Dr. R. Gläser / Prof. Dr. Kopinke	*Studying of diffusion in reacting catalytic systems by means of NMR spectroscopic methods*
M.Sc. Phys. Guillermo Zecua Ramirez	Prof. Dr. K. Kroy / Prof. Dr. T. Pompe	*Inelastic mechanics of the cytoskeleton and cell morphology*

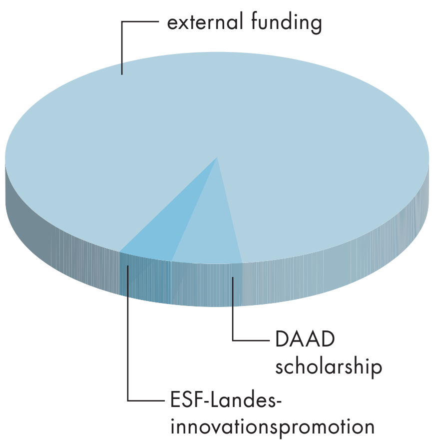
Alumni 2015

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Ariyan Arabi-Hashemi	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Ion beam assisted deposition of intelligent and adaptive surfaces*
Dr. rer. nat. Salma Begum	Prof. Dr. H. Krautscheid / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Metal-organic frameworks based on phosphonate linkers*
Dr. rer. nat. Solveig Boehnke	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaborane derivatives in tumour therapy and diagnosis*
Dr. rer. nat. David Böhme	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Cytotoxic neuropeptide Y-conjugates for the development of new therapeutical approaches of metastasing breast cancer*
Dr. rer. nat. Felix Daume	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Degradation of flexible* $Cu(In,Ga)Se_2$ *solar cells*
Dr. rer. nat. Thomas Heinze	Prof. Dr. R. Gläser / Prof. Dr. B. Kirchner	*Noble metal nanoparticles on ordered porous supports for the in-situ synthesis and conversion of* H_2O_2 *in supercritical carbon dioxide*
Dr. rer. nat. Sven Hofmann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of peptides*
Dr. rer. nat. Fabian Klüpfel	Prof. Dr. M. Grundmann / Prof. Dr. A. Käs	*Transparent active multi-electrode arrays for the measurement of nerve cell signals*
Dr. rer. nat. Paul Neumann	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Switchable dendritic ferrocenyl phosphines*
Dr. rer. nat. Wilma Neumann	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Overcoming cisplatin resistance of tumour cells with cytotoxic cyclo-oxygenase inhibitor conjugates*
Dr. rer. nat. Mareen Pagel	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of surfaces for novel biomaterials*
Dr. rer. nat. Stefan Puttnins	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*The influence of inhomogeneities in* $Cu(In,Ga)Se_2$ *thin film solar cells*
Dr. rer. nat. Dennis Richter	Prof. Dr. R. Gläser / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Heterogeneous photocatalysis: water splitting with visible-light irradiation*

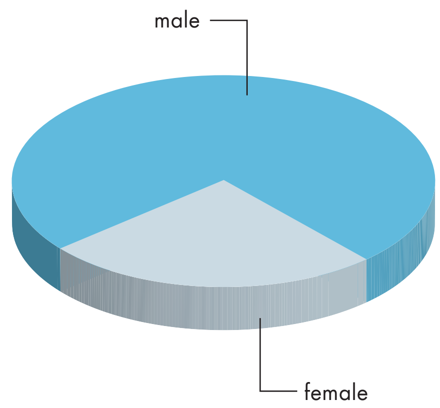
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Stefan Richter	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*New selective cytostatics*
Dr. rer. nat. Friedrich-Leonhard Schein	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Fabrication and characterisation of bipolar heterostructures with oxidic semiconductors*
Dr. rer. nat. Jörg Schnauß	Prof. Dr. J. Käs / Prof. Dr. A.G. Beck-Sickinger	*Biomimetic actin networks*
Dr. rer. nat. Tim Stangner	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Investigation of receptor/ligand interactions on the level of single contacts using high-resolution optical tweezers*
Dr. rer. nat. Erik Thelander	Prof. Dr. B. Rauschenbach/ Prof. Dr. M. Grundmann	*Synthesis of nanostructures using laser ablation*
Dr. rer. nat. Zhaoyang Wang	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	*Metal-organic frameworks based on linkers with hard and soft donor groups*
Dr. rer. nat. Johannes Zierenberg	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Aggregation of polymers in crowded confinement with correlated disorder*

Statistics

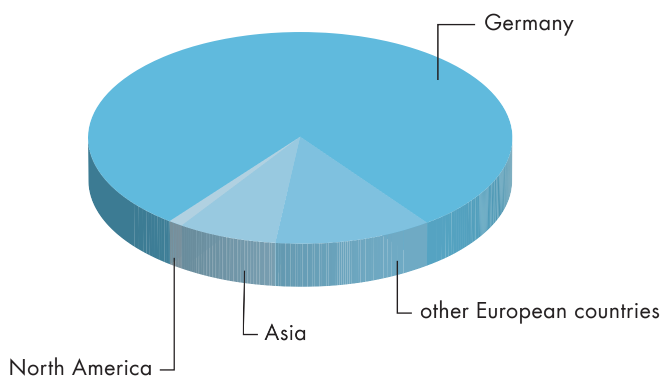
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:



Biophysical and macromolecular chemistry

Prof. Dr. Bernd Abel
M.Sc. Chem. Anika Gladytz, M.Sc. Chem. Thomas Gladytz

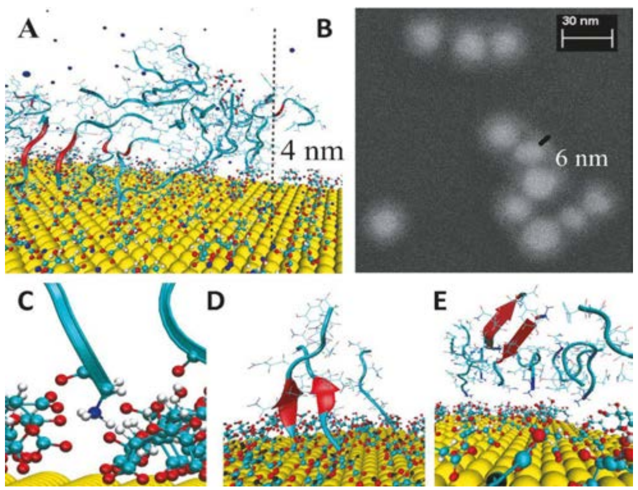
The Abel group at the IOM and the Universität Leipzig works in the fields of biophysical chemistry and macromolecular chemistry, as well as smart functional materials and surfaces. Structure and dynamics are investigated with the long-term goal of obtaining fundamental knowledge about light-matter and particle-matter interaction and about new smart functional materials. Another goal is also to develop new molecular and analytical probes for fundamental research and to develop advanced materials and analytical devices for industry and industrial applications.

Within BuildMoNa we investigate amyloid aggregation and fibrillation with nanoscale imaging and spectroscopic techniques and we aimed at monitoring structures of aggregated proteins near interfaces of nanoparticles to resolve the question whether nanoparticles may induce Alzheimer's disease (A. Gladytz).

Together with A. Beck-Sickinger's group and A. Robitzki's group we also study and develop biofunctionalised surfaces, i.e., proteins/peptides and biomolecules such as enzymes immobilised and bound to oxidic and metal surfaces for biocompatible interfaces and biomolecule assays as well as electronic devices. Peptide based multifunctional molecules are employed as anchors for cells near inorganic interfaces. Molecular adsorption and structure formation are investigated via a number of novel imaging and spectroscopic techniques (A. Gladytz).

Another big research focus of the Abel group at BuildMoNa at present is time-resolved dynamics and structure of chemical and biological molecular systems at water interfaces (T. Gladytz). The analytical tools here are mainly ultrafast laser systems.

With J. Meijer and P. Esquinazi we are currently pushing instrument development towards nanoscale (magnetic) imaging at surfaces based opon cryo-AFM/CFM sensors.



⇐ Molecular dynamics simulation (A. Gladytz / H. J. Risselada) of peptide aggregation and structure formation near gold nanoparticles.

⇒ *Expansion Dynamics of Supercritical Water Probed by Picosecond Time-Resolved Photoelectron Spectroscopy*
T. Gladytz, B. Abel, K.R. Siefermann / Phys. Chem. Chem. Phys. (2015) **17** 4926

⇒ *Structure-Making Effects of Metal Nanoparticles in Amyloid Peptide Fibrillation*
A. Gladytz, M. Wagner, T. Haupl, C. Elsner, B. Abel / Part. Part. Syst. Charact. (2015) **32** 573

⇒ *Intermediates Caught in the Act: Tracing Insulin Amyloid Fibril Formation in Time by Combined Optical Spectroscopy, Light Scattering, Mass Spectrometry and Microscopy*
A. Gladytz, E. Lugovoy, A. Charvat, T. Häupl, K.R. Siefermann, B. Abel / Phys. Chem. Chem. Phys. (2015) **17** 918

⇒ *Supramolecular Assembly of Functional Hybrid Fibrils with Peptide-pi-System-Peptide Monomers Near Silver-Nanoparticles*
C. Elsner, D. Hintzen, A. Prager, K.R. Siefermann, B. Abel / Z. Phys. Chem. (2015) **229** 427

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Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger
Dr. David Böhme, M.Sc. Chem. Milos Erak, M.Sc. Chem. Jan-Patrick Fischer, Dr. Sven Hofmann, Dipl.-Pharm. Cathleen Jendrny, Dr. Mareen Pagel, Dipl.-Biol. Ria Anne-Rose Schönauer, M.Sc. Biochem. Dennis Worm

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

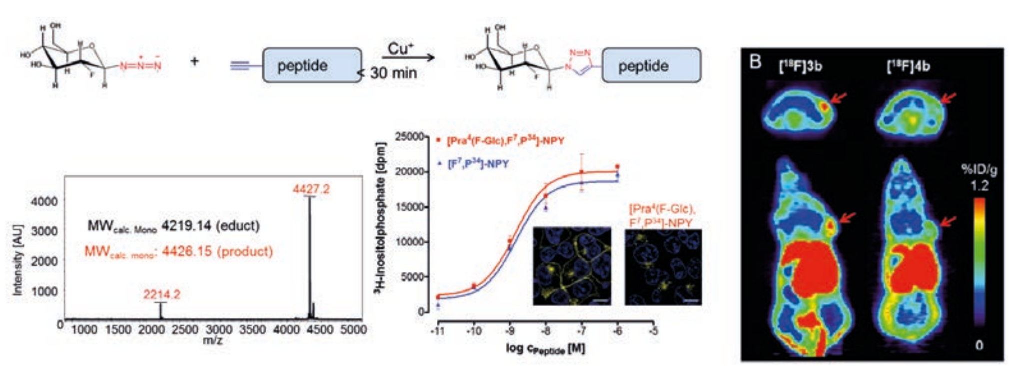
In 2015 Sven Hofmann and David Böhme finished their PhD theses. Sven Hoffmann (M.Sc. Biochem.) and David Böhme (M.Sc. Chem.) worked on the development of novel anti-tumour peptides by conjugation with carbaboranes or cytotoxic

compounds. The peptides are used as shuttle systems to allow tumour specific uptake as the respective peptide receptors are overexpressed on tumour cells and internalise after agonist binding. Both could achieve major advances in 2015. Sven could demonstrate by using a fluorine-18 glucose-azide and peptides with propargylglycine that efficient labelling is possible. This was applied to animal studies and used to specifically label and trace a breast tumour. David developed an internal release system of cytotoxic drugs. He could identify that enzymatic cleavage leads to the most successful endocytotic drug release and thus to the highest specific toxicity.

In the field of chemical modification of proteins Ria Schönauer (Dipl.-Biol.) and Cathleen Jendrny (Dipl.-Pharm.) were very successful. They worked on adrenomedullin and vaspin. Whereas vaspin has been obtained by recombinant technologies, adrenomedullin is achievable by semi-synthetic and fully synthetic approaches.

The field of biomaterial approaches was extremely successful in 2015. Mareen Pagel (Dipl.-Chem.) worked on chemically modified peptides and proteins to improve the properties of biomaterials. She has developed a novel biocompatible ligation method, the inverse Diels-Alder reaction, and successfully applied this to the derivatisation of inorganic surfaces. She could impressively show that cells prefer coated surfaces. Mareen finished her PhD work as well in 2015.

In addition, several papers of former BuildMoNa-members have been published, including Verena Ahrens, Lars Baumann and Sylvia Els-Heindl. The work achieved during their PhD projects was delayed in publication owing to collaborators.



⇑ Specific modification of breast cancer specific neuropeptide Y derivative with F-18 glucose azide by click-chemistry. Chemical, biochemical and biomedical characterisation proved the concept (S. Hofmann et al. / Mol. Pharm. (2015) **12** 1121)

⇒ *Receptor-Mediated Uptake of Boron-Rich Neuropeptide Y Analogues for Boron Neutron Capture Therapy*
V. Ahrens, R. Frank, S. Boehnke, C.L. Schütz, G. Hampel, D.S. Iffland, N.H. Bings, E. Hey-Hawkins, A.G. Beck-Sickinger / Chem. Med. Chem. (2015) **10** 1645

⇒ *High Metabolic in vivo Stability and Bioavailability of a Palmitoylated Ghrelin Receptor Ligand Identified by Mass Spectrometry*
K.B. Kostelnik, S. Els-Heindl, N. Klöting, S. Baumann, M. von Bergen, A.G. Beck-Sickinger / Bioorg. Med. Chem. (2015) **23** 3925

⇒ *Synthesis, in Vitro and in Vivo Evaluation of an 18F-Labeled Neuropeptide Y Analogue for Imaging of Breast Cancer by PET*
S. Hofmann, S. Maschauer, T. Kuwert, A.G. Beck-Sickinger, O. Prante / Mol. Pharm. (2015) **12** 1121

⇒ *Integrating Solid State NMR and Computational Modeling to Investigate the Structure and Dynamics of Membrane-Associated Ghrelin*
G. Vortmeier, S.H. DeLuca, S. Els-Heindl, C. Chollet, H.A. Scheidt, A.G. Beck-Sickinger, J. Meiler, D. Huster / PLoS One (2015) **10** e0122444

⇒ *Controlling Toxicity in Peptide-Drug Conjugates by Different Chemical Linker Structures*
D. Böhme, A.G. Beck-Sickinger / Chem. Med. Chem. (2015) **10** 804

⇒ *Rational Design of Dual Peptides Targeting Ghrelin and Y_2 Receptors to Regulate Food Intake and Body*
T.M. Kilian, N. Klöting, R. Bergmann, M. Clément-Ziza, S. Els-Heindl, S. Babilon, Y. Zhang, A.G. Beck-Sickinger, C. Chollet / J. Med. Chem. (2015) **58** 4180

⇒ *A Cleavable Cytolysin–Neuropeptide Y Bioconjugate Enables Specific Drug Delivery and Demonstrates Intracellular Mode of Action*
V. Ahrens, K. Kostelnik, R. Rennert, D. Böhme, M. von Bergen, L. Weber, A.G. Beck-Sickinger / J. Control. Release (2015) **209** 170

⇒ *Ubiquitin is a Versatile Scaffold Protein for the Generation of Molecules with de Novo Binding and Advantageous Drug-Like Properties*
F. Job, F. Settele, S. Lorey, C. Rundfeld, L. Baumann, A.G. Beck-Sickinger, U. Haupts, H. Lilie, E. Bosse-Doenecke / FEBS Open Bio. (2015) **5** 579

⇒ *Bioorthogonal Labeling of Ghrelin Receptor to Facilitate Studies of Ligand-Dependent Conformational Dynamics*
M. Park, B.B. Sivertsen, S. Els-Heindl, T. Huber, B. Holst, A.G. Beck-Sickinger, T.W. Schwartz, T.P. Sakmar / Chem. Biol. (2015) **22** 1431

⇒ *Fluorescently Labeled Adrenomedullin Allows Real-Time Monitoring of Adrenomedullin Receptor Trafficking in Living Cells*
R. Schönauer, A. Kaiser, C. Holze, S. Babilon, J. Koebberling, B. Riedl, A.G. Beck-Sickinger / J. Pept. Sci. (2015) **21** 905

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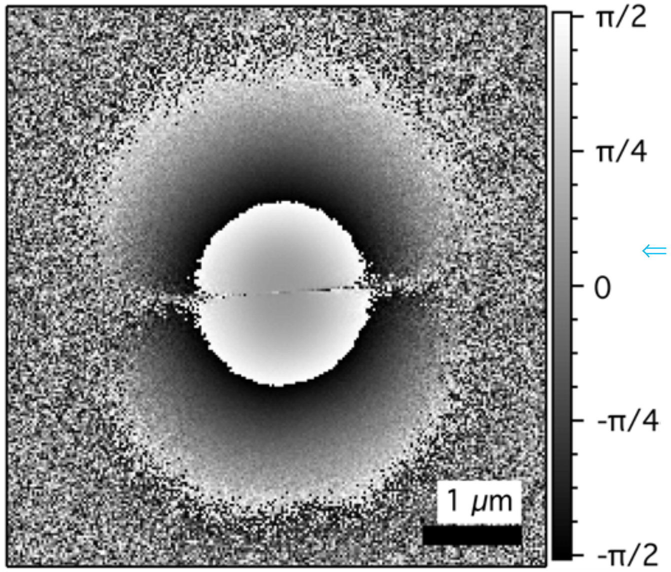
Optical detection of local thermal diffusivities

Prof. Dr. Frank Cichos
Dipl.-Phys. Marco Braun, M.Sc. Phys. André Heber

Fluorescence microscopy on single molecules allows access to spatial and dynamic heterogeneity of materials at the nanoscale. In particular, the application of single molecule fluorescence detection to biological materials, which are intrinsically heterogeneous, has opened new possibilities from measuring protein function to complex transport pathways in cells. Biological systems involve many physical-chemical processes which dissipate energy and where the details of the heat generation and transport in living cells are not explored. On one side, this is due to the lack of suitable methods to measure heat transport at the nanoscale. During the past years, we have continuously developed new techniques which employ the energy conversion in gold nanoparticles to inject heat into various condensed matter systems locally. This heat injection has now been used for the first time to measure the heat transport in polymers and liquids with the help of a single gold nanoparticle. For this purpose, heat is injected periodically at a frequency *f* into the system. The heat causes a local change in the refractive index around the heat source due to the thermal expansion of the material. This local refractive index change can be mapped with a scanning laser beam. As the heat propagates with a finite speed given by the heat diffusivity, the refractive index change is delayed with respect to the oscillation at the source. With the help of this delay, we can directly measure the local heat diffusivity even in complex materials. The figure shows an example of the phase delay caused by the heat conduction. The heat source is a single 60 nm gold nanoparticle centred in the middle of the image. The scanning laser is moving along the y-direction to probe the phase delay. The circular symmetry of the phase delay reveals an isotropic heat conduction which is expected for this particular system. Extracted quantitative values do well agree with the bulk value. Thus, the method is now suitable to map local thermal diffusivities in living cells.



⇐ Optically detected phase delay caused by thermal transport in the surrounding of a harmonically heated gold nanoparticle.

⇒ *Thermal Diffusivity Measured Using a Single Plasmonic Nanoparticle*
A. Heber, M. Selmke, F. Cichos / Phys. Chem. Chem. Phys. (2015) **17** 20868

⇒ *Single Molecules Trapped by Dynamic Inhomogeneous Temperature Fields*
M. Braun, A. Bregulla, K. Günther, M. Mertig, F. Cichos / Nano Lett. (2015) **15** 5499

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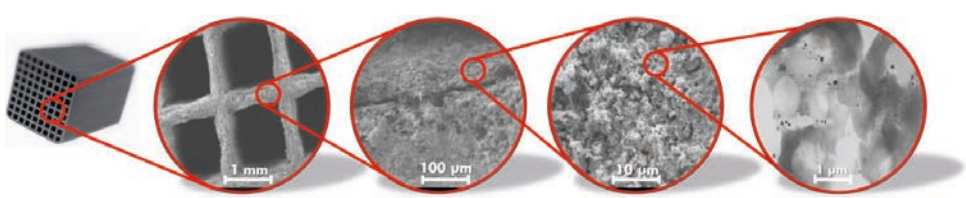
Nano-scale investigations on innovative catalytic systems

Prof. Dr. Roger Gläser
Dr. Thomas Heinze, M.Sc. Chem. Ulrike Junghans, Dipl.-Chem. Ing. Felix Link, M.Sc. Chem. Michael Marx, M.Sc. Chem. Georgia Mhanna, M.Sc. Phys. Marcus Purfürst, Dr. Dennis Richter, M.Sc. Nanosc. Ayman Zaheer

Innovative catalytic systems continue to play a key role for the solution of major current challenges in heterogeneous catalysis, such as energy efficiency, stability and mass transfer. The research in our group is centred on nanoporous materials with defined porosity and tunable active components. Following the principle approaches of the Graduate School, we apply different strategies to rationally design novel materials for the use as catalysts and catalyst supports. In addition to the synthesis of these materials, mass transfer effects and deactivation processes on the nano-scale are in the scope of our research. Mass transfer and diffusion are major challenges when using solid porous catalysts. These phenomena are investigated within two different, industrially relevant fields. On the one hand, in the field of alternative fuels, we apply in-situ monitoring of reaction dynamics and transport of reactants during the transesterification of oils into biodiesel by multinuclear NMR techniques. On the other hand, in the field of emission reduction, we investigate the influence of soot deposited on catalytically coated diesel particle filters on the mass transfer of reactants to the catalytic layer. Moreover, we study the deactivation of catalysts for the selective catalytic reduction of nitrogen oxides by trace compounds that deposit on the catalyst surface. Therefore, field-aged diesel exhaust catalysts are characterised on the nano-scale by microscopy and spectroscopic methods. Another focus is on the immobilisation of multi-enzyme conjugates on hierarchically structured hexagonal mesoporous silicates to enhance the stability and the enzymatic activity. Moreover, the partial oxidation of hydrocarbons on microporous metal-organic frameworks containing transition-metals is studied under continuous-flow conditions in the liquid-phase.



⇑ From the macro- to the nanoscale: microscopic characterisation of a field-aged catalyst monolith for diesel exhaust after treatment.

⇒ *Selective Oxidation of Cyclooctene over Copper-Containing Metal-Organic Frameworks*
U. Junghans, C. Worch, J. Lincke, D. Lässig, H. Krautscheid, R. Gläser / Micropor. Mesopor. Mat. (2015) **216** 15124359

⇒ *Polymer-Based Spherical Activated Carbons in Combination with TS-1 as Efficient Epoxidation Catalysts*
P.C. With, N. Wilde, A. Modrow, S. Fichtner, B. Böhringer, R. Gläser / Chem. Eng. Technol. (2015) **38** 1671

⇒ *Conversion of Carbon Dioxide along with Methanol to Dimethyl Carbonate over Ceria Catalyst*
P. Kumar, P. With, V.C. Srivastava, R. Gläser, I.M. Mishra / J. Environ. Chem. Eng. (2015) **3** 2943

⇒ *Glycerol Carbonate Synthesis by Hierarchically Structured Catalysts: Catalytic Activity and Characterisation*
P. Kumar, P. With, V.C. Srivastava, R. Gläser, I.M. Mishra / Ind. Eng. Chem. Res. (2015) **54** 12543

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Bipolar oxide devices – Putting pn-heterostructures to work

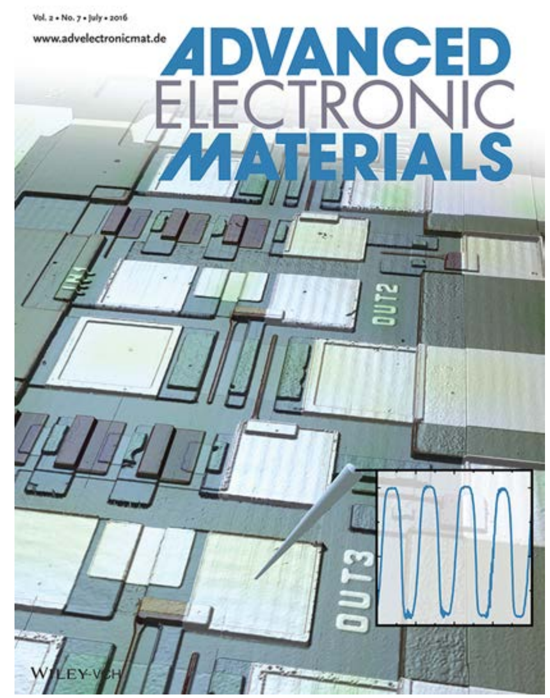
Prof. Dr. Marius Grundmann
M.Sc. Phys. Michael Bonholzer, Dr. Felix Daume, M.Sc. Phys. Robert Karsthof, Dr. Fabian Klüpfel, M.Sc. Phys. Tom Michalsky, Dr. Stefan Puttnins, M.Sc. Phys. Steffen Richter, Dr. Friedrich-Leonhard Schein, M.Sc. Phys. Peter Schlupp, M.Sc. Phys. Daniel Thomas Splith, Dipl.-Phys. Martin Thunert, M.Sc. Phys. Marcel Wille

The class of materials nowadays known as transparent conductive oxides (TCO) was discovered and investigated as early as 1906 by Karl Bädeker when he was post-doc in Leipzig and prepared his Habilitation thesis. Among the transparent and conductive materials he investigated were cadmium oxide and cuprous iodide as well as many other semiconductors such as CdSe or PbS. A detailed biography and historical account of his discoveries and their impact can be found in [M. Grundmann: *Karl Bädeker (1877–1914) and the Discovery of Transparent Conductive Materials* / Phys. Status Solidi A (2015) **212** 1409]. A great push to the field of TCO was the recent discovery of amorphous TCOs with controllable carrier density, also known as transparent amorphous oxide semiconductors (TAOS), by Hosono and coworkers.

Several BuildMoNa doctoral candidates in the Semiconductor Physics Group have achieved decisive progress in the use of such materials by building various electronic devices previously thought to be impossible. The combination of n-type and p-type oxides in bipolar diode structures has yielded unexpectedly high

performance devices and facile fabrication schemes. Also the use of amorphous semiconductors and the deposition of thin films at room temperature enables the use of amorphous substrates, in particular cost-economic glass, and flexible polymeric substrates such as plastic foils for wearable electronics. These properties are explored in and supported through a Horizon 2020 project "Large cost-effective OLED microdisplays and their applications (LOMID)" and newly within the DFG-funded Schwerpunktprogramm 1796 "High Frequency Flexible Bendable Electronics for Wireless Communication Systems (FFlexCom)".

Peter Schlupp adds a further twist to the story as he abandoned all materials that are overly toxic, rare and expensive by only resorting to metal oxides from abundant metals like tin, zinc and cobalt. He fabricated fully amorphous bipolar diodes from zinc-tin-oxide as the n-type materials and zinc-cobalt-oxide as the p-type material [P. Schlupp, F.-L. Schein, H. von Wenckstern, M. Grundmann: *All Amorphous Oxide Bipolar Heterojunction Diodes from Abundant Metals* / Adv. Electr. Mater. (2015) **1** 1400023]. Zinc-cobalt oxide was explored by Friedrich L. Schein who has in the meantime successfully finished his BuildMoNa curriculum and received his doctoral degree. All layers in the new diodes are deposited at room temperature and the starting materials are powders of the respective materials with the optimised metal ratios (i.e. Zn/Sn [S. Bitter, P. Schlupp, M. Bonholzer, H. von Wenckstern, M. Grundmann: *Influence of the Cation Ratio on Optical and Electrical Properties of Zinc-Tin-Oxide Thin Films from Pulsed-Laser Deposition* / ACS Comb. Sci. (2016) **18** 188] and Zn/Co). The amazing result is that such pn-diodes easily outperform



⇐ Ring oscillators based on junction field-effect transistors with ZnO channels and $ZnCo_2O_4$. Oscillation frequencies up to 1.1 MHz are observed for 3-stage circuits and related to easily measurable device properties by a simple analytical model. The cover image is generated from laser scanning microscope images of a 5-stage device.

any previous reported approach [M. Grundmann, F. Klüpfel, R. Karsthof, P. Schlupp, F.-L. Schein, D. Splith, Ch. Yang, S. Bitter, H. von Wenckstern: *Oxide Bipolar Electronics: Materials, Devices and Circuits* / J. Phys. D: Appl. Phys. (2016) **49** 213001], including even devices fabricated with sophisticated growth methods such as molecular beam epitaxy (MBE) and high temperature deposition and annealing.

Fabian Klüpfel has extended his work on inverters based on JFETs [F.J. Klüpfel, A. Holtz, F.-L. Schein, H. von Wenckstern, M. Grundmann: *All-Oxide Inverters Based on ZnO Channel JFETs with Amorphous $ZnCo_2O_4$ Gates* / IEEE Transact. Electr. Dev. (2015) **62** 4004] to a fully operational ring oscillator based on JFETs and bipolar level shifter diodes from $ZnCo_2O_4$/ZnO [F.J. Klüpfel, H. von Wenckstern, M. Grundmann: *Ring Oscillators Based on ZnO Channel JFETs and MESFETs* / Adv. Electr. Mater. (2016) **2** 1500431] (see figure). Fabian has in the meantime finished his doctoral degree.

Building on the great success of particularly our p-type amorphous oxides, BuildMoNa doctoral candidate Robert Karsthof has also explored amorphous nickel oxide as contact in bipolar diodes. He has found that NiO is equally useful as $ZnCo_2O_4$ with the added advantage of transparency [M. Grundmann, R. Karsthof, H. von Wenckstern: *The Recombination Current in Type-II Heterostructure Bipolar Diodes* / ACS Appl. Mat. & Interf. (2014) **6** 14785]. Robert has subsequently built transparent transistors using a NiO/ZnO gate electrode (JFETs) [R. Karsthof, H. von Wenckstern, M. Grundmann: *Transparent JFETs Based on p-NiO/n-ZnO Heterojunctions* / IEEE Transact. Electr. Dev. (2015) **62** 3999] and also has achieved an UV (ultraviolet) solar radiation energy harvester (transparent solar cell) with a a maximum external quantum efficiency of 55% and a power conversion efficiency of about 3% in the UV region for the local power-up of fully transparent electronics [R. Karsthof, P. Räcke, Z. Zhang, H. von Wenckstern, M. Grundmann: *Semi-Transparent n-ZnO/p-NiO UV Solar Cells* / Phys. Status Solidi A (2016) **213** 30].

⇒ *Properties of Schottky Barrier Diodes on $(In_xGa_{1-x})_2O_3$ for $0.01 \leq x \leq 0.85$ Determined by Using a Combinatorial Approach*
H. von Wenckstern, D. Splith, A. Werner, S. Müller, M. Lorenz, M. Grundmann / ACS Comb. Sci. (2015) **17** 710

⇒ *pn-Heterodiodes with n-Type In_2O_3*
H. von Wenckstern, D. Splith, S. Lanzinger, F. Schmidt, S. Müller, P. Schlupp, R. Karsthof, M. Grundmann / Adv. Electr. Mater. (2015) **1** 1400026

⇒ *All Amorphous Oxide Bipolar Heterojunction Diodes from Abundant Metals*
P. Schlupp, F.-L. Schein, H. von Wenckstern, M. Grundmann / Adv. Electr. Mater. (2015) **1** 1400023

⇒ *Comparison of Schottky Contacts on β-Gallium Oxide Thin Films and Bulk Crystals*
S. Müller, H. von Wenckstern, F. Schmidt, D. Splith, F.-L. Schein, H. Frenzel, M. Grundmann / Appl. Phys. Expr. (2015) **8** 121102

⇒ *Maxwell Consideration of Polaritonic Quasi-Particle Hamiltonians in Multi-Level Systems*
S. Richter, T. Michalsky, L. Fricke, C. Sturm, H. Franke, M. Grundmann, R. Schmidt-Grund / Appl. Phys. Lett. (2015) **107** 231104

⇒ *Magnetic Spin Structure and Magnetoelectric Coupling in $BiFeO_3$-$BaTiO_3$ Multilayer*
V. Lazenka, M. Lorenz, H. Modarresi, M. Bisht, R. Rüffer, M. Bonholzer, M. Grundmann, M. J. Van Bael, A. Vantomme, K. Temst / Appl. Phys. Lett. (2015) **106** 082904

⇒ *Modeling the Conductivity Around the Dimensionality-Controlled Metal-Insulator Transition in $LaNiO_3$/ $LaAlO_3$ (100) Superlattices*
H. Wei, M. Jenderka, M. Bonholzer, M. Grundmann, M. Lorenz / Appl. Phys. Lett. (2015) **106** 042103

⇒ *Low Frequency Noise of ZnO based MESFETs*
F.J. Klüpfel, H. von Wenckstern, M. Grundmann / Appl. Phys. Lett. (2015) **106** 033502

⇒ *Study of the Negative Magneto-Resistance of Single Proton-Implanted Lithium-Doped ZnO Microwires*
I. Lorite, C. Zandalazini, P. Esquinazi, D. Spemann, S. Friedländer, A. Pöppl, T. Michalsky, M. Grundmann, J. Vogt, J. Meijer, S.P. Heluani, H. Ohldag, W.A. Adeagbo, S.K. Nayak, W. Hergert, A. Ernst, M. Hoffmann / J. Phys. Condens. Matter (2015) **27** 256002

⇒ *Antiferromagnetic Phase Transition in the Temperature-Dependent NIR-VUV Dielectric Function of Hexagonal $YMnO_3$*
S. Richter, S.G. Ebbinghaus, M. Grundmann, R. Schmidt-Grund / arxiv: (2015) 503.04043

⇒ *Discrete Relaxation of Exciton-Polaritons in an Inhomogeneous Potential*
T. Michalsky, H. Franke, C. Sturm, M. Grundmann, R. Schmidt-Grund / arxiv: (2015) 1501.02644

⇒ *Room-Temperature Condensation in Whispering Gallery Microresonators Assisted by Longitudinal Optical Phonons*
C.P. Dietrich, R. Schmidt-Grund, T. Michalsky, M. Lange, M. Grundmann / arxiv: (2015) 1501.01255

⇒ *All-Oxide Inverters Based On ZnO channel JFETs with Amorphous $ZnCo_2O_4$ Gates*
F.J. Klüpfel, A. Holtz, F.-L. Schein, H. von Wenckstern, M. Grundmann / IEEE Transact. Electr. Dev. (2015) **62** 4004

⇒ *Transparent JFETs Based on p-NiO/n-ZnO Heterojunctions*
R. Karsthof, H. von Wenckstern, M. Grundmann / IEEE Transact. Electr. Dev. (2015) **62** 3999

⇒ *Study of the Negative Magneto-Resistance of Single Proton-Implanted Lithium-Doped ZnO Microwires*
I. Lorite, C. Zandalazini, P. Esquinazi, D. Spemann, S. Friedländer, A. Pöppl, T. Michalsky, M. Grundmann, J. Vogt, J. Meijer, S.P. Heluani, H. Ohldag, W.A. Adeagbo, S.K. Nayak, W. Hergert, A. Ernst, M. Hoffmann / J. Phys.: Condens. Matter (2015) **27** 256002

⇒ *Parametric Relaxation in Whispering-Gallery Mode Exciton-Polariton Condensates*
C.P. Dietrich, R. Johne, T. Michalsky, C. Sturm, P. Eastham, H. Franke, M. Lange, M. Grundmann, R. Schmidt-Grund / Phys. Rev. B (2015) **91** 041202(R)

⇒ *Doping Efficiency and Limits in (Mg,Zn)O:Al,Ga Thin Films with Two-Dimensional Lateral Composition Spread*
A. Mavlonov, S. Richter, H. von Wenckstern, R. Schmidt-Grund, J. Lenzner, M. Lorenz, M. Grundmann / Phys. Status Solidi A (2015) **212** 2850

⇒ *Long-Throw Magnetron Sputtering of Amorphous Zn-Sn-O-Thin Films at Room Temperature*
H. Frenzel, T. Dörfler, P. Schlupp, H. von Wenckstern, M. Grundmann / Phys. Status Solidi A (2015) **212** 1482

⇒ *Electronic Defects in In_2O_3 and In_2O_3:Mg Thin Films on r-Plane Sapphire*
F. Schmidt, D. Splith, S. Müller, H. von Wenckstern, M. Grundmann / Phys. Status Solidi B (2015) **252** 2304

⇒ *Structural and Optical Properties of $(In,Ga)_2O_3$ Thin Films and Characteristics of Schottky Contacts Thereon*
H. von Wenckstern, D. Splith, M. Purfürst, Z. Zhang, C. Kranert, S. Müller, M. Lorenz, M. Grundmann / Semic. Sci. Technol. (2015) **30** 024005

⇒ *From High-T_C Superconductors to Highly Correlated Mott Insulators – 25 Years of Pulsed Laser Deposition of Functional Oxides in Leipzig*
M. Lorenz, H. Hochmuth, M. Keiß, M. Bonholzer, M. Jenderka, M. Grundmann / Semic. Sci. Technol. (2015) **30** 024003

⇒ *Impact of Sodium on the Device Characteristics of Low Temperature-Deposited CIGSe-Solar Cells*
S. Puttnins, M.S. Hammer, J. Neerken, I. Riedel, F. Daume, A. Rahm, A. Braun, M. Grundmann, T. Unold / Thin Solid Films (2015) **582** 85

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Investigation of the properties of modern materials with magnetic resonance

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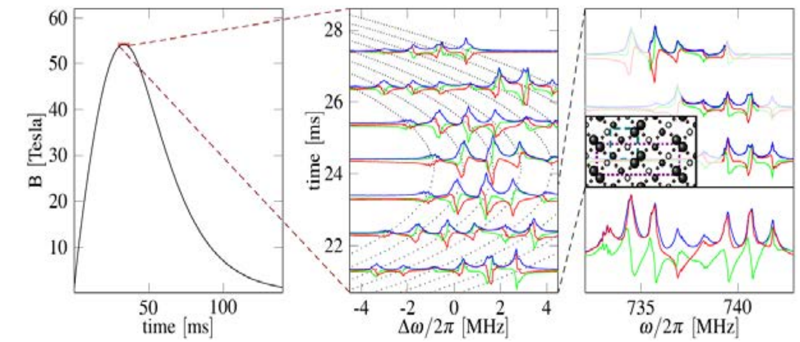
Our group employs Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR) to investigate the physical and chemical properties of materials. Among those are, most notably, high-temperature superconductors and topological insulators, but also porous materials like metal-organic frameworks (MOFs). Alongside the application of magnetic resonance in materials research, we also engage in the development of new magnetic resonance techniques that offer unique insight into material properties.

One of our two BuildMoNa doctoral candidates is engaged in the investigation of the magnetic response of the high-temperature superconducting cuprates, where we could distinguish for the first time three different uniform magnetic responses. This means that these materials are far more complicated than is assumed by most theories. This work contributed the last evidence for the failure of such single-component physics, since it concerned the mercury-based family of materials that exhibits the highest temperatures of superconductivity.



⇑ Broadband NMR in pulsed magnets using field-stepped free induction decays to sample the spectrum. At high fields and low temperatures an electronic superstructure emerges in $SrCu_2(BO_3)_2$ and spectra spanning 9 MHz are reconstructed.

In another effort we further developed a new technique that aims at using magnetic resonance at the highest magnetic fields, by employing pulsed magnets. This is the only possibility to obtain fields up to the 100 T regime. Within a collaboration with the Dresden High Magnetic Field Laboratory we develop and apply the necessary tools for pulsed field NMR where the time-dependence of the magnetic field is especially challenging. We were able to show the feasibility of shift and relaxation measurements as well as obtain broad frequency spectra caused by a field-induced superstructure in $SrCu_2(BO_3)_2$.

Topological insulators (TIs) are of great interest as they exhibit a new electronic state of matter characterised by an insulating bulk band gap coexisting with dissipationless conducting surface states. NMR as a bulk but local probe of electronic properties can be used to study both, bulk as well as surface, and corresponding signals have been reported, but not yet fully understood. Our work focused on studying the model 3D TIs Bi_2Se_3 and Bi_2Te_3 using samples with different bulk doping levels and surface-to-volume ratios. With ^{77}Se NMR on Bi_2Se_3 single crystals we have discovered a hitherto unknown magnetic coupling caused by interband excitations of bulk electrons. These findings, together with the first identification and characterisation of signals from distinct lattice sites, shed new light on the properties of these materials, and necessitate a revision of the interpretations of literature data (published in 2016, arXiv in 2015).

⇒ *Electronic Spin Susceptibilities and Superconductivity in $HgBa_2CuO_{4+\delta}$ from Nuclear Magnetic Resonance*
D. Rybicki, J. Kohlrautz, J. Haase, M. Greven, X. Zhao, M.K. Chan, C.J. Dorow, M.J. Veit / Phys. Rev. B (2015) **92** 081115

⇒ *Anomalous Longitudinal Relaxation of Nuclear Spins in CaF_2*
C.M. Kropf, J. Kohlrautz, J. Haase, B.V. Fine / arxiv: (2015) 1510.06589

⇒ *Se Nuclear Magnetic Resonance of Topological Insulator Bi_2Se_3*
N.M. Georgieva, D. Rybicki, R. Guehne, G.V.M. Williams, S.V. Chong, K. Kadowaki, I. Garate, J. Haase / arxiv: (2015) 1511.01727

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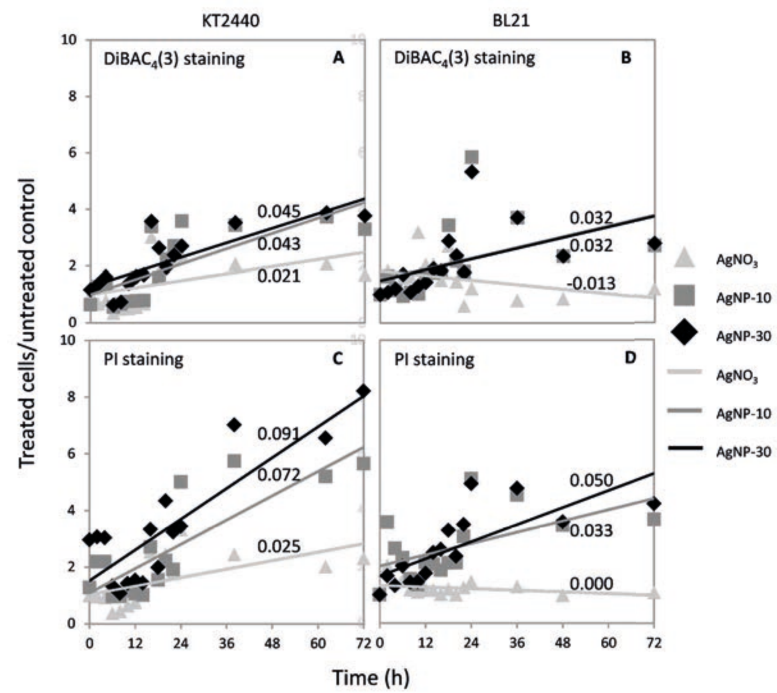
Nanoparticle interactions with microorganisms on the molecular level

Prof. Dr. Hauke Harms
M.Sc. Chem. Yuting Guo

Tons of anthropogenic silver nanoparticles (AgNPs) are assumed to be released into the environment due to their use in many consumer products. AgNPs are known to be toxic towards microorganisms and may harm their functions in ecosystems. In a recent study we explored the impact of AgNPs on functioning of single cells in microbial populations. Results were shown in a manuscript submitted to the Journal of Nanobiotechnology.

Overall, the toxicity of AgNPs is low and predominantly caused by dissolved Ag. A particle effect was found that additionally contributed to increased dead and membrane-compromised cell counts (see figure). Exponential cells were found to be more susceptible to the toxicity of AgNPs than resting cells. Although the loss of silver into the environment may cause death and inhibit energy metabolism of cell fractions, this study did not disclose immediate jeopardy for bacterial survival and metabolic activity, respectively at Ag concentrations typically found in the environment.



Particle-related effects for *Pseudomonas putida* KT2440 and *Escherichia coli* BL21 at EC_{50} concentrations tested for 72 h. Particle-related effects were shown by ratio changes of membrane-depolarised ($DiBAC_4(3)$) or compromised cells (PI) by comparing Ag-treated to untreated control cells. The slopes (k) were shown for each strain.

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

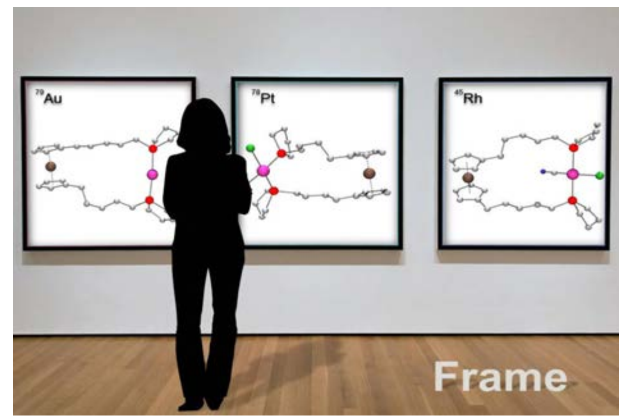
Prof. Dr. Dr. h.c. Evamarie Hey-Hawkins
M.Sc. Chem. Anup Kumar Adhikari, M.Sc. Chem. Eng. Paul Cosmin Boar, Dr. Solveig Boehnke, M.Sc. Chem. Antonio Buzharevski, M.Sc. Chem Marta Gozzi, M.Sc. Chem. Toni Grell, M.Sc. Chem. Reinhard Hoy, M.Sc. Chem. Robert Kuhnert, M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon, Dr. Paul Neumann, Dr. Wilma Neumann, Dr. Stefan Richter, M.Sc. Chem. Stefan Saretz, M.Sc. Chem. Andy Schmied, M.Sc. Chem Axel Straube

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

Smart Catalysts: Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups

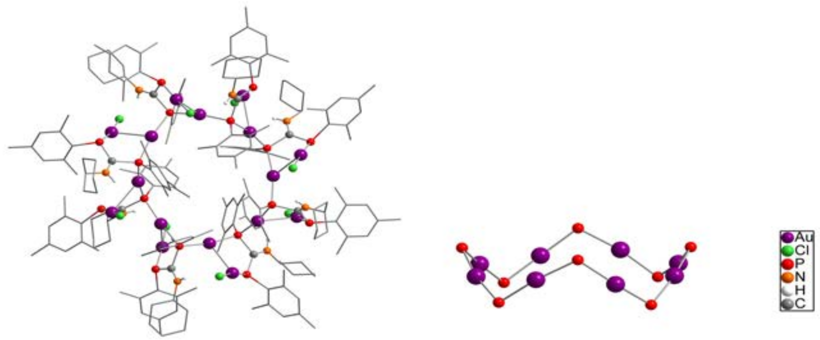
(ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way ”switchable“ phosphines for catalytic applications (P. Neumann). A new approach includes C_3-symmetric ligands (A. Straube).

Another approach focuses on the use of selective phosphorus-based macrocycles or nano-frames (P. C. Boar, R. Hoy, A. Schmied; see figure), and containers, or cavities (functionalised (*S*)-BINOL as linkers) in metal-organic frameworks (MOFs) with well-defined structure and porosity (J. A. Navarro). These compounds can be used as receptors for catalytically active transition metals, generating molecular nanosized reactors that should allow specific interactions of the cavity with substrates during a catalytic process. Variation of the coordinated metal atom or the size of the cavity will influence the selectivity in catalytic processes.



⇐ Self-assembly of heterobimetallic complexes with highly flexible 1,1'-bis(phospholanoalkyl)ferrocene ligands.

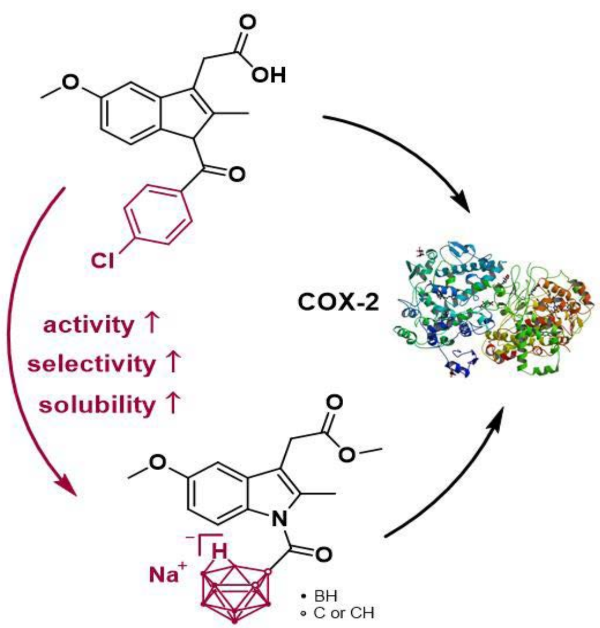
From Molecules to Novel Materials:
Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of *functionalised building blocks* for organometallic or phosphorus-based polymers are: strained inorganic phosphorus-based rings (T. Grell), alkylene- and arylene-bridged bis-phospholanes (P. C. Boar, R. Hoy, A. Schmied) or (planar-chiral) ferrocene derivatives (A. Straube) and bis-, tri- and tetrakis-carboxylates of conjugated aromatic systems as ligands in optically active coordination polymers or MOFs (A. Aleksovska).
Molecular Precursors: Binary metal phosphides MP_x often exhibit interesting optical, electronic and magnetic properties and thus have a wide range of applications,



⇑ The reaction of *cyclo*-[$Mes_4P_4C(NCy)$] with two equivalents of [AuCl(tht)] (Cy = cyclohexyl, tht = tetrahydrothiophene) resulted in cleavage of P–P bonds and formation of this unusual sixteen-membered Au–P macrocycle (top view and side view of the Au_8P_8 ring), by self-assembly of 8 monomeric di(gold(I)) moieties.

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 (A. K. Adhikari, T. Grell) as molecular precursors (see figure).

Inorganic Building Blocks in Medicinal Chemistry: Carbaboranes 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 entity in cyclooxygenase (COX) (W. Neumann, S. Saretz, A. Buzharevski) or lipoxygenase inhibitors (R. Kuhnert) or for boron neutron capture therapy as



⇑ Replacement of a chlorophenyl ring in indomethacin by a *nido*-dicarbaborate cluster gives a highly potent and selective inhibitor (*nido*-indoborin) of the pathogenic isoform cyclooxygenase-2 (COX-2).

conjugates with tumour-targeting entities, such as a Y_1 receptor-selective neuropeptide Y (NPY) derivative (S. Boehnke).

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. To increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. NPY (S. Richter) or COX inhibitors (W. Neumann; see figure). A new approach utilises the *nido* cluster (carbollide, $[C_2B_9H_{11}]^{2-}$, which is isolobal to cyclopentadienide) as ligand in metal complexes that exhibit anticancer properties (M. Gozzi).

⇒ *Receptor-Mediated Uptake of Boron-Rich Neuropeptide Y Analogues for Boron Neutron Capture Therapy*
V.M. Ahrens, R. Frank, S. Boehnke, C.L. Schütz, G. Hampel, D.S. Iffland, N.H. Bings, E. Hey-Hawkins, A.G. Beck-Sickinger / Chem. Med. Chem. (2015) **10** 164

⇒ *Redox Control of a Dendritic Homogeneous Catalyst*
P. Neumann, H. Dib, A.-M. Caminade, E. Hey-Hawkins / Angew. Chem. (2015) **127** 316; Angew. Chem. Int. Ed. (2015) **54** 311

⇒ *Conjugation of Cisplatin Analogues and COX Inhibitors to Overcome Cisplatin Resistance*
W. Neumann, B.C. Crews, M.B. Sárosi, C.M. Daniel, K. Ghebreselasie, M.S. Scholz, L.J. Marnett, E. Hey-Hawkins / Chem. Med. Chem. (2015) **10** 183

⇒ *Carbaborane-Based Alkynylphosphines and Phospholes*
A. Kreienbrink, M.B. Sárosi, R. Kuhnert, P. Wonneberger, A. Arkhypchuk, P. Lönnecke, S. Ott, E. Hey-Hawkins / Chem. Commun. (2015) **51** 836, Inside Back Cover

⇒ *One-Pot Synthesis of an Indole-Substituted 7,8-Dicarba-nido-dodecahydroundecaborate(–1)*
W. Neumann, R. Frank, E. Hey-Hawkins / Dalton Trans. (2015) **44** 1748

⇒ *Carbaboranes – More Than Just Phenyl Mimetics*
R. Frank, V. Ahrens, S. Boehnke, S. Hofmann, M. Kellert, S. Saretz, S. Pandey, M.B. Sárosi, Á. Bartók, A.G. Beck-Sickinger / Pure and App. Chem. (2015) **87** 163

⇒ *Phosphaindazole: A Novel Phosphorus–Carbon Aromatic Heterocycle*
I. Jevtovikj, M.B. Sárosi, A.K. Adhikari, P. Lönnecke, E. Hey-Hawkins / Eur. J. Inorg. Chem. (2015) 2046

⇒ *Ruthenium Complexes with Dendritic Ferrocenyl Phosphanes – Synthesis, Characterisation and Application in the Catalytic Redox Isomerisation of Allylic Alcohols*
P. Neumann, H. Dib, A. Sournia-Saquet, T. Grell, M. Handke, A.-M. Caminade, E. Hey-Hawkins / Chem. Europ. J. (2015) **21** 6590

⇒ *Reduction of Hydroxy-Functionalised Carbaboranyl Carboxylic Acids and Ketones by Organolithium Reagents*
W. Neumann, M. Hiller, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2015) **44** 6638, Invited Contribution, Special Issue Dedicated to Professor Kenneth Wade

⇒ *A Convenient Route Towards Deoxygalactosyl-Functionalised Ortho-Carbaborane: Synthesis of a Building Block for Peptide Conjugation*
R. Frank, E. Hey-Hawkins / J. Organomet. Chem. (2015) **798** 46, Invited Contribution, Special Issue Dedicated to Professor Russell N. Grimes

⇒ *Heterobimetallic Complexes with Highly Flexible 1,1'-Bis(phospholanoalkyl)ferrocene Ligands*
A. Schmied, A. Straube, T. Grell, S. Jähnigen, E. Hey-Hawkins / Dalton Trans. (2015) **44** 18760, Inside Front Cover

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Surface functionalisation of Layer-by-Layer coated colloidal microcarriers for specific cell uptake

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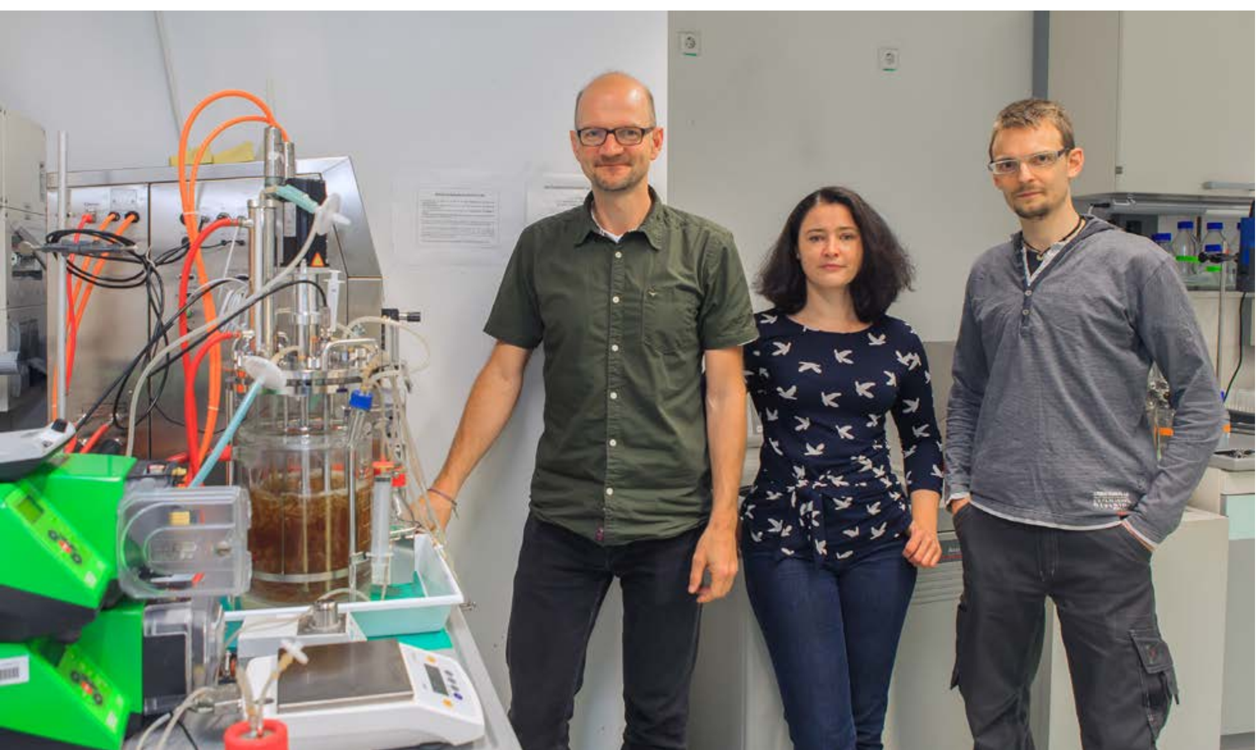
Dipl.-Phys. Martin-Patrick Göse

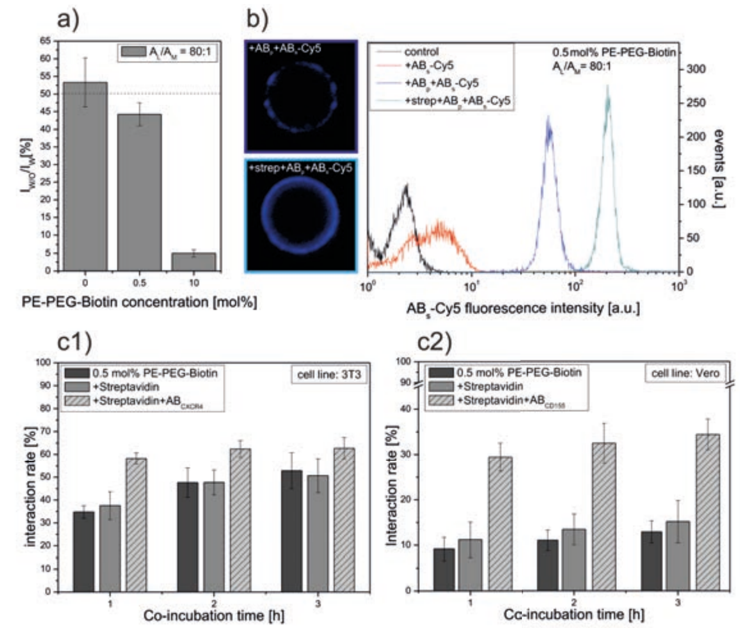
This research project focuses on the development of new drug delivery systems to exhibit a targeted transport and time controlled release as well as which are able to transport multiple active agents safely and in a defined dosage in just one carrier system.

One promising approach which provides all these features is based on the combination of the Layer-by-Layer technique (LbL) and the Liposome-Spreading technique (LS) equipped with a terminal antibody surface modification. However, for the fabrication of an effective microcarrier system it is essential to create a homogeneous and regular lipid bilayer on top of the microcarrier to inhibit unspecific serum protein interaction and to reduce microcarrier uptake by non-targeted cells.

Using SiO_2-microparticles as templates and a LbL multilayer consisting of protamine sulfate and dextran sodium sulfate, it could be shown that the lipid bilayer formation is strongly influenced by the applied lipid mixture as well as the LS coating conditions. Nevertheless, a homogeneous and dense supported lipid bilayer which cannot be penetrated even by small molecules in the size range of 1kDa could be achieved by using POPS/POPC in 1:1 molar ratio as well as a low amount of the functional lipid PE-PEG-Biotin (0.5 mol%) (see figure, a). Subsequently, a streptavidin mediated highly specific coupling of biotinylated antibodies could be achieved (see figure, b).

Finally, the co-incubation with two different cell lines (3T3 and Vero cells) has proven the targeted and accelerated interaction behavior of the optimised microcarrier system (see figure, c), which cannot be achieved in this quality using known strategies of LbL antibody assembly.





⇑ a) Flow Cytometry investigations of SiO_2-microcarrier fluorescence intensity (POPS/POPC 1:1, A_L/A_M of 80:1, 0.1 mol% PE-Fluorescein and 0 mol%, 0.5 mol% or 10 mol% PE-PEG-Biotin) after Trypan Blue (MW = 872 Da) quenching. b) Flow Cytometry and Confocal Laser Scanning Microscopy investigations of specific antibody binding using biotinylated antibodies (AB_p) to be attached to the microcarrier surface via biotin/streptavidin sandwich binding. The design is verified by specific secondary antibody binding (AB_s-Cy5). c1, c2) Flow Cytometry investigations of antibody-functionalised microcarriers previously equipped with a POPS/POPC + 0.5 mol% PE-PEG-Biotin lipid bilayer (striped bars) interacting with c1) 3T3 and c2) Vero cells. As control, basic lipid bilayer coated microcarriers with and without streptavidin coupling were used (filled bars).

⇒ *Design of a Homogeneous Multifunctional Supported Lipid Membrane on LbL-Coated Microcarriers*
M. Göse, P. Pescador, U. Reibetanz / Biomacromol. (2015) **16** 757

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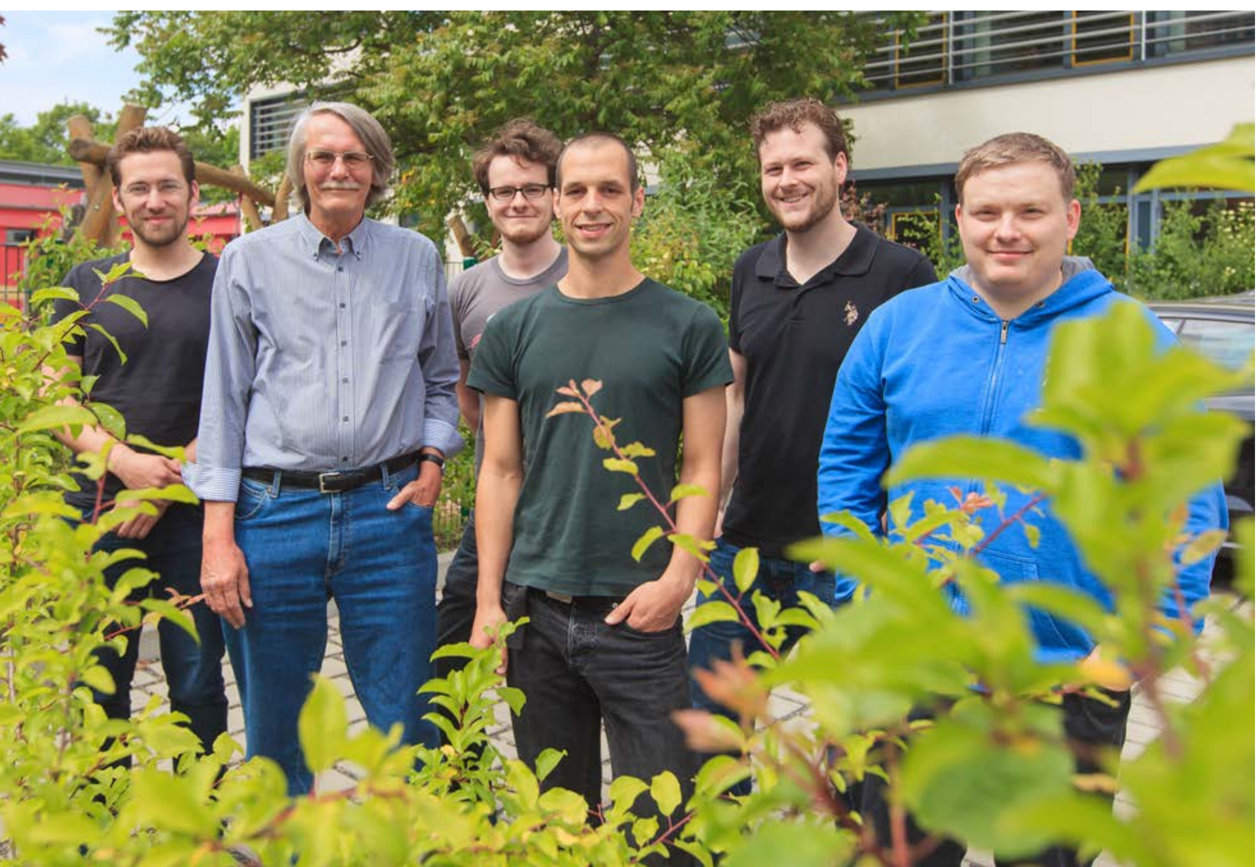
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
M.Ed. Math./Phys. Johannes Bock, Dipl.-Phys. Niklas Fricke, Dipl.-Phys. Martin Marenz, M.Sc. Phys. Philipp Schierz, Dr. Johannes Zierenberg

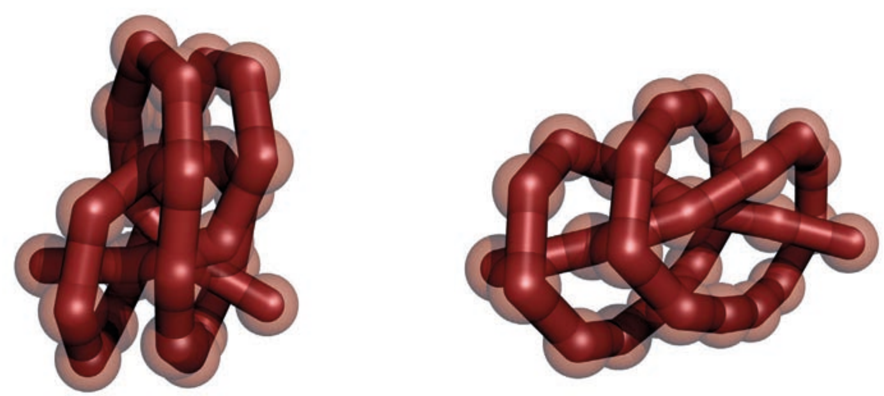
The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on several interrelated subprojects. In most projects, the employed methodology relies mainly on sophisticated Monte Carlo computer simulations based on multicanonical ensembles and parallel tempering techniques, chain-growth algorithms with population control, thermostated Molecular Dynamics methods and exact enumeration techniques. These methods are adapted and tailored by us to the problems at hand and constantly further improved in order to cope with the complexity of the considered problems:



(i) Johannes Zierenberg uses multicanonical methods to investigate the analogy of condensation phenomena for particle systems with the aggregation process in ensembles of polymers, considering both lattice and off-lattice formulations. Special emphasis is laid on distinguishing differences between flexible and semiflexible macromolecules. In the latter case he found very interesting twisted bundle-like structures for large bending stiffness and low temperatures. In December 2015 he has successfully defended his PhD thesis on this topic.

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

(iii) Niklas Fricke extended our recently proposed novel renormalisation group inspired exact enumeration method for self-avoiding random walks on a percolation cluster, modelling polymers in disordered environments with fractal properties, to up to seven space dimensions. The gain of efficiency implied by the reduction from exponential to polynomial complexity is enormous: enumerating all conformations of a 10000-step self-avoiding walk (typically about 10^{1550} on a two-dimensional cluster) would take over 10^{1500} ages of the universe using the standard enumeration method – our new procedure does it in about twenty minutes. As a main physical result he found that established asymptotic scaling predictions need to be corrected.



⇑ Typical knots of topologies $C_n = 5_1$ (left) and 8_{19} (right) in the phase diagram of a semiflexible bead-stick polymer with 28 beads. Here the integer C counts the minimal number of crossings of any projection of a knot onto a two-dimensional plane and the subscript n distinguishes topologically different knots with the same C.

(iv) Johannes Bock focused 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 doctoral candidate (Sebastian Schöbl) by extending it to the three-dimensional case subject to additional confinement constraints. One goal is to investigate to what extent the disorder can be effectively described by a "renormalised" bending stiffness of the macromolecules.

(v) Philipp Schierz aimed at efficient computer simulations of polymer systems. To this end he investigated the advantages of computations performed on powerful graphics cards (GPUs) over the use of standard CPUs and carefully compared the performances of Molecular Dynamics (MD) and Monte Carlo (MC) implementations for this class of problems. In particular he considered the microcanonical ensemble and showed how conservation laws in MD can be properly treated and related to each other and to MC by reweighting techniques. This turns out to be very important for small systems at the nanoscale.

⇒ *MD Simulations of Hydrogen Diffusion in ZIF-11 with a Force Field Fitted to Experimental Adsorption Data*
P. Schierz, S. Fritzsche, W. Janke, S. Hannongbua, O. Saengsawang, C. Chmelik, J. Kärger / Microporous and Mesoporous Materials (2015) **203** 132

⇒ *From Amorphous Aggregates to Polymer Bundles: The Role of Stiffness on Structural Phases in Polymer Aggregation*
J. Zierenberg, W. Janke / Europhysics Letters (2015) **109** 28002

⇒ *Parallel Multicanonical Study of the Three-Dimensional Blume-Capel Model*
J. Zierenberg, N.G. Fytas, W. Janke / Physical Review E (2015) **91** 032126

⇒ *Polymers in Disordered Environments*
N. Fricke, S. Sturm, M. Lämmel, S. Schöbl, K. Kroy, W. Janke / diffusion-fundamentals.org (2015) **23** 7

⇒ *Exploring Different Regimes in Finite-Size Scaling of the Droplet Condensation-Evaporation Transition*
J. Zierenberg, W. Janke / Physical Review E (2015) **92** 012134

⇒ *Probing the Effect of Density on the Aggregation Temperature of Semi-Flexible Polymers in Spherical Confinement*
M. Mueller, J. Zierenberg, M. Marenz, P. Schierz, W. Janke / Physics Procedia (2015) **68** 95

⇒ *Molecular Dynamics and Monte Carlo Simulations in the Microcanonical Ensemble: Quantitative Comparison and Reweighting Techniques*
P. Schierz, J. Zierenberg, W. Janke / Journal of Chemical Physics (2015) **143** 134114

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Formation of regularly spaced networks as a general feature of actin bundle condensation by entropic forces

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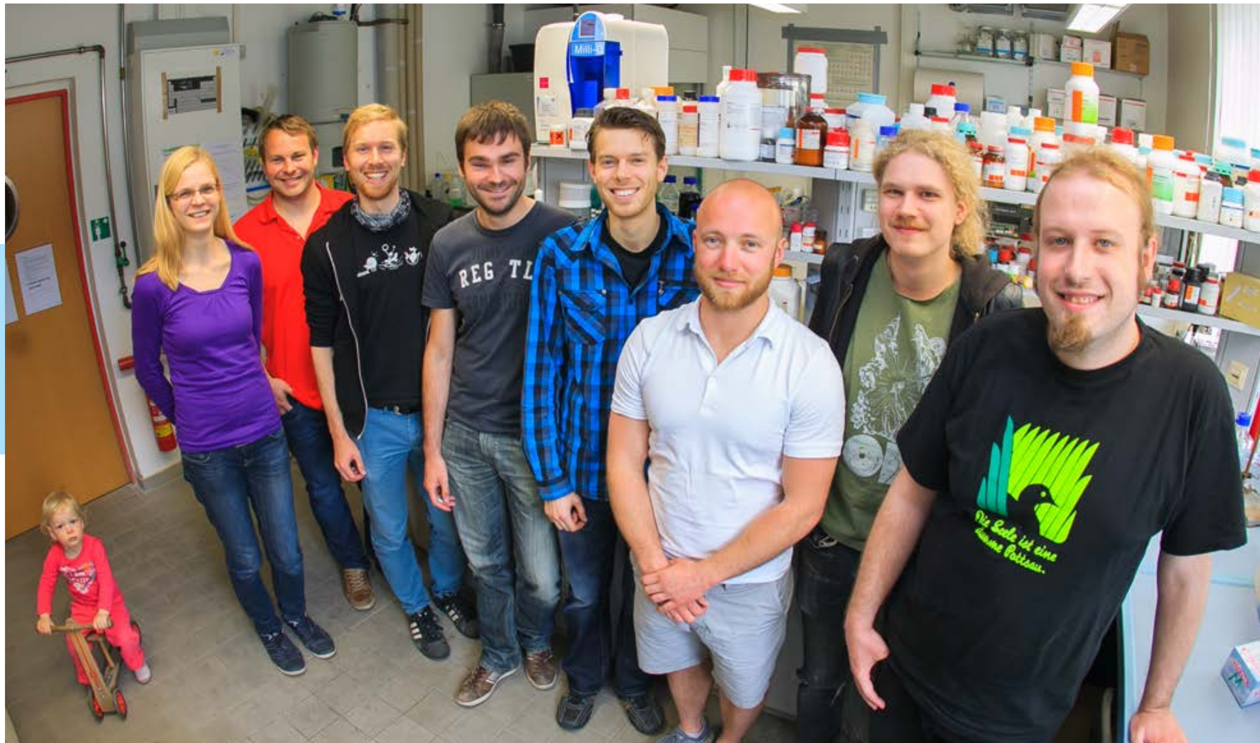
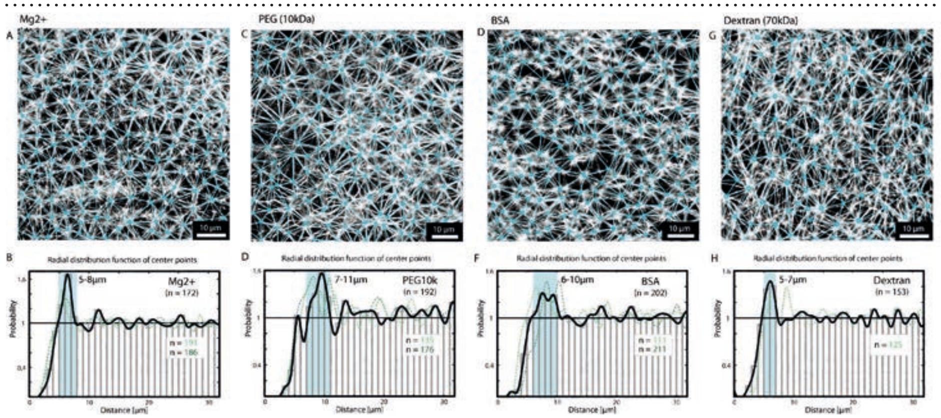
In cells, various functions depend on the properties of the underlying surfaces and differing actin structures. These structures range from loose networks to densely packed bundles and can form clusters in a higher-level assembly like asters and nematic phases. These arrangements have been in focus of many studies and especially aster formation was usually attributed to actin associated proteins. We have shown experimental proof of bundle arrangements in aster-like structures independent of other proteins. In that course, we used known actin bundling mechanisms like counterion condensation and depletion forces to induce attractive effects in solutions with sufficiently high actin concentrations. Emerging patterns revealed that aster formation is a rather general feature when bundling is induced in solu-



tions where filaments are completely isotropical distributed. Biasing the isotropic filament distribution, for instance by flows induced by pipetting, completely random bundle networks appear. Although the physical principles and used chemical agents (which induce the formation) vary inherently, the forming structures appear very similar. By detecting centre points we derived radial distribution functions for all networks, which display an increased probability for finding a next neighbor in a distance of about 5–10 µm. Due to the independency of other proteins, this effect emphasises that structure formations on higher levels of biological complexity can be solely controlled by self-assembly arguments and accordingly by energy minimisation in the system.



⇑ Actin based aster formation without molecular motors or other accessory proteins. Structures are solely formed by counterion condensation or depletion forces and display a probability for finding a next neighbor in a distance of about 5–10 µm.

⇒ *Formation of Regularly Spaced Networks as a General Feature of Actin Bundle Condensation by Entropic Forces*
F. Huber, D. Strehle, J. Schnauß, J.A. Käs / New Journal of Physics (2015) **17** 043029

⇒ *Contractile Cell Forces Deform Macroscopic Cantilevers and Quantify Biomaterial Performance*
U. Allenstein, S.G. Mayr, M. Zink / Soft Matter (2015) **11** 5053

⇒ *Coupling of Metals and Biominerals: Characterising the Interface Between Ferromagnetic Shape-Memory Alloys and Hydroxyapatite*
U. Allenstein, S. Selle, M. Tadsen, C. Patzig, T. Höche, M. Zink, S.G. Mayr / ACS Applied Materials & Surfaces (2015) **7** 15331

⇒ *Pharmacological Targeting of Membrane Rigidity: Implications on Cancer Cell Migration and Invasion*
S. Braig, S.U. Schmidt, K. Ferkaljuk, C. Händel, T. Möhn, O. Werz, R. Müller, S. Zahler, A. Koeberle, J.A. Käs, A.M. Vollmar / New Journal of Physics (2015) **17** 083007

⇒ *Cell Membrane Softening in Human Breast and Cervical Cancer Cells*
C. Händel, S. Schmidt, J. Schiller, U. Dietrich, T. Möhn, T. Kießling, S. Pawlizak, A. Fritsch, L.-C. Horn, S. Briest, M. Höckel, M. Zink, J.A. Käs / New Journal of Physics (2015) **17** 083008

⇒ *Motor-Free Force Generation in Biological Systems*
J. Schnauß, M. Glaser, C. Schuldt, T. Golde, T. Händler, S. Schmidt, S. Diez, J.A. Käs / diffusion-fundamentals.org (2015) **23** 1

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Coordination compounds in supramolecular chemistry and materials chemistry

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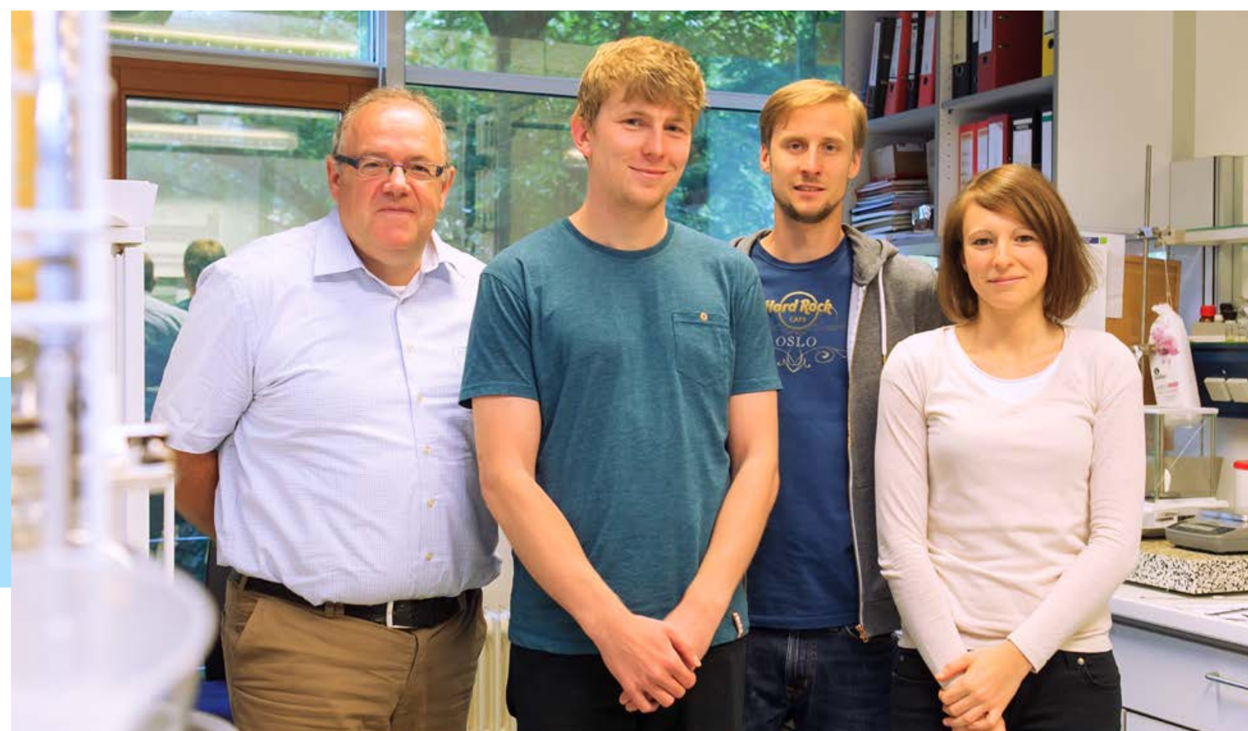
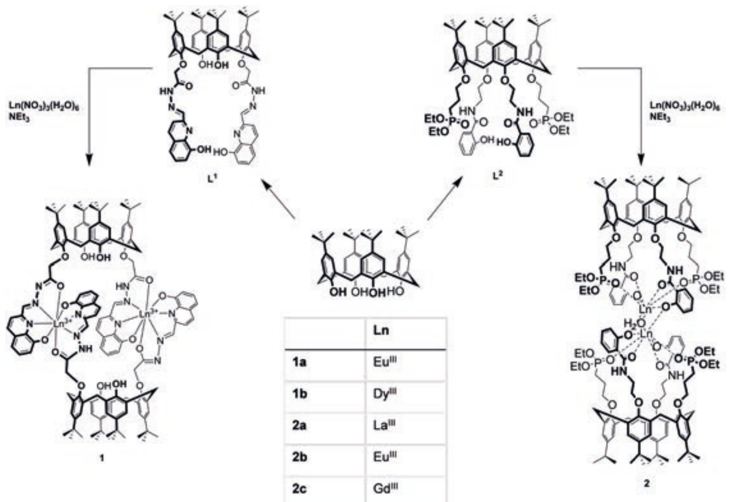
M.Sc. Chem. Florian Glasneck, M.Sc. Chem. Astrid Jäschke, M.Sc. Chem. Steve Ullmann

The studies focus on metal-binding ligands based on calix[4]arenes or macrocyclic N,S-ligands whose abilities as solvent extracting agents in the separation of *f*-metals or the selective binding of anions are investigated. In case of the calix[4]arenes the binding of the metal cations occurs through different ligating groups like phosphonates, amides, carboxylates or heteroaromatic rings. To satisfy the high coordination numbers of *f*-block metals disubstituted derivatives of calix[4]arenes with multidentate aromatic units have been employed recently. Introducing dissimilar ligating groups on the calix[4]arene scaffold opens up further possibilities for fine-tuning and modifying the binding pocket. Employing the synthesised ligands in titration and solvent extraction experiments yields valuable information about the affinity and selectivity of the compounds towards lanthanides and is the basis for further improvement of the ligand structures.

The coordination behaviour of the ligands was also studied in solid state and the properties of the obtained complexes are examined in the light of molecular-based

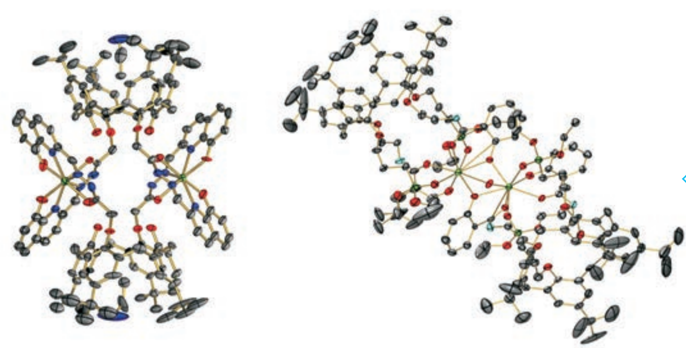




	Ln
1a	Eu[III]
1b	Dy[III]
2a	La[III]
2b	Eu[III]
2c	Gd[III]

⇐ Synthesis of di-, and tetrasubstituted derivatives of calix[4]arenes and their corresponding dinuclear Ln-complexes.

magnetic materials. The Eu(III) centres in **1a** are well-separated from each other (Eu···Eu 8.34 Å) being coordinated by two tetradentate 8-hydroxyquinoline-2-carbaldehyde-hydrazone substituents from two calix[4]arene units. The $\chi_m T$ value at room temperature is found to be 2.77 $cm^3 \cdot K \cdot mol^{-1}$, a value which is close to that expected for two non-interacting Eu(III) ions (2.65 $cm^3 \cdot K \cdot mol^{-1}$), whose magnetic properties are associated with thermal population of the excited terms ($^7F_1$ – $^7F_6$). Thus, the metal centres act like isolated Eu(III) ions. In contrast, temperature dependent magnetic susceptibility measurements reveal antiferromagnetic coupling between the two Eu(III) ions in **2a** which are significantly closer (Eu···Eu 3.97 Å).



⇐ Molecular structures of **1a** (left) and **2a** (right).

⇒ *Cavitands Incorporating a Lewis Acidic Dinickel Chelate Function as Receptors for Halide Ions*
A. Jeremies, U. Lehmann, S. Gruschinski, F. Schleife, M. Meyer, V. Matulis, O.A. Ivashkevich, M. Handke, K. Stein, B. Kersting / Inorg. Chem. (2015) **54** 3937

⇒ *Preparation, Properties and Structures of Pentanuclear [{Ni_2L}$_2$(u-Mcsalen)]$^{2+}$ complexes (L = macrocyclic N_6S_2 donor ligand)*
M. Golecki, B. Kersting / Z. Anorg. Allg. Chem. (2015) **641** 436

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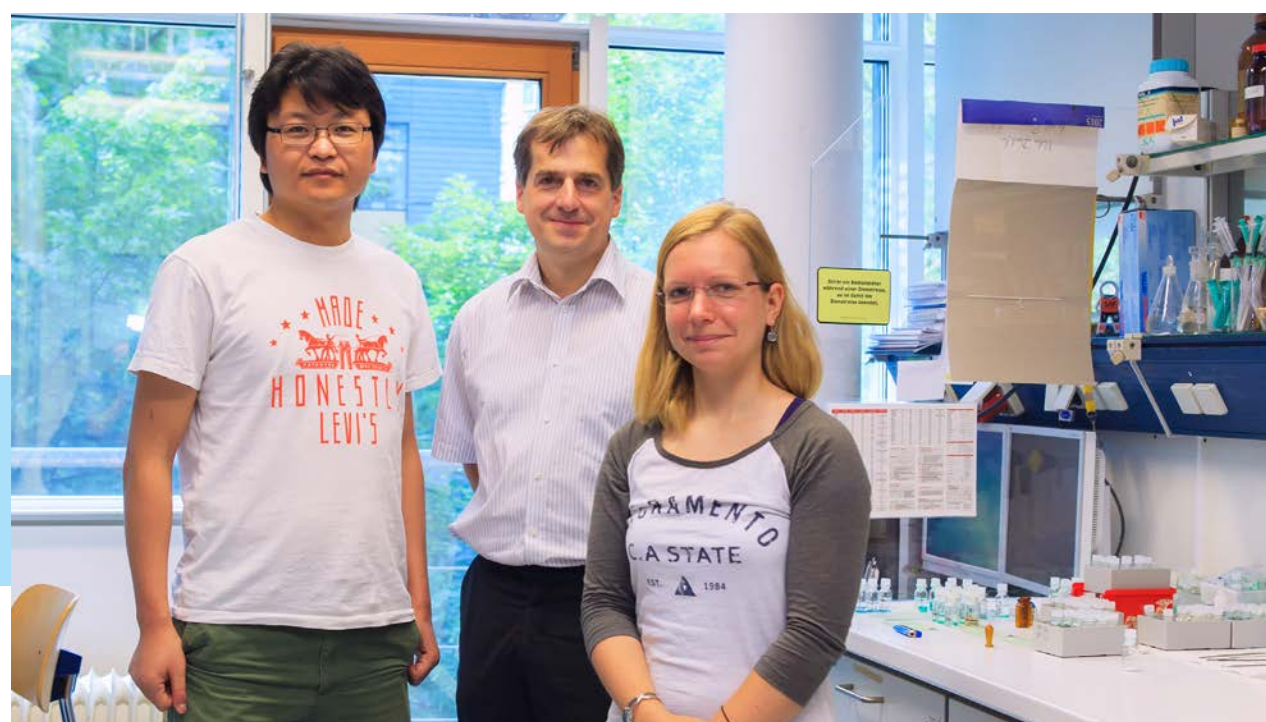
Probing the coordination sphere in metal-organic frameworks by ^{113}Cd solid-state NMR

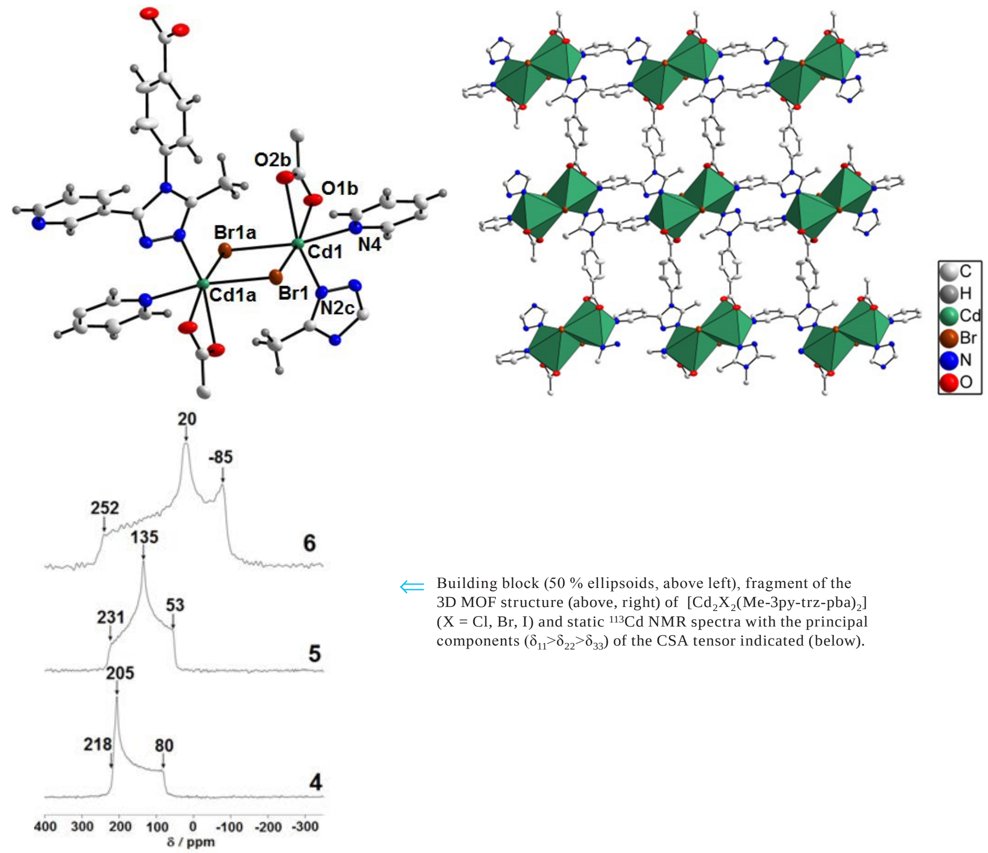
Prof. Dr. Harald Krautscheid
Dr. Salma Begum, M.Sc. Chem. Karolin Stein, Dr. Zhaoyang Wang

Metal-Organic Frameworks (MOFs) as highly porous materials have gained increasing interest because of their high potential for applications in gas separation and storage, heat transformation, as sensors as well as in heterogeneous catalysis.

Despite the toxicity of cadmium compounds the ^{113}Cd nucleus with a nuclear spin I=1/2, a natural abundance of 12.3%, and a fairly high resonance frequency with a gyromagnetic ratio of 9.44 MHz/T provides a powerful probe for structural characterisation of MOFs especially if single-crystalline material is unavailable. In our studies of a series of 27 novel Cd^{2+} based coordination polymers we found that ^{113}Cd solid-state NMR spectroscopy is highly sensitive on coordination number, nature of coordinating groups, and the geometry around the metal ion which is reflected by the isotropic chemical shift and the chemical shift anisotropy (CSA). As an example, the figure on the right exhibits a fragment of the crystal structure of $_\infty^3$[Cd_2Br_2(Me-3py-trz-pba)$_2$]. For the isomorphous MOFs with bridging ligands Cl^-, Br^- or I^- the chemical shift decreases whereas the distortion of the octahedral



coordination of Cd^{2+} ions increases leading to higher CSA. The sensitivity towards the Cd^{2+} environment also allows observing guest induced phase transitions ("gate opening") and supports our understanding of structural flexibility of coordination frameworks.



⇐ Building block (50 % ellipsoids, above left), fragment of the 3D MOF structure (above, right) of $[Cd_2X_2(Me\text{-}3py\text{-}trz\text{-}pba)_2]$ (X = Cl, Br, I) and static ^{113}Cd NMR spectra with the principal components ($\delta_{11}>\delta_{22}>\delta_{33}$) of the CSA tensor indicated (below).

⇒ *Water Stable Triazolyl Phosphonate MOFs; Steep Water Uptake and Facile Regeneration*
S. Begum, S. Horike, S. Kitagawa, H. Krautscheid / Dalton Trans. (2015) **44** 118727

⇒ *Synthesis of $CuInS_2$ Nanocrystals from a Molecular Complex – Characterisation of the Orthorhombic Domain Structure*
J.L. Cholula-Diaz, G. Wagner, D. Friedrich, O. Oeckler, H. Krautscheid / Dalton Trans. (2015) **44** 14227

⇒ *A Series of Isomorphous Metal–Organic Frameworks with rtl Topology – Metal Distribution and Tunable Sorption Capacity via Substitution of Metal Ions*
J. Bergmann, K. Stein, M. Kobalz, M. Handke, M. Lange, J. Moellmer, F. Heinke, O. Oeckler, R. Gläser, R. Staudt, H. Krautscheid / Micropor. Mesopor. Mater. (2015) **216** 56

⇒ *Selective Oxidation of Cyclooctene over Copper-Containing Metal-Organic Frameworks*
U. Junghans, C. Worch, J. Lincke, D. Laessig, H. Krautscheid, R. Glaeser / Micropor. Mesopor. Mater. (2015) **216** 151

⇒ *^{113}Cd Solid-State NMR for Probing the Coordination Sphere in Metal-Organic Frameworks*
A. Viswanath Kuttatheyil, M. Handke, J. Bergmann, D. Lässig, J. Lincke, J. Haase, M. Bertmer, H. Krautscheid / Chem. Eur. J. (2015) **21** 1118

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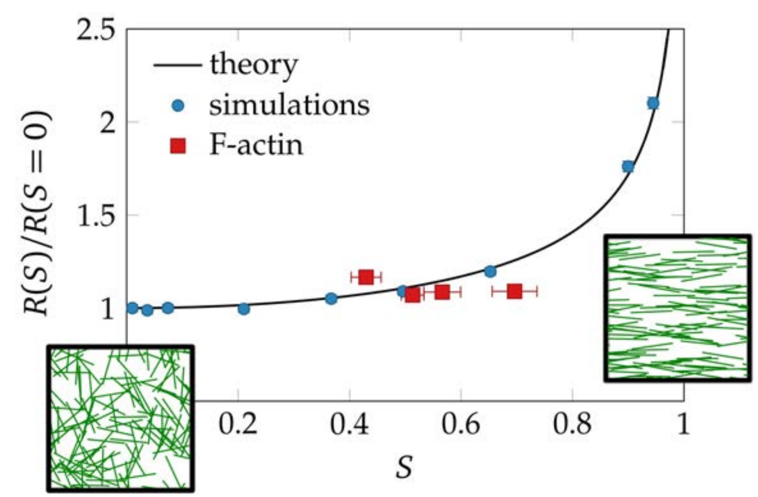
Non-isothermal Brownian motion and rapid force spectroscopy

Prof. Dr. Klaus Kroy
Dipl.-Phys. Jakob Tómas Bullerjahn, M.Sc. Phys. Gianmaria Falasco, Dipl.-Phys. Andrea Kramer, Dipl.-Phys. Marc Lämmel, M.Sc. Phys. Guillermo Zecua Ramirez

Our activities focus on the dynamics of various coarse-grained mesoscopic systems, such as the non-equilibrium diffusion of laser-heated tracer particles and the influence of shear deformations on the packing structure of entangled biopolymer solutions.

Concerning the hot Brownian particles, we start from the fluctuating hydrodynamics of a solvent in local equilibrium but with a global temperature gradient and derive the stochastic equation of motion for a heated colloidal particle, including its fluctuation statistics. The coupling between the hydrodynamic modes excited by the hot particle itself results in a characteristic temperature spectrum that can be used to express the energy content of the particle's velocity and position in terms of effective temperatures.

In the project on sheared biopolymers, we investigate the non-affine response of the polymer solution's local packing structure to a finite shear deformation. Our analysis is based on the so-called tube model for semiflexible polymers, where



⇑ Entangled semiflexible polymers are aligned by a finite large shear deformation, as quantified by the nematic order parameters *S*. The strain-induced tube dilation is characterised in terms of the tube radius *R(S)*. The theoretical prediction is obtained from a binary-collision approximation of the complicated many-body problem and compared to computer simulations and experiments with F-actin.

caging effects on a test polymer in a polymer meshwork are accounted for on a mean-field level, namely by a confinement tube. Per predictions how the size and shape of this tube changes under shear were found to be in very good agreement with numerical simulations and experiments with filamentous actin.

Furthermore, in a collaborative paper with the group of Prof. Frauke Gräter from the Heidelberg Institute of Theoretical Studies, J. Bullerjahn applied a model for forcible bond rupture, recently developed in our group, to analyse rupture events from a molecular dynamics simulation of focal adhesion kinase. A fit by the model, using Bayesian methods of data analysis, provided parameter values that characterise the underlying free-energy landscape of the protein and confirm its dynamical behavior as a mechano-sensor. G. Falasco's cooperation on theoretical models for non-isothermal lattices and fluctuation theorems with Prof. Marco Baiesi (Padova) resulted in two further publications.

⇒ *About the Role of Chaos and Coarse Graining in Statistical Mechanics*
G. Falasco, G. Saggiorato, A. Vulpiani / Physica A (2015) **418** 94

⇒ *Energy Repartition for a Harmonic Chain with Local Reservoirs*
G. Falasco, M. Baiesi, L. Molinaro, L. Conti, F. Baldovin / Physical Review E (2015) **92** 022129

⇒ *Inflow Rate, a Time-Symmetric Observable Obeying Fluctuation Relations*
M. Baiesi, G. Falasco / Physical Review E (2015) **92** 042162

⇒ *Mechanism of Focal Adhesion Kinase Mechanosensing*
J. Zhou, C. Aponte-Santamaría, S. Sturm, J.T. Bullerjahn, A. Bronowska, F. Gräter / PLoS Computational Biology (2015) **11** e1004593

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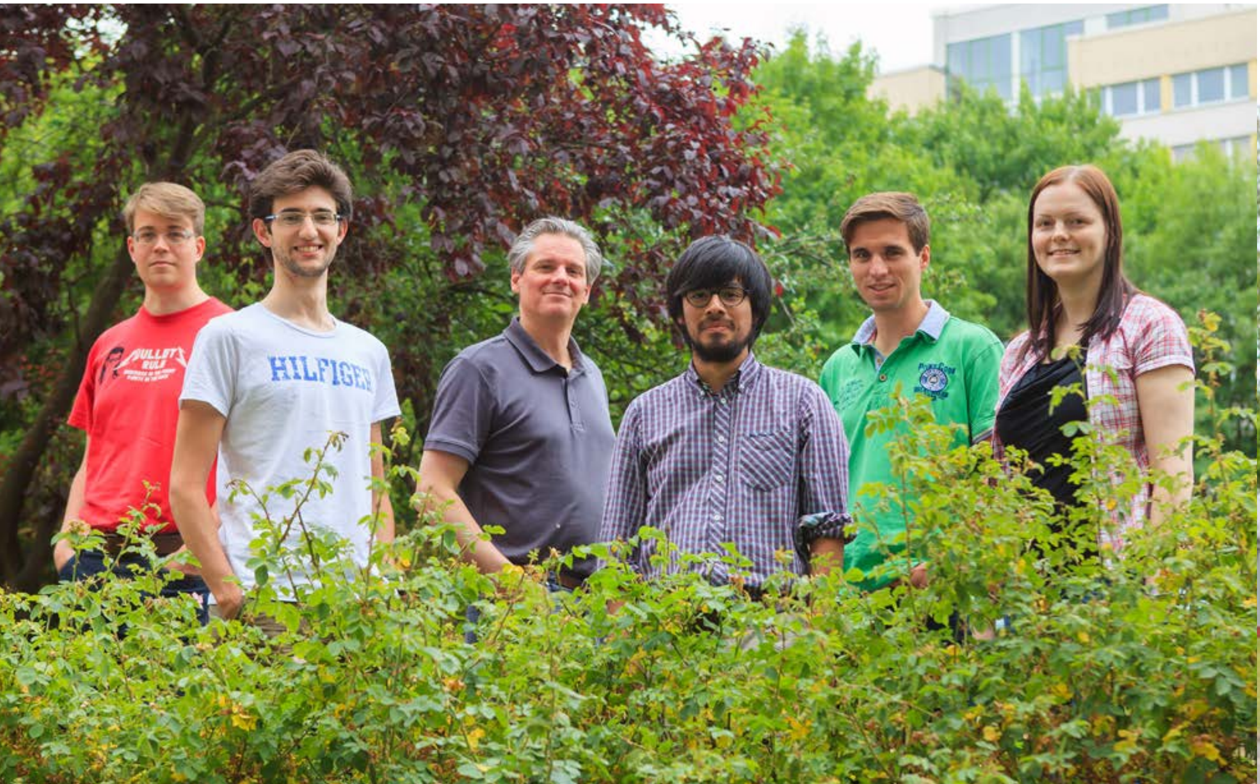


New functional materials for biomedical applications and material physics at the nanoscale

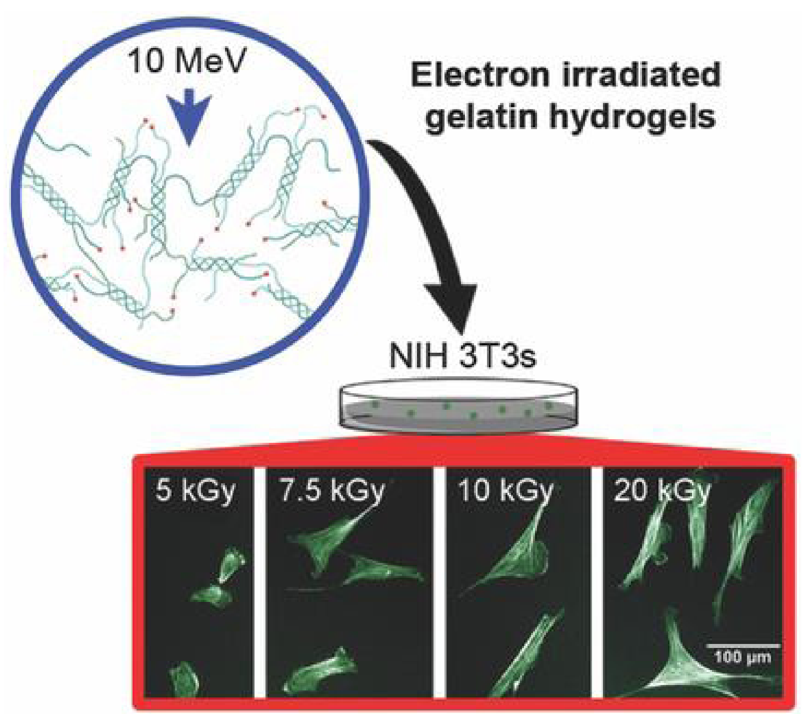
Prof. Dr. Stefan G. Mayr
M.Sc. Phys. Uta Allenstein, Dr. Ariyan Arabi-Hashemi, M.Sc. Phys. Alina Bischoff, Dipl.-Phys. Jörg Buchwald, Dipl.-Phys. Marcel Hennes, Dipl.-Phys. Anja Landgraf, Dipl.-Phys. Fritz Lehnert, M.Sc. Phys. Stefanie Riedel, B.Sc. Eng. Emilia Wisotzki

Biocompatible hydrogels such as gelatin and collagen tailored by electron irradiation represent promising materials in biomedical fields such as regenerative medicine or drug delivery. By modifying the polymeric network using high energy crosslinking, these hydrogels can be adapted to become thermally stable materials with defined structural and mechanical properties. Thereby, electron irradiation represents a fast and non-toxic crosslinking method compared to other methods such as glutaraldehyde crosslinking. Characterisation of the mechanical and structural properties was part of the work. The structure of irradiated gelatin hydrogels was characterised using small angle X-ray scattering (SAXS) in contrast to gelatin

hydrogels of various concentrations, revealing differences in the respective chemical and physical crosslinks.

Additionally, the biocompatibility of high energy irradiated gelatin hydrogels was demonstrated using NIH 3T3 fibroblasts. Cell morphologies were influenced by the irradiation dose via the resulting material viscoelasticity. Furthermore, the ability to transfer microscale patterns onto the hydrogels during irradiation was investigated. Future cell studies will be carried out to investigate the influence of these structures on growth and proliferation. Tuning the microstructure is highly interesting for bio-applications to influence cell adhesion, mobility and viability.

In collaboration with the DFG SPP 1681 project on “Field controlled particle matrix interactions: synthesis multiscale modelling and application of magnetic hybrid materials”, electron irradiation was explored as a method to embed magnetic nanoparticles into the gelatin networks. Magnetic nanoparticles were integrated into the gels before irradiation and investigated across a range of physiologically-relevant temperatures and time scales. By measuring the magnetic response with magnetic particle spectroscopy (MPS) and magnetorelaxometry (MRX), the behavior of the particles was relatively stable after irradiation crosslinking. On the other hand, the



⇑ Biocompatibility tests on gelatin hydrogels irradiated with variable electron doses.

sol-gel transition was visible in the magnetic response of physically crosslinked gelatin ferrogels. MRX relaxation times revealed a slight local softening in the matrix corresponding to the sol-gel transition for a low crosslinking dose of 5 kGy, suggesting a potential of MRX to magnetically detect changes to the local rheology.

⇒ *Stress-Induced Martensitic Transformation, Twin Boundary Mobility and Elastic Properties of Vapor Deposited $Fe_{70}Pd_{30}$ Ferromagnetic Shape Memory Alloy Thin Films*
A. Bischoff, A. Landgraf, S.G. Mayr / Scr. Mat. (2016) **111** 76

⇒ *Coupling of Metals and Biominerals: Characterising the Interface between Ferromagnetic Shape-Memory Alloys and Hydroxyapatite*
U. Allenstein, S. Selle, M. Tadsen, C. Patzig, T. Höche, M. Zink, S.G. Mayr / ACS Applied Materials & Interfaces (2015) **7** 15331

⇒ *Contractile Cell Forces Deform Macroscopic Cantilevers and Quantify Biomaterial Performance*
U. Allenstein, S.G. Mayr, M. Zink / Soft Matter (2015) **11** 5053

⇒ *Equilibrium Segregation Patterns and Alloying in Cu/Ni Nanoparticles: Experiments Versus Modeling*
M. Hennes, J. Buchwald, U. Ross, A. Lotnyk. S.G. Mayr / Phys. Rev. B (2015) **91** 245401

⇒ *Ion Irradiation Assisted Tuning of Phase Transformations and Physical Properties in Single Crystalline Fe_7Pd_3 Ferromagnetic Shape Memory Alloy Thin Films*
A. Arabi-Hashemi, R. Witte, A. Lotnyk, R. Brand, A. Setzer, P. Esquinazi, H. Hahn, R. Averbac, S.G. Mayr / New J. Phys. (2015) **17** 0530298

⇒ *Shifting Martensite Transformation Temperatures of Single Crystalline $Fe_{72}Pd_{28}$ Thin Films by External Magnetic Fields*
A. Arabi-Hashemi, Y. Ma, A. Setzer, P. Esquinazi, S.G. Mayr / Scr. Mat. (2015) **104** 91

⇒ *Elastic Properties of Sub-Stoichiometric Nitrogen Ion Implanted Silicon*
M.F. Sarmanova, H. Karl, S. Mändl, D. Hirsch, S.G. Mayr, B. Rauschenbach / Nucl. Instr. Meth. Phys. Res. B (2015) **349** 169

⇒ *Exploring Electrical Conductivity Anomalies Across the Martensite Transition in Fe_7Pd_3 Ferromagnetic Shape Memory Alloys: Experiments and Ab-initio Calculations*
A. Arabi-Hashemi, S.G. Mayr / Appl. Phys. Lett. (2015) **106** 091906

⇒ *Effect of Microgrooved Surface Topography on Osteoblast Maturation and Protein Adsorption*
A. de Luca, A. Weidt, M. Zink, S.G. Mayr, A.E. Markaki / J. Biomed. Mat. Res. A (2015) **103** 2689

⇒ *Influence of Surface Stresses on Indentation Response*
J. Buchwald, S.G. Mayr / Nanotechn. (2015) **26** 125704

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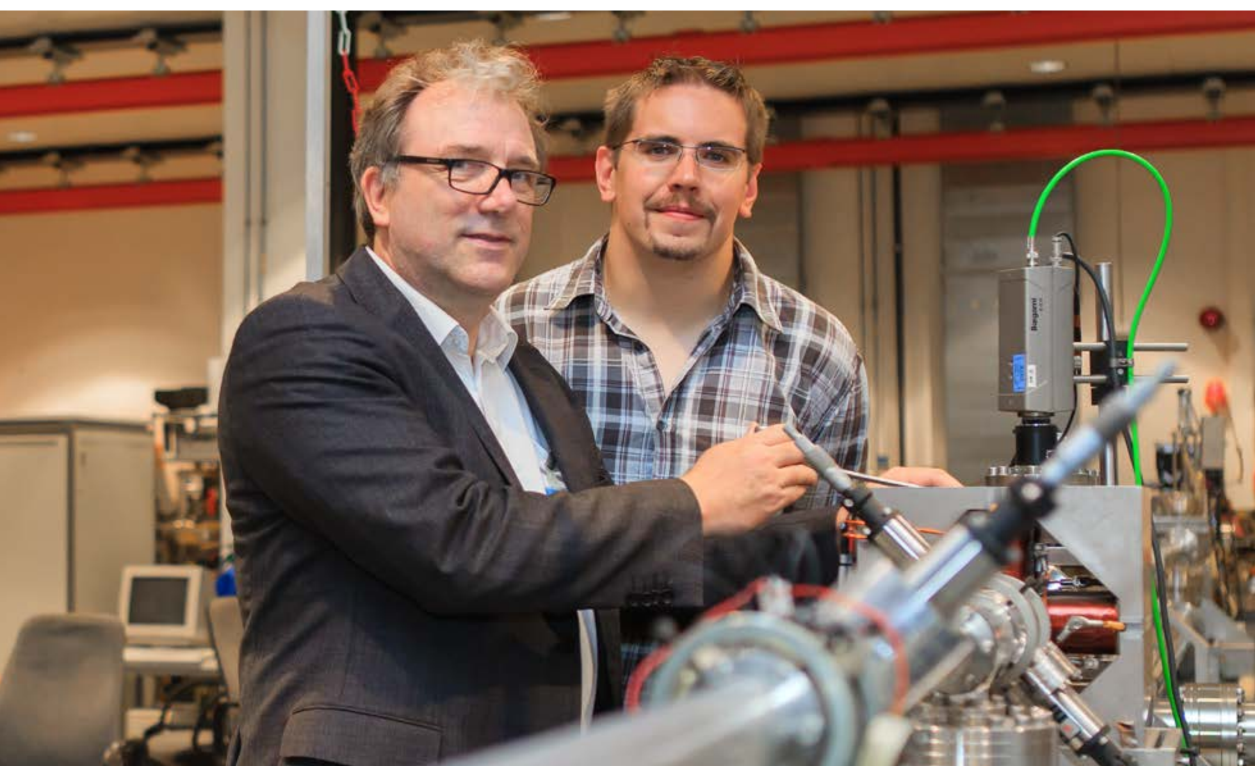
Bright optical centre in diamond with narrow, highly polarised and nearly phonon-free fluorescence at room temperature

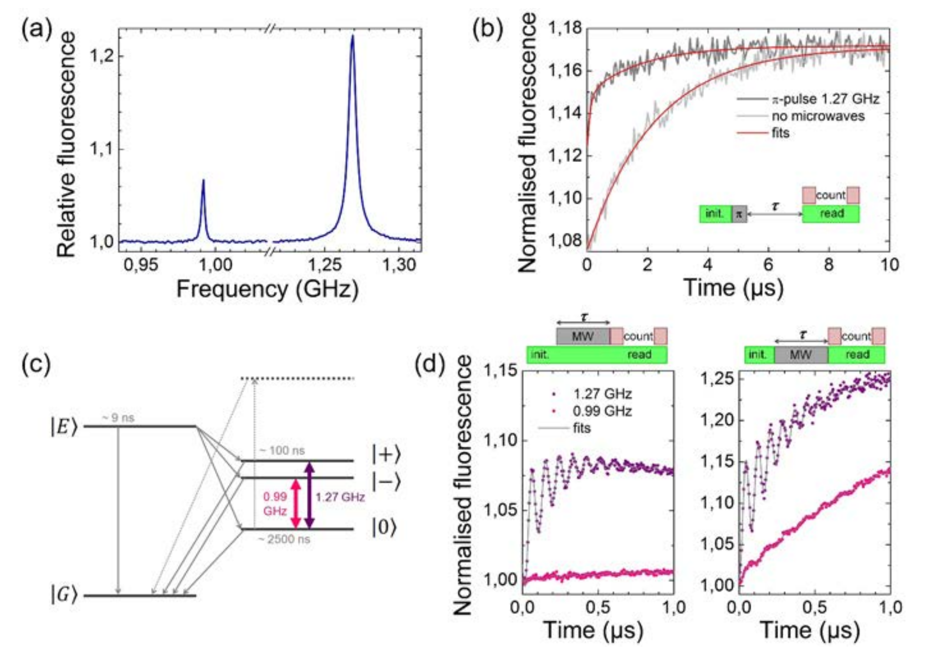
Prof. Dr. Jan Meijer
Dipl.-Math. Roger John

Defect centres in diamond are getting more and more into focus for a large range of applications in physics, material science and bio-technology. Due to its high atomic density and its high Debye temperature, diamond is an ideal candidate for quantum information processing and quantum sensing. The wide transparency range of diamond and the large amount of optically active defect centres also offer the possibility to engineer single-photon sources operating at room temperature. The optical properties of such non-classical light emitters can furthermore be controlled or improved by use of adequate photonic structures. For biomedical applications, fluorescent nano-diamonds containing Nitrogen-Vacancy (NV) centres are widely used for imaging and future therapy schemes. Furthermore, the unique spin and optical properties of the NV centres in diamond have led to single molecule NMR. The



main important features of the NV centre that enable these kinds of applications are the optical readout and coherent control of single spins with extremely long coherence time at room temperature. Among hundreds of defect centres known in diamond, these exceptional properties have been found only for the NV centre and the ST1 centre up to now. Whereas the NV centre can be produced in a controlled way using ion beam implantation or diamond growth, the ST1 centre was found once in a surface etched HPHT diamond and could not be reproduced up to now. Despite its prosperousness, the NV centre has some disadvantages. It is formed after annealing and involves a carbon vacancy, therefore a deterministic fabrication by ion implantation is highly challenging. Additionally, the centre shows a very large phonon coupling. This leads to a broad emission spectrum, thus coherent coupling schemes using photons are hardly achievable with NV centres. In order to find new applicable defect centres, we have set up an ion accelerator which is able to implant all types of elements, at the exception of noble gases. Our aim is to search for all possible diamond (and not only) optical centres created by ion implantation.

Ion implantation addresses single atoms and defects with high spatial resolution in three dimensions. Using this method, the production of an entangled quantum register and quantum sensors at room temperature have already been demonstrated



⇑ (a) Optically Detected Magnetic Resonance (ODMR) spectrum of a single L2 centre at room temperature. (b) Decay curves from which the lifetimes of the spin triplet level can be extracted with a double exponential fit. (c) Tentative level scheme for the L2 centre. (d) Rabi oscillation on the indicated resonance frequency with either constant illumination (left) or pulsed light (right). The measurement scheme is similar to NV centres, but the initialisation laser pulse used was 7 µs long, and the two 250 ns counting windows were 5.5 µs apart to accommodate for the long shelving state lifetime.

using NV centres. Due to the extremely small diffusion constant in diamond, atoms placed by ion implantation remain at the same crystal position even after high temperature treatments. This stability reduces bleaching effects or formation change due to laser irradiation. By applying the ion implantation techniques, we found a new defect centre (the centre was found by Jan Lehnert using an implantation procedure with masses around 26 amu), with narrow yellow fluorescence, emitting mostly at 582 nm (hereafter termed the L1 centre due to the first letter of the city where the discovery took place). This L1 centre was created by ion implantation technique and, to our knowledge, could not be found in any natural diamond. Additionally, another kind of optical centre has been created within the same sample and ion implantation run, with a zero-phonon line emitting at ~ 546 nm and showing electron spin resonance. This hereafter termed L2 centre may be the already reported ST1 centre.

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Engineering biomimetic microenvironments for *in vitro* cell studies

Prof. Dr. Tilo Pompe
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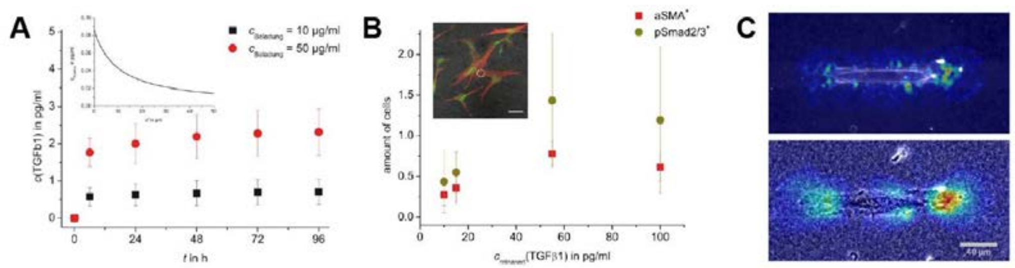
The extracellular microenvironment controls many cellular processes including cell growth, differentiation and apoptosis. For a better understanding of this regulation biomimetic systems are used for in-depth analysis in high-resolution *in vitro* studies. We design and construct material scaffolds to model important extracellular cues like stiffness, viscosity, spatial constraints and gradients of signalling molecules.

In this context M. Ansorge builds and characterises micrometer sized gradients of soluble mediators that regulate hematopoietic stem cells as well as fibroblasts and macrophages during wound healing. He modifies polymer microparticles with various glycosaminoglycans, yielding a controlled and slow release of signalling

molecules like SDF-1, IL-10, and TGF-β1. Thereby short-ranged gradients in 2D and 3D cell culture scaffolds are established. The systems are used to study local, single cell behaviour within these gradients in terms of migration, proliferation and differentiation.

A. Müller uses synthetic hydrogel layers to model the impact of materials stiffness, ligand affinity and spatial constraints on cell adhesion. The latter are introduced by micropatterning the top of the polymer coated hydrogels. The correlation of traction force generation with actin stress fibre formation of constrained adherent cells is monitored *in situ* in a time-resolved manner to better understand mechanobiology of adherent cells.



⇑ A) Tuning the release of TGF-β1 from microparticles over 96 hours by loading concentration (10/50 µg/ml) and the respective calculated local diffusion gradient around a microparticle (inset). B) Fibroblast differentiation into myofibroblasts (positive for alpha smooth muscle actin (aSMA, red) and Smad2/3 in nucleus (green)) is stimulated by the local and sustained release of TGF-β1 from microparticles inside 3D collagen networks at two orders of magnitude lower concentration than standard global TGF-β1 supplement. (scale bar: 50 µm). C) Live cell tracking of adherent cells on patterned hydrogel substrates to characterise traction force evolution and stress fibre formation (white) (top - traction stress, bottom - displacement field).

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Ion and laser beam induced thin films and nanostructures

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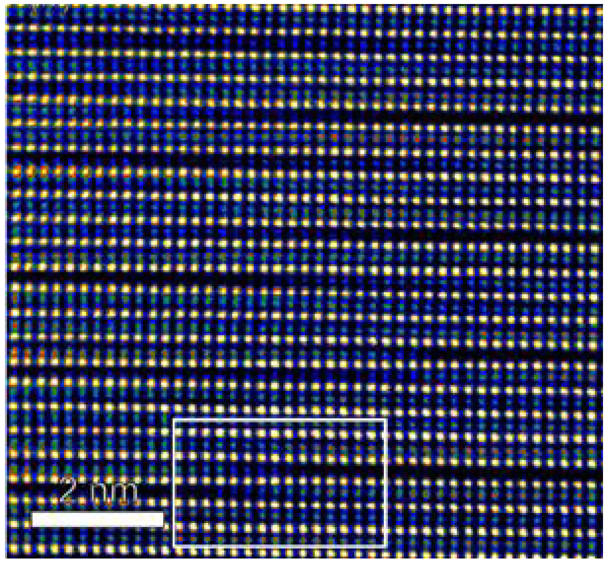
With the accelerated demands on new non-volatile memories in terms of high speed, high endurance and low power, one of the most promising candidates are chalcogenide-based phase change materials (PCMs). PCMs can rapidly and reversibly be switched between an amorphous and different crystalline phases. Since the phase changes are characterised by very different optical and electrical properties, these materials can be employed for rewritable optical and electrical data storage.

In the research project, we aim to investigate the growth of PCMs as thin films and the deposition dependent effects on optical and electrical properties. Additionally, the effects of miniaturisation (nano-structures) on switching speed

and reversibility will be investigated. Pulsed laser ablation will be used to prepare /optimise the phase change material and miniaturisation are accomplished with in-house facilities (laser irradiation / focused ion and electron beam techniques). The crystallisation behavior of the material is investigated with thermal annealing experiments, whereas the reversible switching is studied either by ultra-fast laser pulse irradiation laser or by resistive measurements. Selected samples are investigated with HRTEM to obtain a correlation between structure and experimental parameters.



⇐ High-resolution high-angular angle dark field scanning transmission electron microscopy (HAADF-STEM) images of stacking-disordered hexagonal GST in [011¯0] zone axis. The 180° rotation twin domains as well as the prevalence of 4-, 5- and 6-fold Te stacking are clearly visible. Inset shows quantitative image simulations of a $Ge_2Sb_2Te_5$ block.

⇒ *Elastic Properties of Sub-Stoichiometric Nitrogen Ion Implanted Silicon*
M.F. Sarmanova, H. Karl, S. Mändl, D. Hirsch, S.G. Mayr, B. Rauschenbach / Nucl. Instr. Meth B (2015) **349** 169

⇒ *Crystallisation Kinetics of GeTe Phase-Change Thin Films Grown by Pulsed Laser Deposition*
X. Sun, E. Thelander, J.W. Gerlach, U. Decker, B. Rauschenbach / J. Phys. D: Appl.Phys. (2015) **48** 295304

⇒ *Focused High- and Low-Energy Ion Milling for TEM Specimen Preparation*
A. Lotnyk, D. Poppitz, U. Ross, J.W. Gerlach, E. Thelander, S. Bernütz, B. Rauschenbach / Microelectronics Reliability (2015) **55** 2119

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Coherent transport in quantum condensates: from quantum Hall nano-structures to exciton-polariton condensates

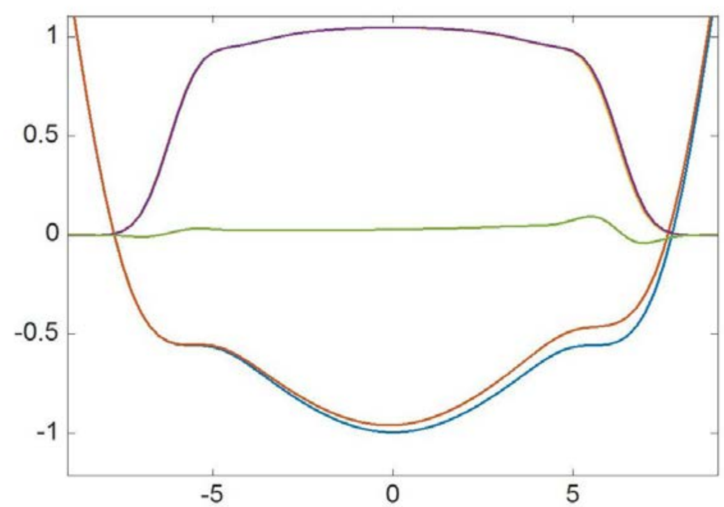
Prof. Dr. Bernd Rosenow
Dipl.-Phys. Alexander Janot, M.Sc. Phys. Martin Treffkorn

Research in the group is focused on the analysis of quantum condensates, their low-energy excitations, and topological quantum systems. Examples for quantum condensates are quantum Hall fluids, superconductors and exciton-polariton condensates. The common characteristic of these states of matter is the existence of a macroscopic wave function, which describes the collective quantum dynamics of the system.

Topological quantum systems exhibit a novel phase of matter, which cannot be characterised by standard order parameters. As a hallmark, for example, they exhibit perfectly conducting, topologically protected edge states.

The Quantum spin Hall (QSH) insulator is a system which allows for such phenomena. In contrast to the quantum Hall effect, as investigated in another work of our group (see below), this topological phase additionally requires time reversal symmetry (TRS). Then, in a topologically nontrivial state, the edge states are protected against perturbations. If TRS is broken (or the gap is closed), a transition into the trivial phase may occur and the edge states are no longer robust against disorder. Contrary to these fermionic systems, for bosons in two dimensions the existence of a topological nontrivial phase is ruled out by the existing topological classification. We studied the light-matter coupling in a QSH insulator. Remarkably, for such a QSH cavity we observed a topologically nontrivial phase of bosonic polaritons. At a first glance, this may sound rather unexpected, however it turns out that the emerging polaritons can inherit the non-trivial topological structure from the underlying electronic system, and that this system does not fall into the existing topological classification. Furthermore, our work presents details about possible experimental realisations and the emerging polaritonic edge states.

The low energy excitations of the quantum Hall condensate at filling factor 5/2



⇑ Equilibrium vs. non-equilibrium results for electrons inside a two dimensional electron gas, confined by a gate potential, and with a perpendicular magnetic field of 2*T*. A bias of 0.1 $\hbar\omega_c$ is applied to one of the edge channels to obtain the non-equilibrium data. We show the respective potentials (blue, red), densities (yellow, violet), and the local non-equilibrium current distribution (green).

are believed to be quasiparticles with non-abelian statistics, an exotic generalisation of bosonic and fermionic statistics. Currently, experimental efforts are under way to prove the existence of these particles through interference experiments in submicron scale devices. Important building blocks of such interferometers are quantum point contacts, which allow tunneling between counter-propagating edge states. As a result of such tunneling, oscillations of the conductance as a function of gate voltage or magnetic field arise. The model of edge states passing through or being reflected at the quantum point contact is well accepted, but little is known about details, such as exact position and width of individual edge states inside the point contact. Recent experiments managed to image the quantum Hall edge states by scanning gate microscopy. With this technique one can analyse the detailed structure of edge states.

We are now able to construct self-consistent potentials of a gate induced quantum point contacts taking into account Coulomb interactions between electrons at finite temperature in different approximations. The simplest way of taking electron-electron interactions into account is introducing a Hartree potential. Solving the self-consistent equations, we end up with alternating compressible and incompressible strips. In this picture the compressible strips are very wide, which is in extreme contrast to the non-interacting case, where the edge channels are quasi-one-dimensional. Furthermore, we are able to produce self-consistent potentials in the local spin density approximation, which also takes exchange interactions into account. In this case, compressible strips are less pronounced. An open question is, whether the LSDA is able to produce edge reconstruction, as it is the case with Hartree-Fock theory of the quantum Hall system. After calculating self-consistent potentials, it is now possible for us to compute local non-equilibrium current distributions, and we will use our algorithms in the future to analyse non-equilibrium current distributions inside quantum point contacts.

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Experiences

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

Prof. Dr. Bernd Rosenow

As someone who was a late-comer to BuildMoNa, I can report that the warm welcome in the Graduate School very much helped me to appreciate both the breadth and the depth of research performed in Leipzig. The open and collaborative environment of the BuildMoNa Graduate School brings out the best in all participants in terms of creativity, openness of mind, and acquisition of new working techniques. I vividly remember how much I was impressed with both the quality of research and its presentation, which was presented at the first BuildMoNa Annual Conference I attended, and I continue to enjoy the impressive display of successful research at BuildMoNa conferences.

My students are excited to be members of the BuildMoNa community, and both friendships and collaborations have been forged during participation in BuildMoNa events. Being a member of the Graduate School is always viewed as a privilege.

An important part of the scientific life are the various scientific and training modules. They enrich the education of both BuildMoNa doctoral candidates and Principal Investigators by giving the opportunity to host distinguished speakers from around the world. Poster sessions integrated into the advanced modules give students the possibility to discuss their research with experts from abroad, and these discussions often have provided an essential stimulus for my students' research projects. In this way, modules serve the double purpose of bringing new ideas to Leipzig, and to further secure Leipzig's place on the scientific map. In this way, both the further development of well established research directions is secured, and an exposition to novel research is possible.

The Graduate School BuildMoNa continues to focus on shared research interests and provides a glue between a wide range of researchers from physical, chemical, and biochemical research institutions, in addition to its contributions to enriching the education of students described above. I look forward to many more years of being a member of this scientific family.

Prof. Dr. Bernd Rosenow

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

M.Sc. Phys. Martin Glaser

The interdisciplinary Graduate School BuildMoNa aims to increase the communication between young scientists from various fields like physics, chemistry, biology, and biochemistry. Their studies, both from a theoretical or experimental background, can range from designing molecules or nano-objects to the micrometer scale and even to multicellular approaches. This broad field of interest surpasses, what is usually taught during undergraduate studies in each specific field. Therefore, a constant scientific training including basic and highly specialised courses is offered.

During these classes, well-known experts on the respective subjects give lectures, which introduce general concepts as well as brand new scientific results. One of the major advantages of these courses is the possibility to discuss results and ideas on a personal level, which is often not possible in the crowded rooms of bigger international conferences. This provides the unique possibility for the doctoral candidates to get direct feedback on their work. Additionally, these workshops help to gain knowledge beyond the usual frame of your doctoral project, which is – in my opinion – absolutely crucial, especially when working in an interdisciplinary field.

The later examination, which is also required during training, sometimes misses that opportunity for a direct feedback. Since most exams are in written form, the doctoral candidates can hardly reflect their broad knowledge and apply the newly acquired skills to their own field of research. Beyond the subject-specific training a wide range of so-called 'soft skills' are offered in collaboration with, for example, the Research Academy Leipzig (RALeipzig). Courses like 'Presentation workshop', in which the doctoral candidate is filmed during a scientific talk, can greatly improve the performance of young researchers when presenting their findings.

For me, BuildMoNa is a good example for an interdisciplinary doctoral program, which helps young researchers to extend their knowledge and gives a platform to increase the important dialog between the different research fields.

M.Sc. Phys. Martin Glaser

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, TRM (Translational Centre for Regenerative Medicine) and 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
Annual BuildMoNa Conference	R		C											
Literature seminars	R/E			S		S		S		S		S		S
Guest lectures/colloquia	E	5	L	L	L	L	L	L	L	L	L	L	L	L
Tutoring	R/E			T	T	T	T			T	T	T	T	
Research stays abroad	E		flexible during the whole year (1 week up to a few months)											
Summer/winter schools	E													
Industrial training	E													
Active participation in conferences/workshops	R/E		flexible during the whole year (1 up to a few days)											
Transferable (generic) skills	R/E	5		S	S	S	S			S	S	S	S	
					M		M				M		M	

BuildMoNa training programme: M, C, 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 chemistry (2015-B1)

30 / 31 March 2015,
written exam, 2 credit points, yearly recurrence, 10 participants

This module for non-chemists introduced the basic concepts in chemistry needed for actively participating in the thematic and advanced modules (T1–T6, A1, A2). The doctoral researchers was given an introduction into the way chemists interpret atomic properties, structures and bonding.

Responsible Scientists/Lecturers:
Prof. Dr. B. Kersting, Prof. Dr. H. Krautscheid, Prof. Dr. F. Kremer

Contents:
⇒ Periodicity: atomic models, orbitals, electron configuration, periodic table and associated properties of the elements: atom and ion size, ionisation energy, electron affinity, electronegativity, oxidation number, groups and rows
⇒ Chemical bonds: concepts, characteristics, breaking chemical bonds, and experiments. Ionic bonds, covalent bonds, *d*- and *f*-orbitals in chemical bonding, van der Waals bonds, hydrogen bonding, hydrogen bonds in bio-systems, electronic and IR-spectroscopy to probe chemical bonding, chemistry: the change of chemical bonds
⇒ Coordination chemistry: *d* electrons, ligands & ligand types, coordination number, complex composition and structure, bonding, valence bond theory, Lewis-acid/-base theory, crystal field theory, crystal field splitting parameter Δ_o, spectrochemical series, high-spin & low-spin complexes, spin-only paramagnetism

Basic concepts in biochemistry (2015-B2)

09 / 10 March 2015,
written exam, 2 credit points, yearly recurrence, 15 participants

Doctoral researchers without a background in biochemistry or biology were brought up to a level necessary to understand the thematic and advanced modules (T1–T6, A2, A1). The module introduced basics in bioactive molecules and biomacromolecules, including their structure and (bio)chemical properties, as well as cell biology. The doctoral researchers learned how proteins are produced, how mutations are introduced and which types of chemical and physical data can be obtained from these types of experiments.

Responsible Scientist:
Prof. Dr. H. Harms, Prof. Dr. D. Huster

Lecturers:
Dr. A. Chatzinotas, UFZ, Leipzig, Germany; Dr. L. Wick, UFZ, Leipzig, Germany; Dr. F. Harnisch, UFZ, Leipzig, Germany; Dr. P. Schmidt, Universität Leipzig, Germany; Dr. U. Krug, Universität Leipzig, Germany; Dr. G. Künze, Universität Leipzig, Germany

Contents:
⇒ Basic bioactive molecules and macromolecules (DNA, RNA, peptides, proteins, carbohydrates, lipids)
⇒ Cell structure and metabolism
⇒ Methods in molecular biology (recombinant DNA, PCR, tools to produce DNA or proteins)
⇒ Proteins (biochemical and biophysical characteristics, folding and stability)
⇒ Cell membranes
⇒ Protein chemistry
⇒ Tissue culturing and biological assays
⇒ Fluorescence microscopy

Basic concepts in molecular spectroscopy (2015-B4)

16 / 17 June 2015,
written exam, 2 credit points, yearly recurrence, 15 participants

This module 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 and single molecule fluorescence detection.

Responsible Scientists/Lecturers:
Prof. Dr. F. Cichos, Prof. Dr. D. Huster, Prof. Dr. F. Kremer

Contents:
⇒ Quantum mechanical foundation of infrared spectroscopy
⇒ Experimental principles of Fourier transform infrared spectroscopy

- ⇒ 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
- ⇒ 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

Multifunctional scaffolds: Biopolymer scaffolds to study dynamic cell function (2015-T2)

11 / 12 June 2015,
written exam, 2 credit points, bi-yearly recurrence with modification, 19 participants

The basic background in passive and active soft matter physics was taught to enable the students to use highly dynamic polymer scaffolds as an organising matrix for smart nanoelements and active proteins. A particular focus was to build mechano-sensing, force-generating, moving, polymeric machines, inspired by active and passive biopolymer networks.

Responsible Scientists/Lecturers:
Prof. Dr. T. Pompe

Lecturers:
Dr. M. Bailly, University College London, UK; Dr. U. Freudenberg, IPF Dresden, Germany; Dr. J. Galle, Universität Leipzig, Germany; Dr. M. Hacker, Universität Leipzig, Germany; Dr. K. Wolf, Radboud University Medical Center, Nijmegen, The Netherlands

Contents:
- ⇒ Physical concepts (statistical and polymer physics, nonlinear dynamics)
- ⇒ Biochemistry of protein filaments
- ⇒ Self-assembly and organisation (cytoskeleton and its architectures, asters and molecular motors, bead motility, counterion cloud condensation)
- ⇒ Semiflexible polymers (individual filaments, entangled and cross-linked solutions, nematics, transients bonds, linear and nonlinear elastic as well as inelastic and plastic mechanics, active networks with molecular motors)
- ⇒ From Brownian to directed motion (diffusion, thermal ratchets, entropic forces)
- ⇒ Cell motility (forces, traction, mechanosensitivity)
- ⇒ Bottom-up approach to cell mechanics (rheological properties, viscoelasticity, glassy behaviour, functional modules)
- ⇒ Liquid crystal physics of lipid membranes (self-assembly, phase diagrams, vesicles, Langmuir monolayers, supported bilayers)
- ⇒ Nanomuscles (active and passive filament bundles, contractile structures, bending stiffness)

Methods:
- ⇒ Rheology (microrheology, plate rheometer, colloidal probe scanning microscopy, optical and magnetical tweezers, optical stretcher)
- ⇒ Microscopy (single molecule and particle imaging, digital polarisation microscopy, confocal/multiphoton microscopy, STED, thermophoretic microscopy)
- ⇒ Dielectric spectroscopy
- ⇒ Soft lithography and microfluidics
- ⇒ Theory and modelling (polymers in di-confinements effects, computer simulation methodologies for (semi)flexible polymers [chain-growth algorithms, Monte Carlo methods, scaling theories, etc.])
- ⇒ Concepts from many-body physics to address entangled and cross-linked solutions
- ⇒ Active hydrodynamics

Complex nanostructures: Active nanostructures (2015-T3)

27 - 29 May 2015,
written exam, 2 credit points, bi-yearly recurrence with modification, 15 participants

The module aimed to provide participants with some understanding of the chemical and physical properties of active nanoparticles and nanostructures, such as their synthesis, experimental control, theoretical description, numerical modeling, including specific nano-scale effects and interactions, and emerging complexity. It aimed at generating an interdisciplinary perspective covering chemical, physical, experimental, computational, and theoretical aspects.

Responsible Scientists:
Prof. Dr. F. Cichos, Prof. Dr. K. Kroy

Lecturers:
Prof. Dr. I. Pagonabarraga, University of Barcelona, Spain; Dr. R. Wittkowski, Uni-

versität Düsseldorf, Germany; Dr. D. Chakraborty, IISER Mohali, India; Dr. J.-B. Fleury, Universität des Saarlandes, Saarbrücken, Germany; Dr. M. Selmke, Princeton University, USA; Ass. Prof. J. Palacci, UC San Diego, USA

Contents:
⇒ Driven and self-propelled transport of nanoparticles and nanostructures
⇒ Thermal and solute gradients and related thermodynamic forces
⇒ (Self-)phoresis in driven systems
⇒ Hydrodynamics
⇒ Wet electrostatics
⇒ Topological and geometric effects
⇒ Energy transfer mechanisms and strong light-matter interactions
⇒ The emergence of complexity
⇒ Collective dynamics
⇒ Networks and swarm properties
⇒ Active matter
⇒ Theoretical, experimental, and computer simulation methods were introduced along with the phenomenological and conceptual overview

Methods:
⇒ Single-particle techniques
⇒ Nano-optics
⇒ Theory
⇒ Computer simulations

Smart and active assemblies (2015-A1)

03 / 04 December 2015,
written exam, 2 credit points, bi-yearly recurrence with modification, 15 participants

This module linked molecular sciences to catalysis on complex, multicomponent and multifunctional active sites. It imparted knowledge on the interaction of active sites and active nanocatalysts with their local environment and the catalytic reaction system, and discussed cutting-edge applications in modern homogeneous, heterogeneous and biocatalysis with the goal of understanding emerging catalytic applications for future needs.

Responsible Scientists:
Prof. Dr. Dr. h.c. E. Hey-Hawkins, Prof. Dr. A.G. Beck-Sickinger, Prof. Dr. A. Robitzki, Prof. Dr. R. Gläser

Lecturers:
Prof. Dr. M. Hartmann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Prof. Dr. V. Urlacher, Heinrich-Heine Universität Düsseldorf, Germany; Prof. Dr. R. Goss, University of St. Andrews, UK

Contents:
⇒ Complex assemblies (specific synthesis, modification, structure and catalytic properties, various environments with optimised catalytic activity, selectivity and stability
⇒ Conductive and semi-conductive electrode materials
⇒ Complex catalysts (functionalised surfaces, enzymes, biofilms, biological systems, immobilisation of catalysts on solid or liquid supports)
⇒ Complex biocatalysts (developing of engineered enzymes, immobilisation of enzymes, surface modification, improved tailor-made biocatalysts, biomimetic catalyst assemblies [zeozymes, artizymes, cells, organisms])
⇒ Catalytic activation by smart assemblies (activation of unreactive molecules [CO_2, hydrocarbon bonds (methane), water splitting], enantioselective catalysis)

Methods:
⇒ Active site assemblies (synthesis, genetic engineering, characterisation of textural, electronic and structural properties by spectroscopy, protein characterisation, potentiometric and impedimetric analysis, electrical conductivity)
⇒ Catalysts (porosity analysis, assays, spectroscopy under working conditions, advanced testing)

Chemical biology and biophysics of cancer: Physics of cancer (2015-A2)

07 - 09 September 2015,
written exam, 2 credit points, bi-yearly recurrence with modification, 15 participants

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

Responsible Scientist:
Prof. Dr. A. Käs

Lecturers:
Prof. Dr. Dr. h.c. E. Bodenschatz, MPI for Dynamics and Self-Organisation, Göttingen, Germany; Dr. K. Chalut, University of Cambridge, UK; Prof. Dr. E. Chen, Johns Hopkins University, Baltimore, USA; Prof. Dr. C. Dahmann, Technical University Dresden, Germany; Ass. Prof. Dr. M. Das, Rochester Institute of Technology, USA; Dr. A. del Campo, MPI for Polymer Research, Mainz, Germany; Dr. M. Faivre, University of Lyon 1, France; Prof. Dr. J. Guck, Technical University Dresden, Germany; Dr. C. Jamora, inStem, Bangalore, India; Prof. Dr. L. Kreplak, Dalhousie University, Halifax, Canada; Prof. Dr. Dr. K. Kruse, Saarland University, Saarbrücken, Germany; Assoc. Prof. Dr. L. Manning, Syracuse University, USA; Dr. L. Nagahara, National Cancer Institute, Bethesda, USA; Prof. Dr. M. Narasimha, Tata Institute of Fundamental Research, Mumbai, India; Prof. Dr. E. Paluch, University College London, UK; Dr. S. Raghavan, inStem, India; Prof. Dr. H. Rieger, Saarland University, Saarbrücken, Germany; Prof. Dr. M. Ritsch-Marte, Innsbruck University, Austria; Prof. Dr. I. Sack, Charité, Berlin, Germany; R. Sinkus, King´s College London, UK

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

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

Scientific minisymposium

Quantum coherent structures: Unconventional superconductivity (2015-A3)

30 September – 01 October 2015

The sixth BuildMoNa Minisymposium was organised by the research groups of Prof. Dr. M. Grundmann and Prof. Dr. B. Rosenow and dealt with macroscopic coherent quantum states such as superfluids, superconductors or Bose-Einstein condensates that hold great promise for applications such as frictionless, dissipationless transport or ultralow threshold lasers, if brought to room temperature. It also elucidated the role of spins (“spintronics”), topological band structures, and light-matter interactions (nanophotonics) in nanoscience. The field is partly a challenge in materials physics, partly a challenge in theoretical understanding. The fundamentals of the field and several practical examples were considered. The speakers were:

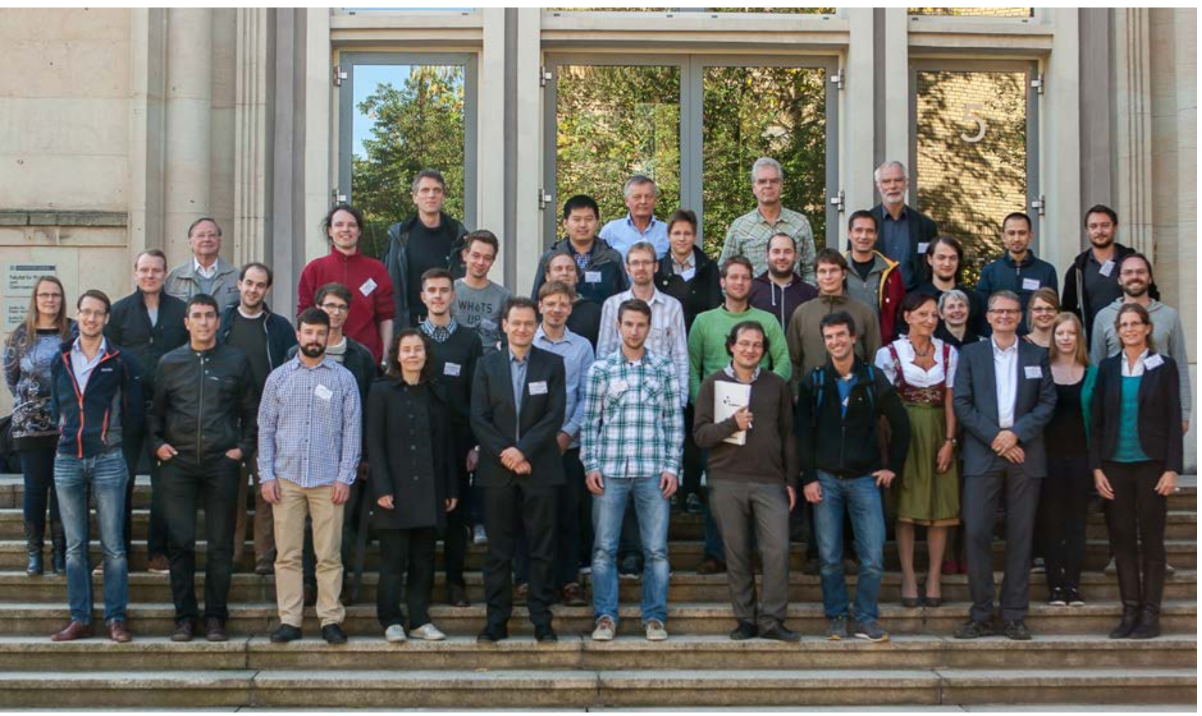
⇒ A. Beukman, TU Delft, The Netherlands, *Experimental Studies of InAs/GaSb Heterostructures as a 2D Topological Insulator*
⇒ P. Brouwer, Freie Universität Berlin, Germany, *Majorana Wires*
⇒ Dr. C. Brüne, Universität Würzburg, Germany, *Transport and Induced Superconductivity in the Topological Surface and Edge States of HgTe*
⇒ Dr. M. Eremets, Max-Planck-Institut für Chemie, Mainz, Germany, *Superconductivity at 200K*
⇒ Dr. M. Houzet, CEA Grenoble, France, *Multi-Terminal Josephson Junctions as Topological Materials*
⇒ Prof. Dr. T. Ihn, ETH Zurich, Switzerland, *Magnetotransport in the Topological Insulator Candidate InAs/GaSb*
⇒ Prof. Dr. F. Kuemmeth, University of Copenhagen, Denmark, *Transport*

Spectroscopy of Semiconductor-Superconductor Quantum Devices

⇒ Prof. Dr. F. Laussy, Universidad Antónoma de Madrid, Spain, *Superconductivity: The Sandwich Mechanism*

⇒ Prof. Dr. G. Malpuech, Institut Pascal, CNRS Aubière, France, *Spin-Orbit Coupling in Photonic Systems: From Optical Spin Hall Effect to Z Topological Insulator*

⇒ Prof. Dr. P. Törmä, Aalto University, Espoo, Finland, *Superfluidity in Topologically Nontrivial Flat Bands*



⇑ Participants of the scientific minisymposium

Transferable skills workshops

Presentation workshop

Dr. Frank Lorenz, Rhetoric Excellence,
12 / 26 March 2015 in combination with the Annual BuildMoNa Conference,
12 participants

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

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Lutz Thrams	*PTB Berlin, Germany*	Magnetische Messtechnik an magnetischen Nanopartikeln	29 January 2015	*Leibniz Institute of Surface Modification*
Prof. Dr. Katsumi Matsuzaki	*Kyoto University, Japan*	Coiled-coil labeling method: A useful tool for membrane protein imaging	22 July 2015	*Faculty of Biosciences, Pharmacy and Psychology*
Prof. Dr. Cristina Marchetti	*Syracuse University, USA*	Active Glasses: From colloids to living cells	30 October 2015	*Faculty of Physics and Earth Sciences*

Annual BuildMoNa Conference

The third annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held on 23 and 24 March 2015 at the Faculty of Chemistry and Mineralogy. The following renowned guest speakers from science gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Oliver Benson, Humboldt-Universität zu Berlin, Germany:
Defect Centres in Nanodiamonds: Fundamental Building Blocks for Quantum Technology & Sensing Applications

⇒ Prof. Dr. Muriel Hissler, Université de Rennes 1, France:
Molecular Materials for (Opto)electronic Devices

⇒ Prof. Dr. Regina Palkovits, RWTH Aachen, Germany:
From Lignocellulose to Novel Monomers

⇒ Prof. Dr. Tanja Weil, Universität Ulm, Germany:
Macromolecular Therapeutics by Programmed Self-Assembly

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

⇑ Participants of the Annual BuildMoNa Conference

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

Niklas Fricke (Institute for Theoretical Physics) received the first prize for his work on polymers in disordered environments, published in:
Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters
N. Fricke, W. Janke / Phys. Rev. Lett. (2014) **113** 255701

André Heber (Institute for Experimental Physics I) received the second prize for his work on the development of a photothermal light modulator, published in:
Metal Nanoparticle Based All-Optical Photothermal Light Modulator
A. Heber, M. Selmke, F. Cichos / ACS Nano (2014) **8** 1893

Jakob Tómas Bullerjahn (Institute for Theoretical Physics) was awarded the third prize for his work on the theory of dynamic force spectroscopy, published in:

Theory of Rapid Force Spectroscopy

J.T. Bullerjahn, S. Sturm, K. Kroy / Nat. Commun. (2014) **5** 4463

17 doctoral candidates presented their scientific results with short talks. Presentations covered the whole research profile of the graduate school: Development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. Mechanisms of material formation from building blocks, e.g. self-organisation, were also included.

For the 12 participants of the Presentation Workshop by Dr. Frank Lorenz this was the opportunity to directly apply their newly acquired knowledge in that area. Their talks were filmed and critically discussed afterwards. At the end of the workshop a jury selected the three best presentations given by the doctoral candidates.

⇑ Winners of the BuildMoNa Awards 2015: Niklas Fricke, Jakob Tómas Bullerjahn, André Heber (from right to left)

The first prize was awarded to Toni Grell for his presentation “Novel donor–acceptor complexes with phosphines and amines”, the second to Emilia Wisotzki for her presentation “Tailoring the material properties of electron irradiated gelatin hydrogels” and the third to Peter Schlupp for “Room-temperature fabricated amorphous oxide heterodiodes on glass and flexible substrates”.

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference: Toni Grell, Emilia Wisotzki, Peter Schlupp (from right to left)

Funding of doctoral candidates

DFG

WR
WISSENSCHAFTSRAT

Europa fördert Sachsen.
ESF
Europäischer Sozialfonds

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