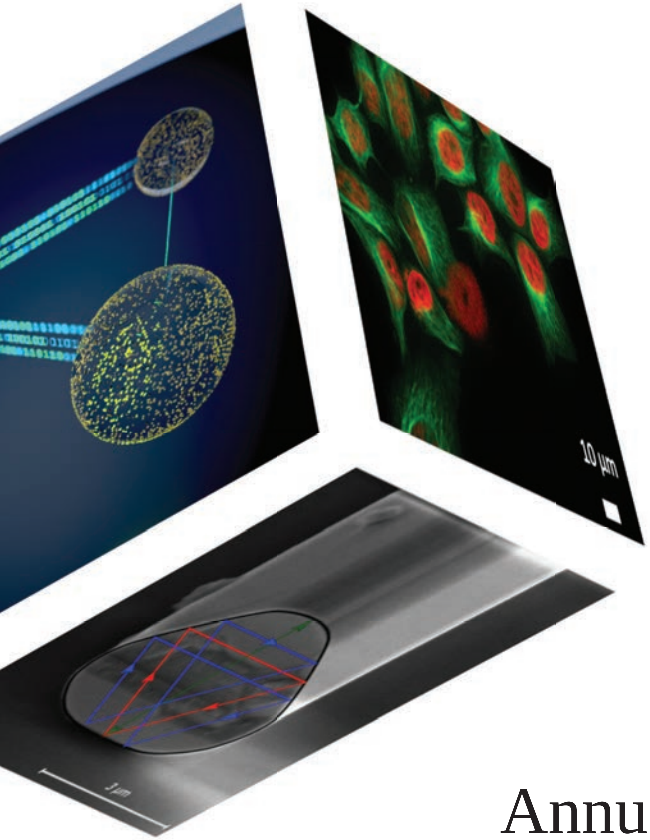
UNIVERSITÄT
LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2017

Cover image:

⇒ *Left:* Three symmetric microswimmers decorated with gold nanoparticles. The information flow between the particles sketched by binary number streams is realized in the experiment by a real time detection of the position of the microswimmers.

⇒ *Right:* Adherent epithelial cells. The green stain represents the actin cytoskeleton and red shows the cell nucleus.

⇒ *Bottom:* Scanning electron microscopy image of copper iodide microwire and its cross-section.Schematically different optical modes are superimposed.

UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects

Annual Report 2017

Founded as DFG Graduate School 185 in 2007

⇒ Publisher: Graduiertenschule "Leipzig School of Natural Sciences - Building with Molecules and Nano-objects (BuildMoNa)"
Universität Leipzig, Johannisallee 29, 04103 Leipzig, Germany
Tel.: +49 341 97-36015, Fax.: +49 341 97-39317
buildmona@uni-leipzig.de, www.buildmona.de

⇒ Authors: Prof. Dr, A.G. Beck-Sickinger, Prof. Dr. F. Cichos, Prof. Dr. R. Gläser, Prof. Dr. M. Grundmann, Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins, Prof. Dr. W. Janke, Prof. Dr. J.A. Käs, Prof. Dr. B. Kersting, Prof. Dr. K. Kroy, Prof. Dr. S.G. Mayr, Prof. Dr. J. Meijer, Prof. Dr. T. Pompe, Prof. Dr. Dr. h.c. B. Rauschenbach, PD Dr. U. Reibetanz, Prof. Dr. B. Rosenow, Prof. Dr. R. Seidel

⇒ Editor: Lukas Trefflich

⇒ Photographers: Swen Reichhold

⇒ Design & Layout: Tim Klinger, Franziska Becker, Leipzig, meantrafik.com

⇒ Production: Merkur Druck- & Kopierzentrum GmbH, Leipzig

Table of contents

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

Preface
Prof. Dr. Marius Grundmann
Coordinator since 1 November 2017
Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Coordinator until 31 October 2017

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

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

Since the establishment of the Graduate School in 2007, 139 young scientists have finished their doctoral studies with a certificate of the Graduate School by the end of 2017. In 2017, 43 doctoral researchers have been enrolled as members of BuildMoNa. Most of them are employed through third-party funded research projects and we are grateful for 7 DAAD and 9 other scholarships.

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

Each year, one of the advanced modules is organised as an international symposium. In 2017, the symposium “Transparent Conductive Oxides - Fundamentals and Applications” (TCO2017) was organised by Prof. Marius Grundmann together with Dr. Holger von Wenckstern of the Semiconductor Physics Group and brought together researchers in the field of transparent materials. These materials are used for ohmic applications such as transparent contacts in displays or solar cells. In addition, semiconducting transparent oxides for diodes and transistors have gained tremendous interest due to applications in transparent and flexible active electronics. TCO2017 was additionally supported by the Deutsche Forschungsgemeinschaft.

Science-related events included the fifth Annual BuildMoNa Conference in March, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School. External speakers, selected and invited by the doctoral researchers of BuildMoNa, covered topics of topological materials, metal-organic frameworks, atomic and molecular scale functional devices and the molecular design of nanocapsules in engaging presentations.

After funding by the Deutsche Forschungsgemeinschaft within the German Excellence Initiative until October 2014, BuildMoNa was financially supported as a class at the Research Academy Leipzig until October 2017 through funds of the Research Profile Area “Complex Matter”.

It is our distinct pleasure to announce that from November 2017 on, BuildMoNa has been permanently established as “Graduate School” (Graduiertenschule) within the Research Academy Leipzig and is funded through an agreement (Zielvereinbarung) between BuildMoNa, the rectorate of Universität Leipzig and the three main faculties forming BuildMoNa. The sustained path established for BuildMoNa will allow us to develop further, widen our reach, flourish in our activities and to continue to supply excellent support and research conditions for our doctoral researchers.

Prof. Dr. Marius Grundmann

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

Organisation and management

RESEARCH ACADEMY LEIPZIG ADVISORY BOARD

Prof. Dr. Manfred Salmhofer
Universität Heidelberg

Prof. Dr. Julia Fischer
Universität Göttingen

Prof. Dr. Michael Geyer
Universität Chicago

Frau Dr. Henrike Hartmann
Volkswagen Stiftung

Prof. Dr. Peter Scherrer
Universität Graz

Prof. Dr. Bernhard Englitz
Radboud University

RESEARCH ACADEMY LEIPZIG

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

BuildMoNa OFFICE

Scientific Managers
Dr. Alexandra Hildebrand
Dr. Anna Reinhardt

Multilingual Secretaries
Isabel Holzke

STEERING COMMITTEE

Speaker of the Graduate School
Prof. Dr. Marius Grundmann
Prof. Dr. Dr. hc. mult. Evamarie Hey-Hawkins (until 31 October 2017)

Deputy
Prof. Dr. Dr. hc. mult. Evamarie Hey-Hawkins
Prof. Dr. Roger Gläser (until 31 October 2017)
Prof. Dr. Marius Grundmann (until 31 October 2017)

Representative of Doctoral Candidates
M.Sc. Phys. Paul Räcke
M.Sc. Phys. Peter Schlupp

Deputy
M.Sc. Biochem. Dennis Worm
M.Sc. Phys. Martin Glaser

Representatives of Principal Investigators
Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Prof. Dr. Daniel Huster
Prof. Dr. Harald Krautscheid
Prof. Dr. Bernd Abel
Prof. Dr. Annette G. Beck-Sickinger
Prof. Dr. Frank Cichos
Prof. Dr. Marius Grundmann
Prof. Dr. Frank-Dieter Kopinke
Prof. Dr. Felix Otto

SPOKESPERSONS OF THE DOCTORAL CANDIDATES

Faculty of Life Sciences
M.Sc. Biochem. Dennis Worm

Faculty of Chemistry and Mineralogy
Dipl.-Chemie-Ingenieur Felix Link
M.Sc. Chem. Antonio Buzharevski

Faculty of Physics and Earth Sciences
M.Sc. Phys. Paul Räcke

Leibniz Institute of Surface Modification
M.Sc. Phys. Stefanie Riedel

Helmholtz Centre for Environmental Research
M.Sc. Chem. Yuting Guo

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

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

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

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

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

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

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Angela Aleksovska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Photoactive metal-organic-frameworks - synthesis and applications*
M.Sc. Phys. Sascha Becker	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*Photoelectrically detected magnetic resonance of nitrogen vacancy centres in diamond*
M.Ed. Math./Phys. Johannes Bock	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Computer simulations of semiflexible polymers in disordered media*
M.Sc. Chem. Antonio Buzharevski	Prof. Dr. Dr. h.c. mult. 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. Phys. Henrik Christiansen	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Nonequilibrium investigation of (bio-)physical systems*
M.Sc. Chem. Peter Coburger	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*1,2-Dicarba-closo-dodecaborane(12) as scaffold for the development of new ligands with application in homogeneous catalysis*
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*
M.Sc. Chem Jan-Patrick Fischer	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Chemical modification and characterisation of therapeuticaly relevant peptide hormones*
M.Sc. Biochem. Tobias Fischer	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. T. Pompe	*Identification of chemerin fuction*
M.Sc. Chem. Martin Fränzl	Prof. Dr. F. Cichos / Prof. Dr. R. Seidel	*Thermoelectric effects at the nanoscale*
M.Sc. Phys. Martin Glaser	Prof. Dr. J. Käs / Prof. Dr. S. Mayer	*Investigation of actin structures*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Tom Golde	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Actin related contractile structures*
M.Sc. Chem. Marta Gozzi	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Nido-carbaborate complexes as cytoxic agents*
M.Sc. Chem. Toni Grell	Prof. Dr. Dr. h.c. mult. 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 molecular level*
M.Sc. Chem. Peter Hahn	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Calix[4]arenes for binding f-elements, synthesis, characterisation and complex formation*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Principles of mechanosensitivity and durotaxis in mammatian cells*
M.Sc. Phys. Constantin Huster	Prof. Dr. K. Kroy / Prof. Dr. T. Pompe	*Bottom-up inelastic cell mechanics*
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.-Math. Roger John	Prof. Dr. J. Meijer / Prof. Dr. B. Rosenow	*Coupling ^{13}C-superlattices to single nitrogen vacancy centres in diamond*
M.Sc. Chem. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Heterogeneously catalyzed liquid phase oxidation of hydrocarbons over metal-organic frameworks*
M.Sc. Phys. Robert Karsthoff	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Transparent photovoltaic cells*
M.Sc. Phys. Max Kneiß	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Optical properties and lateral Ttransport in $Mg_xZn_{(1-x)}O$ quantum well nanostructures: A new approach for diluted magnetic semiconducters*
M.Sc. Chem. David Langer	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Application of dendritic catalyists in tandem catalysis*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Fritz Lehnert	Prof. Dr. S. Mayer / Prof. Dr. Dr. hc. B. Rauschenbach	*Ion-aided synthesis and investigation of nanoporous materials*
M.Sc. Phys. Susann Liedtke	Prof. Dr. Dr. hc. 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. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. J. Käs	*Stochastic analysis of plasma membrane fluctuations of neuonal growth cones*
M.Sc. Phys. Tom Michalsky	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Light-matter interaction in systems of reduced dimensionality*
M.Sc. Chem. Georgia Mhanna	Prof. Dr. R. Gläser/ Prof. Dr. A.G. Beck-Sickinger	*Hexagonal mesoporous silicates for immobilisation of multi-enzyme conjugates*
M.Sc. Phys. Erik Morawetz	Prof. Dr. J. Käs / Prof. Dr. S. Mayer	*Optical deformability and tumour aggressiveness*
M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Metal-organic frameworks with chiral binaphthalene-based linkers*
M.Sc. Chem. John Popp	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Redox-switchable catalysis with P-stereogenic dendritic ferrocenyl phosphine complexes*
M.Sc. Chem. Rafaella Precker	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. D. Huster	*MOFs as drug carriers for cancer therapy*
M.Sc. Phys. 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. Paul Räcke	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	*High precision fabrication of quantum sensor arrays via ion implantation*
M.Sc. Chem. David Rettke	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	*Soft colloidal probe-based biosensors*
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Spin polarization investigations on exciton-polaritons and their condensates*

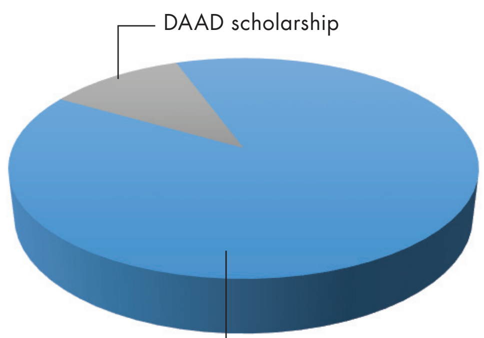
Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Stefanie Riedel	Prof. Dr. S. Mayer / Prof. Dr. J. Käs	*Radiation assisted modification of gelatin and collagen for biomedical applications*
M.Sc. Biotech. Chiara Ruggirello	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Targeted tumor therapy by cell specific receptor internalisation*
M.Sc. Chem. Stefan Saretz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbarborane derivates for medical use*
M.Sc. Phys. Philipp Schiertz	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. Jan Schulz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Carborane-based frustrated lewis pairs for homogeneous catalysis*
M.Sc. Chem. Benedikt Schwarze	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Metal carborate complexes with bioactive ligands as organometallic anticancer agents*
M.Sc. Chem. Axel Straube	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Multi-ferrocene-based phosporus ligands for homogenous catalysis*
M.Sc. Phys. Marcel Wille	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Whispering gallery modes: influence of resonator shape on lasing properties*
M.Sc. Biochem. Philipp Wolf	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. T. Pompe	*Selective drug uptake via peptide-mediated internalization of the endothelin system*
M.Sc. Biochem. Dennis Worm	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	*Synthesis and biochemical evaluation of carbaborane - modified peptide ligands*
M.Sc. Nanoscience Muhammad Ayman Zaheer	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Studying of diffusion in reacting catalytic systems by means of NMR spectroscopic methods*
Dipl.-Math. Heinrich-Gregor Zirnstein	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Topological aspects of dirac Ffermions in condensed matter systems*

Alumni 2017

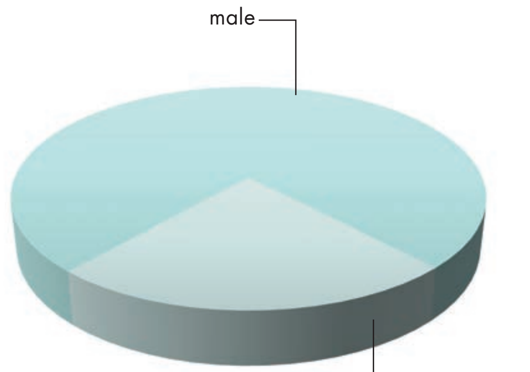
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Anup Kumar Adhikari	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Novel phosphorus-rich compounds - Ssynthesis and reactivity*
Dr. rer. nat. Alina Bischoff	Prof. Dr. S. Mayer / Prof. Dr. M. Grundmann	*Mechanische Charakterisierung freistehender Dünnschichten der magnetischen Formgedächtnislegierung* Fe_7Pd_3
Dr. rer. nat. Paul Cosmin Boar	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Novel copper(I) and silver(I) metallcycles with flexible bis-phospholane ligands: synthesis, characterisation and complexation studies of phospholane-containing bifunctional P,N ligands*
Dr. rer. nat. Florian Glasneck	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Tetrasubstituierte Calix[4]arene mit gemischten Donorgruppen als selektive Liganden für Seltenerdelemente*
Dr. rer. nat. André Heber	Prof. Dr. F. Cichos / Prof. Dr. M. Grundmann	*Application of single optically heated gold nanoparticles to sensing and actuation*
Dr. rer. nat. Reinhard Hoy	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Tridentate Phospholan-Liganden-Synthese und Koordinationsverhalten in Gold(I)-Komplexen*
Dr. rer. nat. Robert Kuhnert	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Synthese, Charakterisierung und biologische Eigenschaften carboranbasierter Lipoxygenaseinhibitoren*
Dr. rer. nat. Anja Landgraf	Prof. Dr. S. Mayer / Prof. Dr. Dr. hc. B. Rauschenbach	*Magnetische und mechanische Eigenschaftenvon epitaktischen Dünnschichten der magnetischen Formgedächtnislegierung Fe-Pd*
Dr. rer. nat. Daniel Thomas Splith	Prof. Dr. M. Grundmann/ Prof. Dr. S. Mayr	*Schottky-Kontakte auf ß-Galliumoxid- und Indiumoxid-Dünnfilmen: Optimierung der Probenstruktur und Modellierung der Diodenkennlinien*
Dr. rer. nat. Xinxing Sun	Prof. Dr. Dr. hc. B. Rauschenbach / Prof. Dr. S. Mayer	*Phase transformation and switching of chalcogenide phase change material films prepared by pulse laser deposition*
Dr. rer. nat. Martin Thunert	Prof. Dr. M. Grundmann / Prof. Dr. B. Rosenow	*Exciton-polaritons in ZnO-based Mmicroresonators: disorder influence and coherence properties*
Dr. rer. nat. Emilia Wisotzki	Prof. Dr. S. Mayer / Prof. Dr. J. Käs	*High energy electron irradiation of gelantin hydrogels: towards the development of a magnetically- driven bioactuator*

Statistics

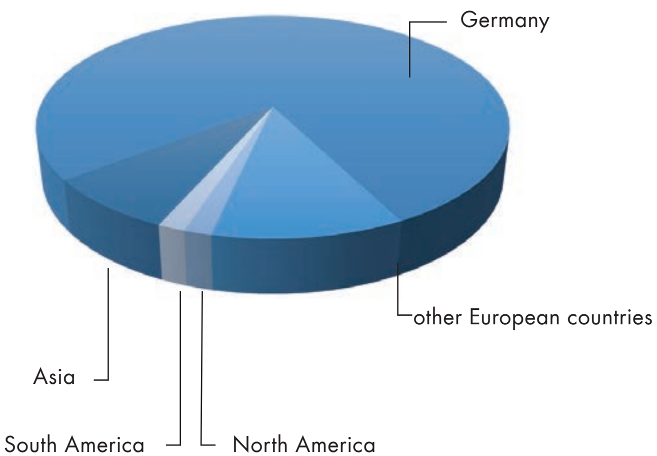
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:

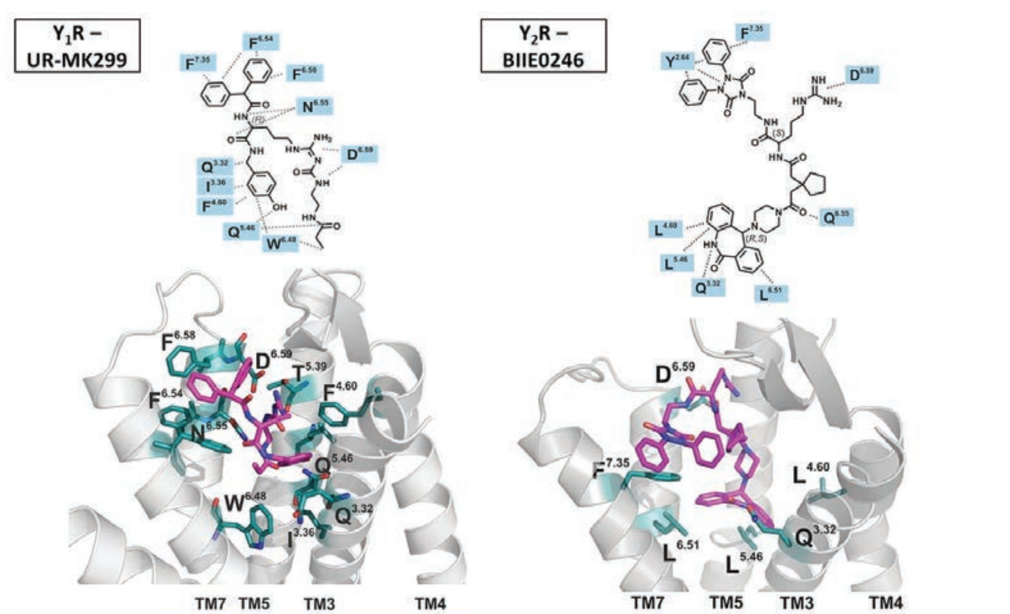


Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger
M.Sc. Chem. Milos Erak, M.Sc. Chem. Jan-Patrick Fischer, M.Sc. Biotech. Chiara Rugirello, 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 tumor 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 2017 Milos Erak and Tristan Zellmann finished their PhD. Wheras Milos worked successfully on the stabilisation of peptides, including small proteins like relaxin, Tristan successfully worked on the development of

small chemerin variants and performed extended molecular modelling of chemerin and the chemerin receptor as well as the neuropeptide Y receptors Y_1 and Y_2. He significantly contributed to the binding site of small antagonists at the Y_2 receptor.The field of chemical modification of peptides and proteins is pursued successfully. Jan-Patrick Fischer further explores the field of adrenomedullin and its interaction with its receptor system. He aims to stabilise different structural elements of the molecule and to evaluate their impact on the selectivity of these peptides. He developed a number of disulphide bond mimetics and tested them for stability and activity. Dennis Worm synthesised and evaluates carbaboranylated neuropeptide Y derivatives that eventually will serve as therapeutics within a boron neutron capture therapy regimen. In addition to neuropeptide Y he worked on ghrelin agonists and antagonists. Chiara Ruggirello joined the group as a DAAD-funded student and works on peptides coupled to nanoparticles. This combines in a unique way peptide synthesis with biomolecular surface approaches. In addition to current members, several papers of former BuildMona-members have been published, including Sylvia Els-Heindl, Cathleen Juhl, Ria Schönauer and Mareen Pagel. Work achieved during their PhD project was delayed in publication owing to collaborators. Maren Pagel was awarded with the Research Prize for Young Scientists by the Max Bergmann Society, which is one of the most prestigious awards in this field.



⇑ Comparison of the binding site of selective antagonists at the Y_1R (left, *Structural basis of ligand binding modes at the neuropeptide Y Y_1 receptor* Yang et al. / Nature (2018) **7702** 520 and Y_2R (right, *A deep hydrophobic binding cavity is the main interaction for different Y_2 R antagonists* Burkert et al. / ChemMedChem. (2017) **12** 75).

⇒ *Deep Hydrophobic Binding Cavity is the Main Interaction of Different Y_2R Antagonists*
K. Burkert, T. Zellmann, R. Meier, A. Kaiser, J. Stichel, J. Meiler, G. K. Mittapalli, E. Roberts, A. G. Beck-Sickinger / ChemMedChem. (2017) **12** 1

⇒ *Development of Potent and Metabolic Stable APJ Ligands with High Therapeutic Potential*
C. Juhl, S. Els-Heindl, R. Schönauer, G. Redlich, E. Haaf, F. Wunder, B. Riedl, N. Burkhardt, A. G. Beck-Sickinger, D. Bierer / ChemMedChem. (2017) **11** 21

⇒ *Functional Characterization, and Solid-State NMR Investigation of the G Protein-Coupled GHS Receptor in Bilayer Membranes*
S. Schrottke, A. Kaiser, G. Vortmeier, S. Els-Heindl, D. Worm, M. Bosse, P. Schmidt, H. A. Scheidt, A. G. Beck-Sickinger, D. Huster / Sci Rep. (2017) **7** 46128

⇒ *Development of Fluorinated Non-Peptidic Ghrelin Receptor Ligands for Potential Use in Molecular Imaging*
R. P. Moldovan, S. Els-Heindl, D. J. Worm, T. Kniess, M. Kluge, A. G. Beck-Sickinger, W. Deuther-Conrad, U. Krügel, P. Brust / Int. J. Mol. Sci. (2017) **18** 4

⇒ *Multifunctional biomaterial coatings: synthetic challenges and biological activity*
M. Pagel, A. G. Beck-Sickinger / Biol Chem. (2017) **398** 1

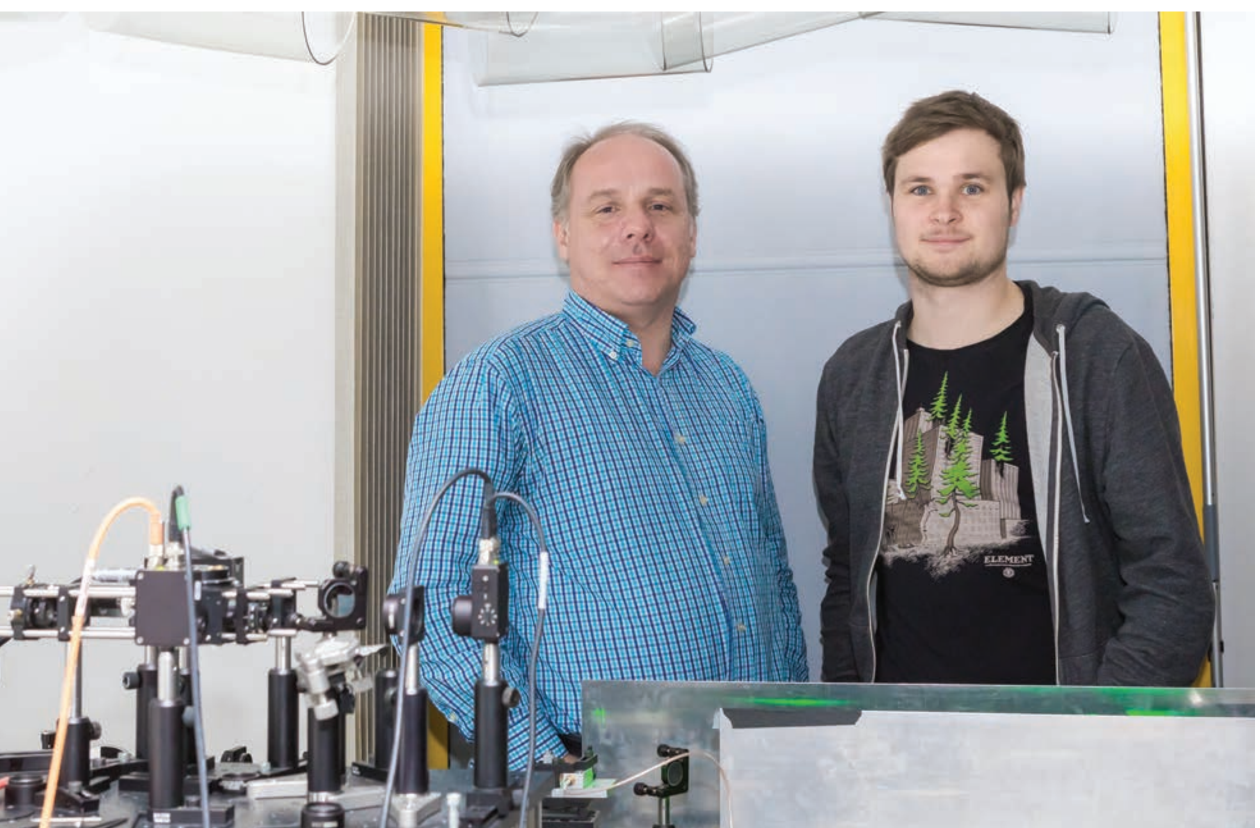
⇒ *Adrenomedullin – new perspectives of a potent peptide hormone*
R. Schönauer, S. Els-Heindl, A. G. Beck-Sickinger / J Pept Sci. (2017) **23** 7

Prof. Dr. Annette G. Beck-Sickinger
Bioorganic Chemistry and Biochemistry
Institute of Biochemistry
http://www.biochemie.uni-leipzig.de/agbs/
E-mail: abeck-sickinger@uni-leipzig.de
Phone: +49 341 97-36900
Fax: +49 341 97-36909

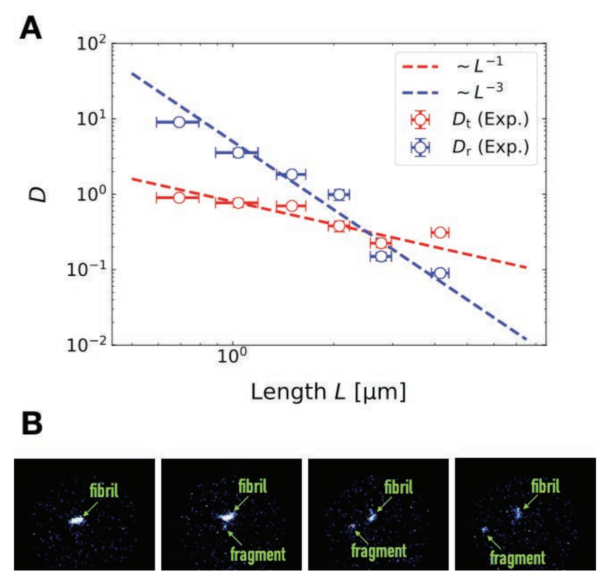
Thermophoretic trapping of single amyloid fibrils

Prof. Dr. Frank Cichos
M.Sc. Phys. Martin Fränzl, M.Sc. Phys. André Heber

The aggregation of soluble proteins into highly ordered, insoluble amyloid fibrils is characteristic for a range of neurodegenerative disorders. At present, no effective medical treatment for these diseases is known. This can be attributed, at least in part, to an insufficient fundamental understanding of the mechanism of aggregation as well as the incomplete characterization of the fibril formation process from mon-omers to oligomers to protofibrils to fibrils, the interactions between aggregates, and the specificities of the various nucleation events. Some recent experiments suggest that amyloid growth involves not only primary nucleation, but various forms of secondary nucleation that enable multiple fibrils to be generated from a single primary nucleation event. However, the microscopic mechanisms that govern such pathways of fibril formation are far from being understood mainly because of a lack of experimental techniques that are capable of disentangling the experimental heterogeneity of fibril growth.



molecules in solutions for extended time periods. This technique is based on a drift of molecules in temperature gradients. These temperature gradients are generated optically by illuminating chrome ring structures of about 10 µm in diameter. The resulting temperature field provides local minima in which molecules and other nano-objects can be stored. Using this type of thermophoretic trapping we are able to confine single Aß40 fibrils for time periods of several 10 minutes. The observation of the fibrillar dynamics is only limited by photo-bleaching of dye molecules intercalating the fibril structure. Using an intermittent probe we have even extended the observation period to more than 2 hours. With the help of the data collected on the motion of single fibrils during these time periods, we are able to characterise the growth of fibrils with the help of the rotational diffusion. With the strong length dependence of the rotational diffusion coefficient we have measured a growth of a few 10 nanometers over a time period of 20 minutes. We have also identified for the first time a break up of an $Aß_{40}$ fibril, which has been suspected to be one of the secondary nucleation processes.



A) Length dependence of the rotational and translational diffusion coefficient together with the theoretical predictions (dashed lines). **B)** Sequence of snapshots (false color) of a single fibril which breaks apart into two pieces. The scale bar in the image is 3 µm.

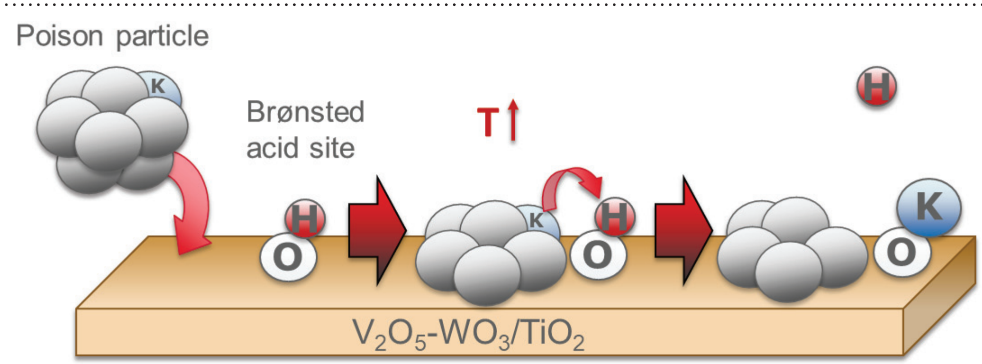
⇒ *Thermal Diffusivities Studied by Single-Particle Photothermal Deflection*
A. Heber, M. Selmke, F. Cichos / ACS Photonics (2017) **4** 681

Prof. Dr. Frank Cichos
Peter Debye Institute for Soft Matter Physics
https://home.uni-leipzig.de/~physik/sites/mona/
E-mail: cichos@physik.uni-leipzig.de
Phone: +49 341 97-32571
Fax: +49 341 97-32598

Novel catalytic systems by nano-scale design

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

Current challenges in heterogeneous catalysis are, among others, the fluctuating feed streams resulting in high demands towards catalyst stability and mass transfer. Innovative nanostructured catalysts with defined porosity on the nanometer scale and tunable active components continue to play a key role for the solution of these challenges. Following the principle approaches of the graduate school, the research in our group is focused on the nano-scale design of materials and their use as catalysts and catalyst supports. In this respect, we investigate hierarchical large-pore mesoporous silicates (LPMS) as carriers for the selective immobilization of multi-enzyme conjugates applied in co-factor regeneration or in cascade reactions. The main challenges include the interconnectivity between the two pore systems. This is crucial for the active sites of the co-immobilized enzymes to be accessible, and, therefore, to achieve high overall activity of the multifunctional biocatalysts. Another research area focuses on catalyst stability and deactivation due to poison deposits present in trace amounts as typical for the selective catalytic reduction of nitrogen oxides in off-gas streams. Brønsted acid sites play a key role for catalytic activity. Alkali metal ions present in nano-sized poison particles loosely attached to the catalyst surface can react with the Brønsted acid sites and lead to irreversible deactivation. Molecular transport processes on the nano-scale is addressed using in-situ and in-operando investigations during the course of catalytic reactions in partially miscible liquid mixtures. Xenon gas, solvated in the reacting mixture, serves as an atomic nano-sensor, along with multinuclear NMR spectroscopy. In addition, molecular transport processes are investigated inside the nanometer-scale pore system of hierarchically structured catalysts.



⇑ Schematic representation of the deactivation of Brønsted acid sites on V_2O_5-WO_3/TiO_2 catalysts for selective catalytic reduction of nitrogen oxides. Poison particles from the gas phase attach loosely to the catalyst surface. High Temperatures favor the reaction of alkali metals from poison particles with Brønsted acid sites leading to unwanted neutralisation.

⇒ *Active Ceria-Calcium Oxide Catalysts for Dimethyl Carbonate Synthesis by Conversion of CO_2*
P. Kumar, V.C. Srivastava, R. Gläser, P. With, I.M. Mishra / Powder Technol. (2017) **309** 13-21

⇒ *Efficient ceria-zirconium oxide catalyst for carbon dioxide conversions: Characterization, catalytic activity and thermodynamic study*
P. Kumar, P. With, V.C. Srivastava, R. Gläser, I.M. Mishra / J Alloy Compd (2017) **309** 718-726

⇒ *In Situ and In Operando Characterization of Mixing Dynamics in Liquid-Phase Reactions by ^{129}Xe NMR Spectroscopy*
M.A. Zaheer, J.C. Zill, J. Matysik, R. Gläser, M. Dvoyashkin / ChemPhysChem. (2017) **18** 1513-1516

⇒ *A Series of Robust Copper-Based Triazolyl Isophthalate MOFs: Impact of Linker Functionalization on Gas Sorption and Catalytic Activity*
U. Junghans, M. Kobalz, O. Erhart, H. Preißler, J. Lincke, J. Möllmer, H. Krautscheid, R. Gläser / Materials (2017) **10** 4 338-355

⇒ *Influence of Soot on Ammonia Adsorption and Catalytic $DeNO_x$-Properties of Diesel Particulate Filters Coated with SCR-Catalysts*
M. Purfürst, S. Naumov, K.-J. Langeheinecke, R. Gläser / Chemical Engineering Science (2017) **168**, 423-436

Prof. Dr. Roger Gläser
Institute of Chemical Technology and
Institute of Non-Classical Chemistry
http://techni.chemie.uni-leipzig.de
E-mail: roger.glaeser@uni-leipzig.de
Phone: +49 341 97-36301
Fax: +49 341 97-36349

Copper iodide - very transparent with many holes and no holes at the same time

Prof. Dr. Marius Grundmann
M.Sc. Phys. Max Kneiß, M.Sc. Phys. Marcel Wille, M.Sc. Phys. Lukas Trefflich, M.Sc. Phys. Peter Schlupp

Copper iodide is the transparent p-type conductor that has the best figure of merit, i.e. the largest conductivity at the highest transparency (Fig. 1a). This is due to the fact that is has many holes in the sense of defect electrons, the positive charge carriers in the valence band of a semiconductor. At the same time the sputtered thin films fabricated in the Semiconductor Physics Group have no holes, i.e. they are compact and cover the substrate completely.

BuildMoNa doctoral candidate Max Kneiß has investigated the conductivity of CuI thin films in detail and has proposed a model that explains the conductivity as a function of carrier density and temperature. Typically, the films exhibit unexpectedly high hole mobilities in the range of 10 cm² V^{-1} s^{-1} even when heavily textured, i.e. in the presence of many grain boundaries. The temperature-dependent resistivity of the textured (111)-oriented films with different carrier concentration are fitted using the fluctuation-induced tunneling conductivity (FITC) model in series with a power law. The FITC model describes barriers at the grain boundaries whereas the power law considers the scattering in the metallic interior of the grains. An n-type inversion layer or a defect band at the interfaces of the grains as origin of a 2D carrier system and the barriers at the grain boundaries is proposed (Fig. 2). This leads to a conclusive description of the electrical transport properties of zincblende-type CuI thin films and explains the high hole mobilities which are due to a suppressed backscattering at the grain boundaries in the presence of tunneling channels [R1].

In [R2] the superior performance of CuI as transparent p-type thermoelectric material was reported. The figure of merit (ZT-value at room temperature) of CuI is compared to other materials in Fig. 1b and clearly outstanding.

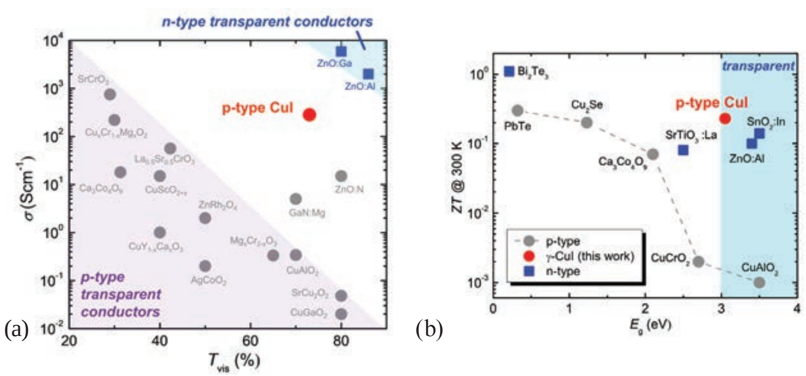


Fig. 1: (a) Conductivity of various reported p-type compounds (circles) vs. their optical transparency. Two n-type TCO's are shown for comparison (squares). (b) ZT-value vs. band gap for various p-type thermoelectric materials (circles). A few n-type thermoelectric materials are shown for comparison (squares). The dashed line is guide to the eyes.

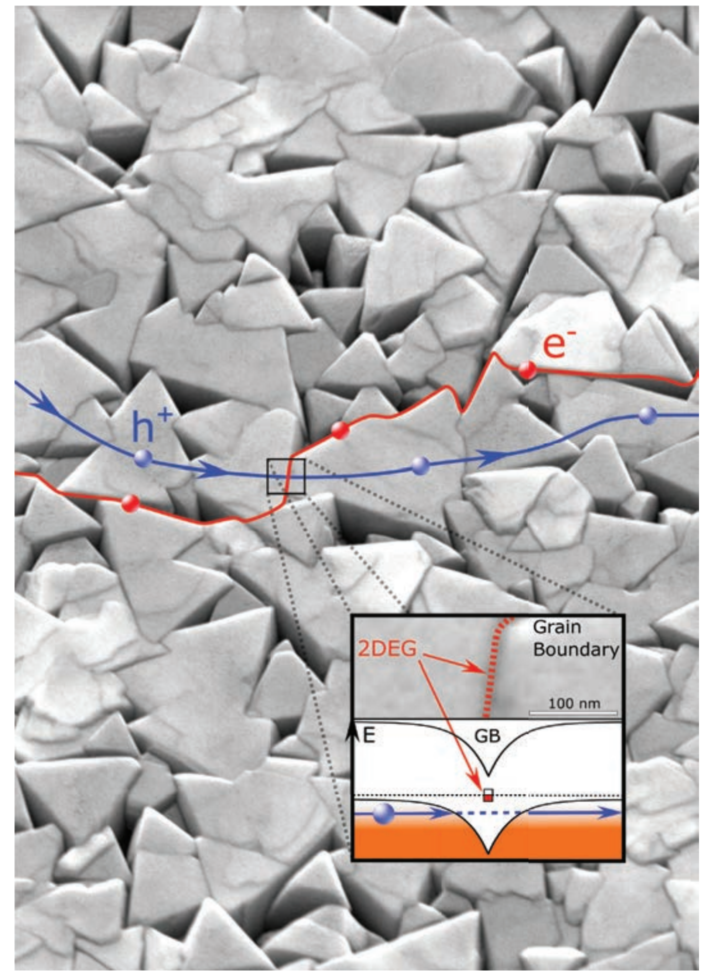


Fig. 2: Secondary electron microscopy image of (111)-oriented CuI thin film with schematic path of a hole (h) and the electron-charged interface between different grains. The inset shows the potential at the grain boundary

The BuildMoNa chemistry-physics cooperation has yielded nice results on CuI nanowires. These have been made with a chemical transport method and their optical properties have been investigated by BuildMoNa doctoral candidates Marcel Wille and Lukas Trefflich. Using optical excitation, lasing on whispering gallery modes could be stimulated up to a temperature of 200 K [R3]. The analysis of the optical modes correlates their energy with the geometrical shape/cross section of the wires. In addition also the dynamics of emission were investigated using time-resolved luminescence methods. Marcel Wille has also investigated nanowires that can be tuned with mechanical stress [R4, R5]. In [R4] it was found that the shift of band gap with mechanical strain has a non-linear component clearly resolved for strain above about 2% in ZnO nanowires. Reversely, in [R5] mechanical stress was used for tuning of the emission wavelength of nanowire lasers from CdS.

Other results of our BuildMoNa doctoral candidates concern the understanding of amorphous oxide semiconductors [R6] and devices based on them [R7].

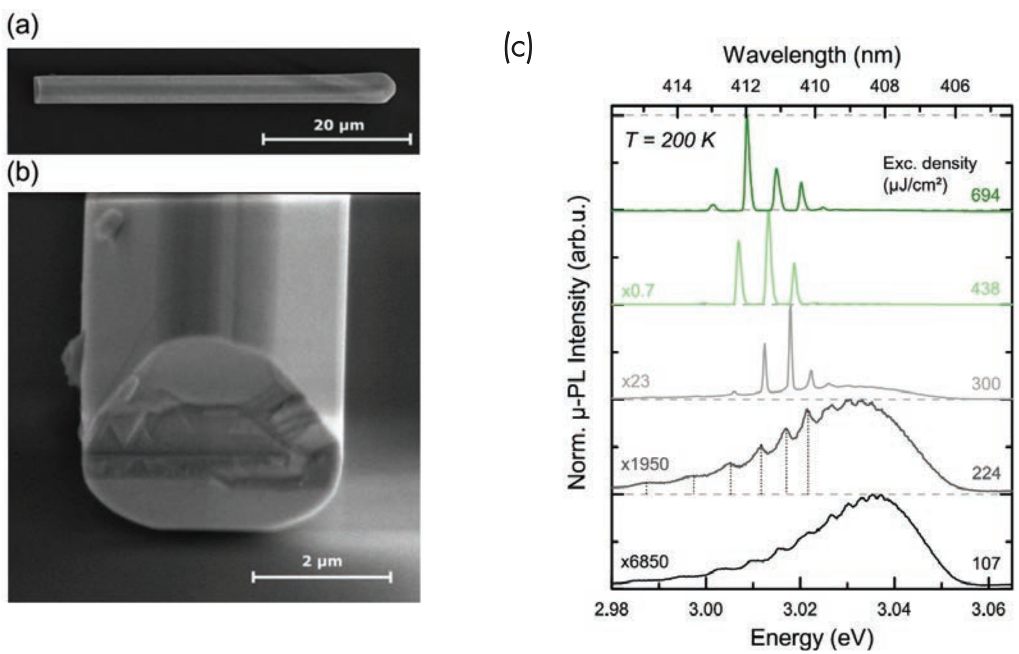


Fig. 3: (a, b) Scanning electron microscopy images of CuI nanowire. (c) Emission spectra at T=200 K for different excitation densities; laser emission is observed in the form of sharp modes.

⇒[R1] *Suppression of grain boundary scattering in p-type transparent γ-CuI thin films due to interface tunneling currents*
M. Kneiß, C. Yang, J. Barzola-Quiquia, G. Benndorf, H. von Wenckstern, P. Esquinazi, M. Lorenz, M. Grundmann / Adv. Mater. Interf. (2018) **5** 1701411 11-12

⇒[R2] *Transparent Flexible Thermoelectric Material Based on Non-toxic Earth-Abundant p-Type Copper Iodide Thin Film*
C. Yang, D. Souchay, M. Kneiß, M. Bogner, H. M. Wei, M. Lorenz, O. Oeckler, G. Benstetter, Y.Q. Fu, M. Grundmann / Nature Commun. (2017) **8** 16076

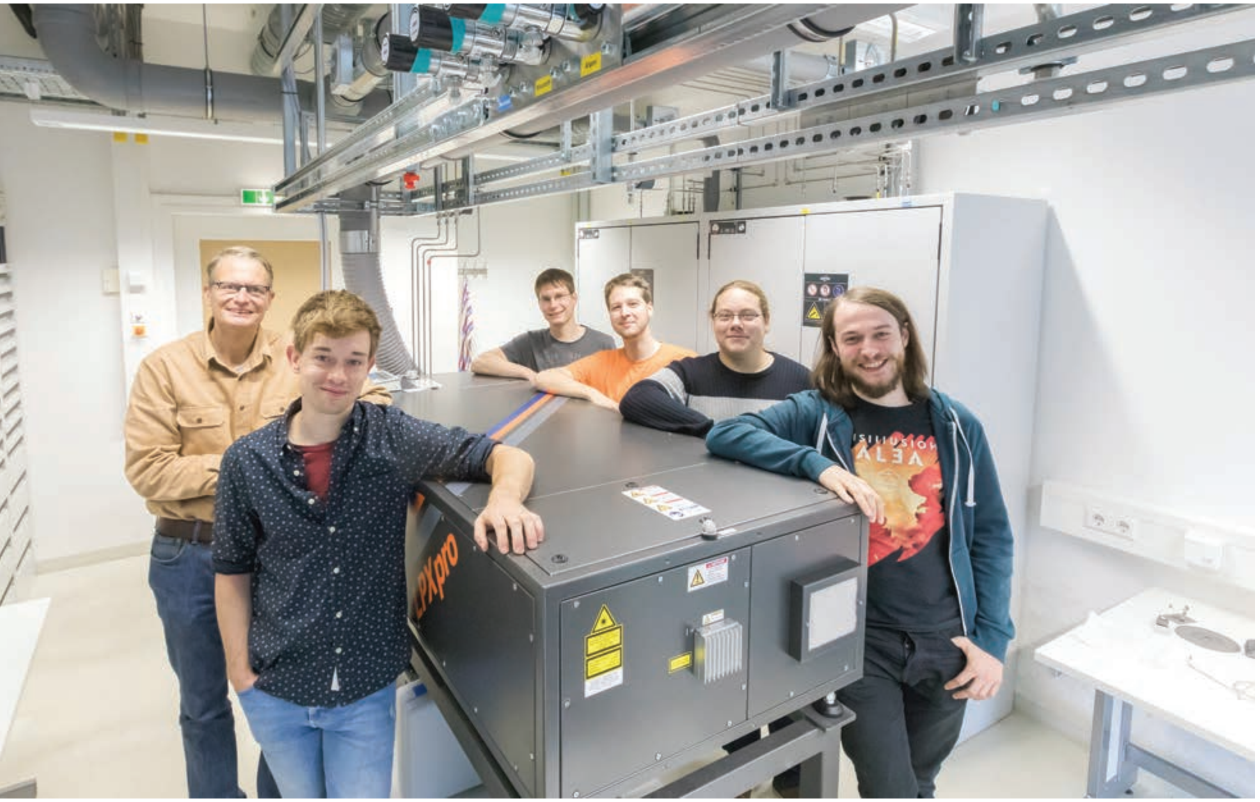
⇒[R3] *Lasing in cuprous iodide microwires*
M. Wille, E. Krüger, S. Blaurock, V. Zviagin, R. Deichsel, G. Benndorf, L. Trefflich, V. Gottschalch, H. Krautscheid, R. Schmidt-Grund, M. Grundmann / Appl. Phys. Lett. (2017) **111** 3 031105

⇒[R4] *Non-linear optical deformation potentials in uniaxially strained ZnO microwires*
C. Sturm, M. Wille, J. Lenzner, S. Khujanov, M. Grundmann / Appl. Phys. Lett. (2017) **110** 062103

⇒[R5] *Dynamical Tuning of Nanowire Lasing Spectra*
M. Zapf, R. Röder, K. Winkler, L. Kaden, J. Greil, M. Wille, M. Grundmann, R. Schmidt-Grund, A. Lugstein, C. Ronning / Dynamical Tuning of Nanowire Lasing Spectra, Nano Lett. (2017) **17** 11 6637-6643

⇒[R6] *The Vital Role of Oxygen for the Formation of Highly Rectifying Schottky Barrier Diodes on Amorphous Zinc-Tin-Oxide with Various Cation Composition*
S. Bitter, P. Schlupp, H. von Wenckstern, M. Grundmann / ACS Appl. Mater. Interfaces (2017) **9** 31 26574-26581

⇒[R7] *Schottky barrier diodes based on room temperature fabricated amorphous zinc tin oxide thin film*
P. Schlupp, H. von Wenckstern, M. Grundmann / Phys. stat. sol. (a) (2017) **214** 10 1700210



Prof. Dr. Marius Grundmann
Felix-Bloch-Institut für Festkörperphysik
http://research.uni-leipzig.de/hlp/
E-mail: grundmann@physik.uni-leipzig.de
Phone: +49 341 97-32650
Fax: +49 341 97-32668

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

Prof. Dr. Evamarie Hey-Hawkins
Dr. Anup Kumar Adhikari, M.Sc. Chem. Angela Aleksovska, Dr. Paul Cosmin Boar, M.Sc. Chem. Antonio Buzharevski, M.Sc. Chem. Peter Coburger, M.Sc. Chem. Marta Gozzi, M. Sc. Chem. Toni Grell, Dr. Reinhard Hoy, Dr. Robert Kuhnert, M.Sc Chem. David Langer, M.Sc. Chem. John Popp, M.Sc. Mater. Sci. Eng. Rafaella Lima de Meneses Precker, M.Sc. Chem. Stefan Saretz, M.Sc. Chem. Jan Schulz, M.Sc. Chem. Benedikt Schwarze, M.Sc. Chem. Axel Straube

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

Smart Catalysts

Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups (ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way ”switchable“ phosphines for catalytic applications (J. Popp). A new approach includes C_3-symmetric (A. Straube) and carborane-based (P. Coburger) phosphine ligands (Fig. 1).

Another approach focusses on the use of selective phosphorus-based macrocycles, nano-frames (P. C. Boar, R. Hoy), containers, or cavities (photoactive linkers) in metal-organic frameworks (MOFs) with well-defined structure and porosity (A. Aleksovska). 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.

Last but not least, complexes containing two different catalytic metal centres can offer exciting chemical and physical properties which can be used in catalysis. The key to designing these “heterobimetallic” complexes is the synthesis of a ligand with distinct coordination sites able to bind suitable metal ions. With such a ligand, and the wide range of metal ions available, the construction of different heterobimetallic complexes is limited only by one’s imagination (D. Langer)

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 (Fig. 2) or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of functionalised building blocks for organometallic or phosphorus-based polymers are: strained phosphorus-based rings (T. Grell, P. Coburger), alkylene- and arylene-bridged bis(phospholanes) (P. C. Boar, R. Hoy) or (planar-chiral) ferrocene derivatives (A. Straube) and bis-, tri- and tetrakis-carboxylates of conjugated aromatic systems as ligands in optically active coordination polymers or MOFs (A. Aleksovska).

Molecular precursors: Binary metal phosphides MP_x often exhibit interesting optical, electronic and magnetic properties and thus have a wide range of applications, such as corrosion resistors, catalysts, semiconductors, electrode materials in lithium-ion batteries, etc. We have developed an approach to this class of compounds starting with volatile phosphorus-rich metal complexes (A. K. Adhikari, T. Grell) as molecular precursors.

Inorganic Building Blocks in Medicinal Chemistry

Carboranes are highly hydrophobic and extremely stable icosahedral carbon-containing boron clusters. The cage framework of these clusters can easily be modified with a variety of substituents, both at the carbon and at the boron atoms and can either be used as pharmacophoric entities in cyclooxygenase (COX) (S. Saretz, A. Buzharevski) or lipoxygenase inhibitors (LOX) (R. Kuhnert) (Fig. 3) or for boron neutron capture therapy (BNCT) as conjugates with tumour-targeting entities, such as a Y_1-receptor-selective neuropeptide Y (NPY) derivative (S. Saretz, R. Kuhnert).

Chemotherapy using platinum-based anti-tumour agents, such as cisplatin, is often associated with strong side effects and is further limited by resistance of tumour cells. Therefore. specific MOFs with large cavities are being studied for targeted drug delivery (R. Precker). Furthermore, to increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. tamoxifen (B. Schwarze)). A new approach utilises the nido cluster (carbollide, $[C_2B_9H_{11}]^{2-}$ (which is isolobal to cyclopentadienide) as ligand in metal complexes that exhibit anticancer properties (M. Gozzi, B. Schwarze).

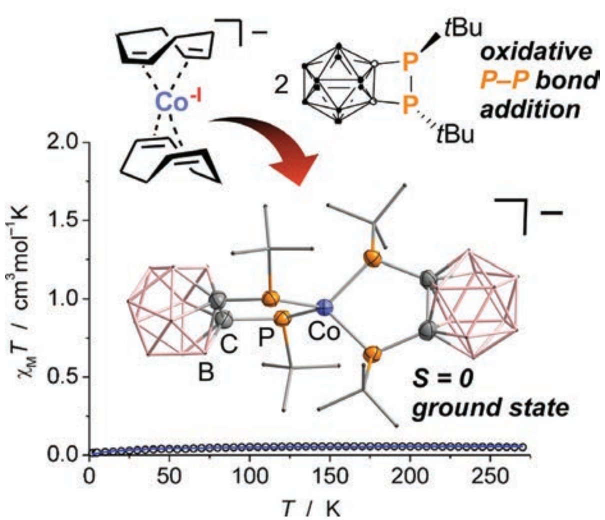
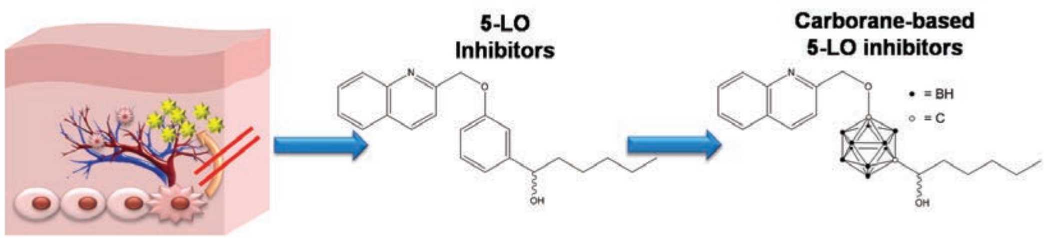


Fig. 1. The first homoleptic cobalt phosphanido complex is formed via consecutive oxidative additions of P–P bonds to cobalt(–I). X-ray crystallography and magnetic measurements show that this new cobalt(III) compound is a rare example of a tetrahedral complex with a low-spin ground state.

Fig. 2. Diastereomerically pure planar-chiral secondary ferrocenylphosphanes derived from Ugi’s amine are of interest as chiral ligands for metal complexes in asymmetric catalysis, and the corresponding phosphino borane derivatives could be suitable precursors for the synthesis of chiral P–B polymers by dehydrocoupling.



⇑ Fig. 3. The progression of cancer is accelerated by processes that are mediated by leukotrienes. Several cancer cell lines overexpress 5-lipoxygenase, which converts arachidonic acid to leukotrienes. The introduction of carboranes as highly hydrophobic and metabolically stable pharmacophores in Rev-5901 generates the first carborane-based inhibitor of the 5-lipoxygenase pathway.

⇒ *Planar-chiral secondary ferrocenyl phosphanes*
S. Pandey, M. B. Sárosi, P. Lönnecke, E. Hey-Hawkins / invited contribution to special issue on "The Multifaceted Chemistry of Ferrocene", Eur. J. Inorg. Chem. (2017) 256-262 Back cover

⇒ *C_2-Symmetric P,N Ligands Derived from Carborane-Based Diphosphetanes: Synthesis and Coordination Chemistry*
P. Coburger, J. Schulz, J. Klose, B. Schwarze, M. B. Sárosi, E. Hey-Hawkins / Inorg. Chem. (2017) **56** 292–304

⇒ *A Sixteen-Membered Au_8P_8 Macrocycle Based on Gold(I) and Diphospha(III)guanidine*
A. K. Adhikari, M. B. Sárosi, T. Grell, P. Lönnecke / E. Hey-Hawkins Angew. Chem. (2017) **129** 4120-4123
Angew. Chem. Int. Ed. 56 (2017) 4061-4064

⇒ *Carboranes as Aryl Mimetics in Catalysis: a Highly Active Zwitterionic NHC Precatalyst*
S. Selg, W. Neumann, P. Lönnecke, E. Hey-Hawkins, K. Zeitler / Chem. Eur. J. (2017) **23** 7932-7937 Front cover

⇒ *CarbORev-5901: The first carborane-based inhibitor of the 5-lipoxygenase pathway*
R. Kuhnert, M.-B. Sárosi, S. George, P. Lönnecke, B. Hofmann, D. Steinhilber, B. Murganic, S. Mijatovic, D. Maksimovic-Ivanic, E. Hey-Hawkins / ChemMedChem (2017) **12** 1081-1086

⇒ *Molecular modeling of the interactions between the carborane-containing analogs of indomethacin and cyclooxygenase-2*
M.-B. Sárosi, W. Neumann, T. P. Lybrand, E. Hey-Hawkins / J. Chem. Inf. Model. (2017) **57** 2056-2067

⇒ *Antiproliferative activity of (η^6-arene)-ruthenacarborane sandwich complexes against HCT116 and MCF7 cell lines*
M. Gozzi, B. Schwarze, M.-B. Sárosi, P. Lönnecke, D. Drača, D. Maksimović-Ivanić, S. Mijatović, E. Hey-Hawkins / Dalton Trans. (2017) **46** 12067-12080

⇒ *Copper(I) Complexes with a Flexible Bis-phospholane Ligand. Route to Paddle Wheel- and Box-type Macrocycles*
P. Boar, M. Streitberger, P. Lönnecke, E. Hey-Hawkins / Inorg. Chem. (2017) **56** 7285-7291

⇒ *Basicity of N-(tetramesityltetraphosphacyclopentylidene)cyclohexylamine – an Unusual Diphospha(III)-guanidine Derivative*
A. K. Adhikari, T. Grell, P. Lönnecke, E. Hey-Hawkins / Eur. J. Inorg. Chem. (2017) 5329-5333 Front coverCover Profile: Eur. J. Inorg. Chem. (2017) 5328

⇒ *Chiral Rhodium(I) Complexes of 1,2-Bis(chloroalkoxyphosphanyl)- and Bis(amidoalkoxyphosphanyl)-1,2-dicarba-closo-dodecaboranes(12)*
S. Bauer, I. Maulana, P. Coburger, S. Tschirschwitz, P. Lönnecke, M. B. Sárosi, R. Frank, E. Hey-Hawkins / ChemistrySelect (2017) **2** 7407-7416

⇒ *Oxidative P–P Bond Addition to Cobalt(–I): Formation of a Low Spin Cobalt(III) Phosphanido Complex*
P. Coburger, S. Demeshko, C. Rödl, E. Hey-Hawkins, R. Wolf / Angew. Chem. Int. Ed. (2017) **56** 15871-15875

⇒ *Oxidative P-P-Bindungsaddition an Cobalt(–I): Bildung eines low-spin-Cobalt(III)- Phosphanidokomplexes*
P. Coburger, S. Demeshko, C. Rödl, E. Hey-Hawkins / R. Wolf, Angew. Chem. (2017) **129** 16087-16091

Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins
Institute of Inorganic Chemistry
http://research.uni-leipzig.de/hh
E-mail: hey@rz.uni-leipzig.de
Phone: +49 341 97-36151
Fax: +49 341 97-39319

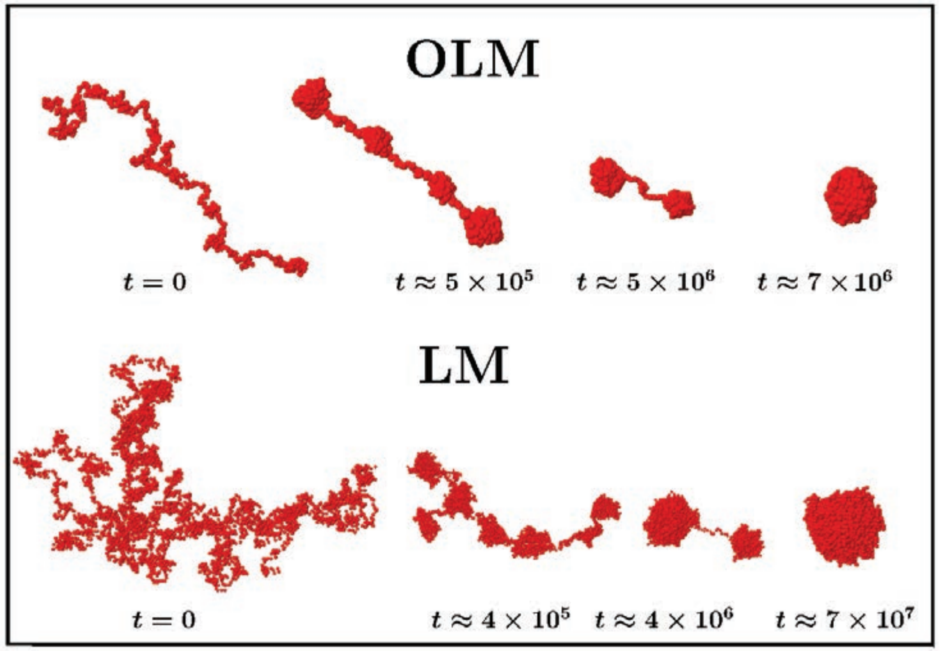
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
Dipl.-Phys. Martin Marenz, M.Sc. Johannes Bock, M.Sc. Phys. Philipp Schierz, M.Sc. Henrik Christiansen

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

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

(ii) Johannes Bock focuses on the intriguing properties of semiflexible polymers and proteins in quenched, disordered environments ("crowded cell problem") and thereby continues the work of a previous BuildMoNa PhD student (Sebastian Schoebl) by extending it from the hitherto considered two-dimensional to the three-dimensional case, subject to additional confinement constraints. One main objective is to investigate by



⇑ Time evolution snapshots of the coarsening dynamics of a polymer, after being quenched from the extended random-coil phase into the globular phase at a temperature well below the collapse transition. The upper row shows results from simulations of an off-lattice model (OLM) and the lower row those from a lattice model (LM).

means of a “breadth-first” chain-growth algorithm to what extent the disorder can be effectively described by a “renormalized” bending stiffness of the macromolecules.

(iii) Philipp Schierz aimed at efficient computer simulations of polymer systems. To this end he investigated the advantages of computations performed on powerful general purpose graphics processing units (GPGPUs) over the use of standard CPUs and carefully compared the performances of MD and MC implementations for this class of problems. In particular he considered the microcanonical ensemble and showed how conservation laws can be properly treated in MD and related to each other and to MC by reweighting techniques. This turns out to be very important for small systems at the nanoscale. Subsequently he investigated MC computer simulations in the so-called “real” microcanonical ensemble which, with a few further developments, promises to become a competitive alternative to generalized ensemble methods in the future.

(iv) Henrik Christiansen employs MC methods for studying coarsening and aging phenomena of polymers. Using a random-coil conformation as the starting point and then suddenly quenching the temperature below the collapse transition of the polymer, the temporal evolution and the emerging coarsening of the polymer morphology are recorded. The aging behavior can be investigated by analysing related two-time correlation functions. The main goal is to elucidate the dynamic scaling laws governing the polymer kinetics.

⇒ *Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation*
J. Zierenberg, P. Schierz, W. Janke / Nature Communications (2017) **8** 14546-1-7

⇒ *Scaling Laws for Random Walks in Long-Range Correlated Disordered Media*
N. Fricke, J. Zierenberg, M. Marenz, F.-P. Spitzner, V. Blavatska, W. Janke / Condensed Matter Physics (2017) **20** 13004-1-11

⇒ *Coarsening and Aging of Lattice Polymers: Influence of Bond Fluctuations*
H. Christiansen, S. Majumder, W. Janke / Journal of Chemical Physics (2017) **147** 094902-1-12

⇒ *Generalized Ensemble Computer Simulations for Structure Formation of Semiflexible Polymers*
W. Janke, M. Marenz, J. Zierenberg / Lobachevskii Journal of Mathematics (2017) **38** 978-985

⇒ *Transition Barrier at a First-Order Phase Transition in the Canonical and Microcanonical Ensemble*
W. Janke, P. Schierz, J. Zierenberg / Journal of Physics: Conference Series (2017) **921** 012018-1-5

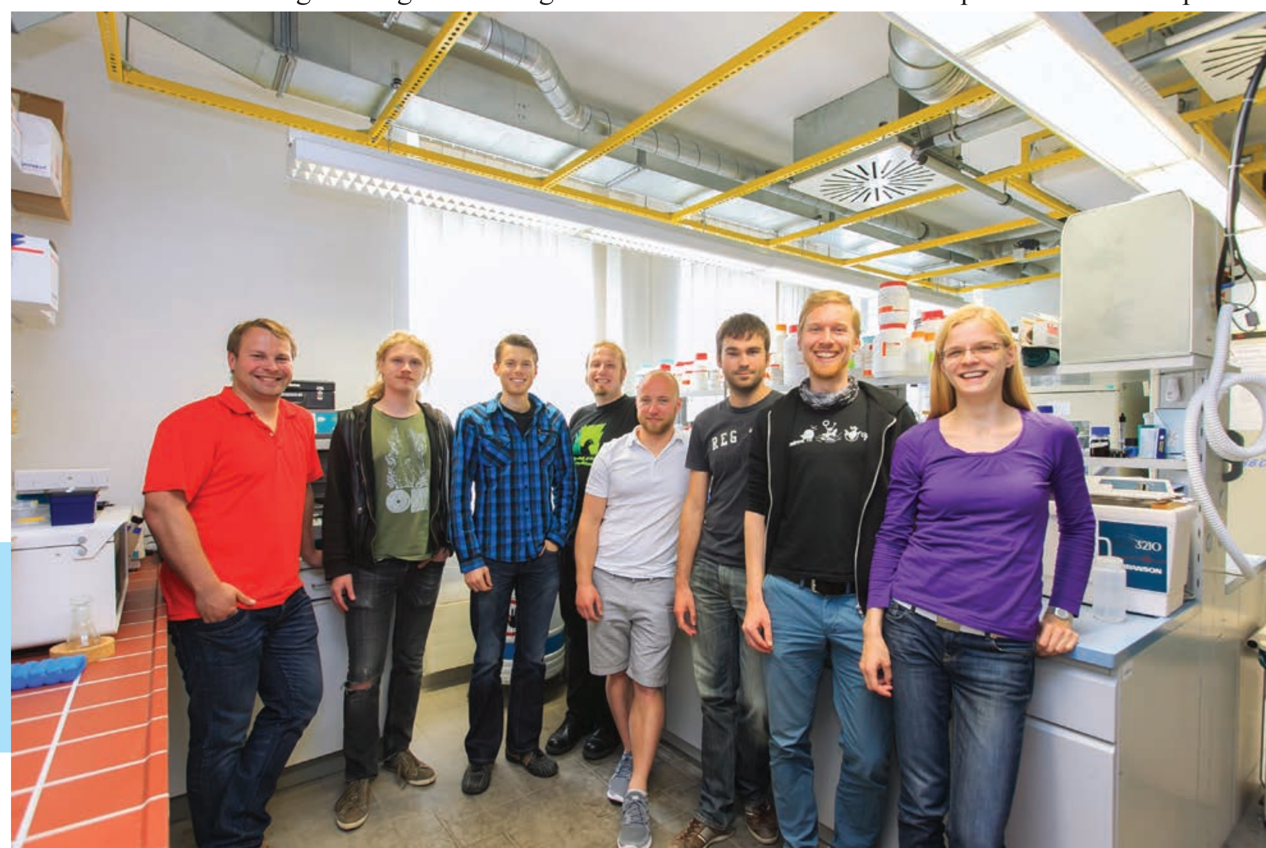
⇒ *Percolation Thresholds and Fractal Dimensions for Square and Cubic Lattices with Long-Range Correlated Defects*
J. Zierenberg, N. Fricke, M. Marenz, F.P. Spitzner, V. Blavatska, W. Janke / Physical Review E (2017) **96** 062125-1-11

Prof. Dr. Wolfhard Janke
Institute for Theoretical Physics
http://www.physik.uni-leipzig.de/index.php?id=cqt
E-mail: janke@itp.uni-leipzig.de
Phone: +49 341 97-32725
Fax: +49 341 97-32548

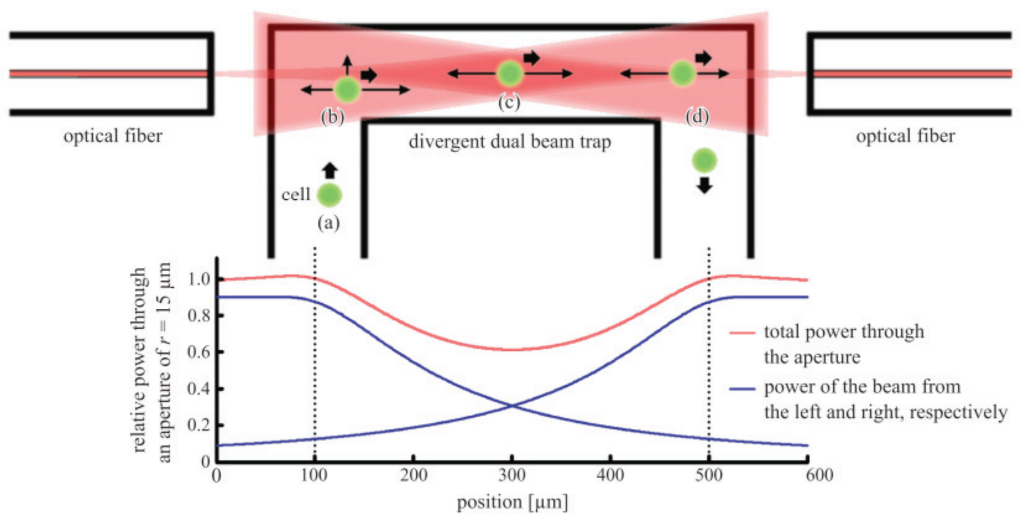
Optical stretching in continuous flows

Prof. Dr. Josef Alfons Käs
M.Sc. Phys. Martin Glaser, M.Sc. Phys. Tom Golde, Dipl.-Phys. Tina Händler,
M.Sc. Phys. Jürgen Lippoldt, M.Sc. Phys. Erik Morawetz

The large majority of tumor diseases become live threatening, once cells start to invade the surrounding tissue. A lot of biochemical triggers that enable a cancerous cell to leave the primary tumor are well explored. and the exact physical requirements are still to be pinpointed. One of the most fundamental and first steps of a malignant transformation in carcinomas is the epithelial to mesenchymal transition (EMT). We investigate the biomechanical change cells undergo in the early EMT by microrheological measurements of living cells, since the fundamental mechanical parameters of cells are known to be altered during the malignant transformation.
Cell rheology with a sensitivity for biochemical markers has developed an increasing need for high throughput measurements. We present the ‘in flow optical stretcher’ (IFOS), a concept of non-invasive optical cytometry capable of high throughput rates, while working in a regime of long measurement times and low frequencies. The setup



deforms whole cells in a continuous flow by optical forces, bypassing steps of cell positioning that are unavoidable in state-of-the-art optical stretcher devices. In a proof of premise experiment, we show that in the IFOS it is possible to deform cells of mammalian origin which have been treated with cytochalasin. All recorded successful experiments took place in less than 2 s each, as opposed to 10–20 s in state-of-the-art optical stretcher devices. Although other microfluidic rheology devices achieve significantly higher throughput rates, they operate in different frequency regimes and probe different mechanical responses. The IFOS still captures viscoelastic properties and active responses of cells while aiming to maximize the throughput at creep times on the order of seconds. It can be assumed that an automatic IFOS reaches a throughput an order of magnitude higher than current devices that are based on optical stretching for cell rheology [1].
Additionally, the Optical Strecher allows for fluorescent staining of epithelial cadherin (E-Cad) in the measured cells, giving an individualized correlation between progress of the EMT and single cell mechanical behavior. By evaluating not only fluorescence



⇑ Principle of the 'in flow optical stretcher': instead of a trap perpendicular to the flow direction of the cells, the flow path is aligned with the propagation path of the Gaussian beams. Thick arrows indicate flow direction; the thin arrows indicate optical forces acting on each single cell. (a) A cell moves towards the optical trap and is centered by fluidic forces. (b) The cell enters the dual beam trap. (c) Subsequently, the cell moves along the flow path while being trapped and exposed to stretching forces. (d) The cell leaves the trap, and the stretching process is finished. The graph below displays the power exerted on a cell of r = 15 µm when moving through the chamber. Values are normalized to the total power passing through the aperture at the points where cells enter or exit the dual beam trap (indicated as dotted lines), respectively.

intensity, but also the clustering of E-Cad on the cell surface, we are able to show that a deactivation and mobilization of E-Cad in the cell membrane is coupled to a softening of the cell body, which is strongly related to increased invasive behavior. These results suggest that E-Cad might be an upstream regulator of cancerous behavior, and its downregulation the very first step towards the physical enabling of cancerous cells to invade the surrounding stroma.

⇒ *Optical stretching in continuous flows*
E. W. Morawetz, R. Stange, T. R. Kießling, J. Schnauß, J. A. Käs/ Convergent Science Physical Oncology (2017) **3** 2 19212

⇒ *DNA Nanotubes as a Versatile Tool to Study Semiflexible Polymers*
J. Schnauß, M. Glaser, J. S. Lorenz, C. Schuldt, C. Möser, M. Sajfutinow, T. Händler, J.A. Käs, D. M. Smith / Journal of Visualized Experiments (2017) **128** 56056

⇒ *Single Actin Bundle Rheology*
D. Strehle, P. Mollenkopf, M. Glaser, T. Golde, C. Schuldt, J. A. Käs, J. Schnauß/ Molecules (2017) **22** 1804

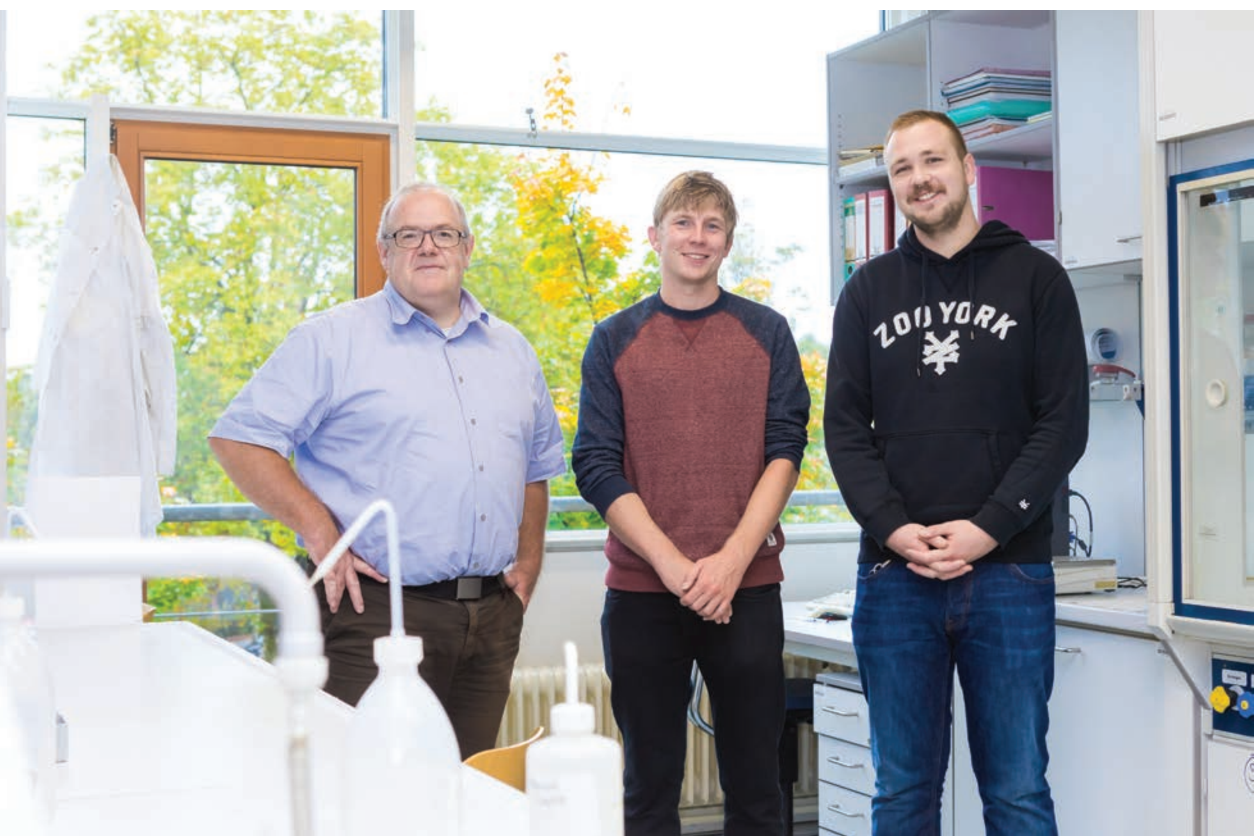
Prof. Dr. Josef Alfons Käs
Peter Debye Institute for Soft Matter Physics
http://www.softmatterphysics.com
E-mail: jkaes@physik.uni-leipzig.de
Phone: +49 341 97-32471
Fax: +49 341 97-32479

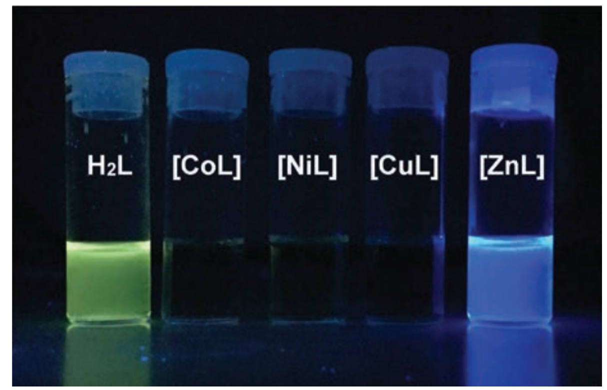
Coordination compounds in supramolecular chemistry and materials chemistry

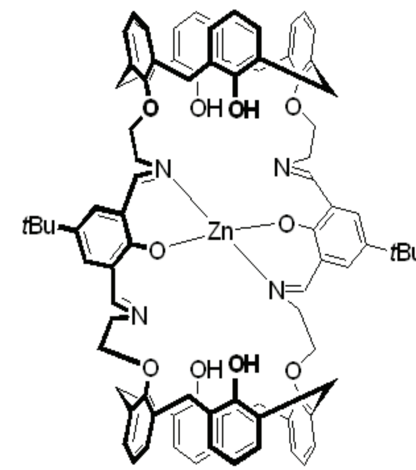
Prof. Dr. Berthold Kersting
M.Sc. Chem. Steve Ullmann, M.Sc. Chem. Florian Glasneck, M.Sc. Chem. Astrid Jäschke, M.Sc. Peter Hahn

Our research is focused on macrocyclic calixarene and thiophenolate-based ligands that are able to coordinate a range of d- and f-block metals. By introducing appropriate binding sites the selectivity of such host systems towards a specific group of guest ions can be modified. Ligating groups with high affinities towards the metal ions are used to obtain potent calix[4]arene-based receptors for d-metal and f-metals, which can be used for solvent extraction or generation of luminescent and magnetic compounds.

A new macrocycle H_2L comprising fluorescent bis(iminomethyl)phenol and calix[4] arene head units has been synthesised and its coordination chemistry examined. H_2L allows the sensitive optical detection of Zn^{2+} among a series of biologically relevant metal ions by a dual fluorescence enhancement / quenching effect in solution. The macrocycle H_2L was obtained in one step by a [2 + 2] Schiff-base condensation reaction between 25,27-bis(aminoethoxy)-26,28-dihydroxy-calix[4]arene (1) and 4-tert-butyl-2,6-diformylphenol (2). Reaction of H_2L with $ZnCl_2$ or $Zn(OAc)_2{\cdot}2H_2O$ in EtOH affords a bright yellow, highly fluorescent compound of composition [ZnL] (3) in almost quantitative yield.. The solid-state structure of 4 shows the presence of a one-dimensional material, in which the calix[4]arene units of adjacent $[ZnL(py)_2]$ monomers self-assemble through

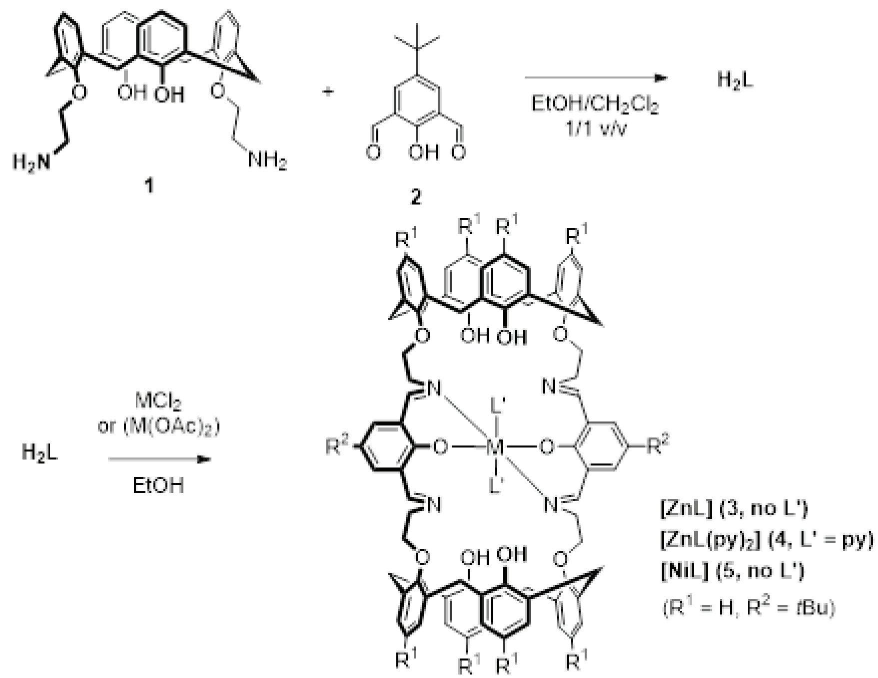


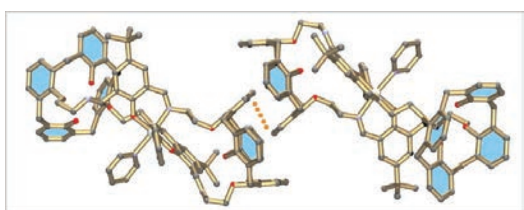


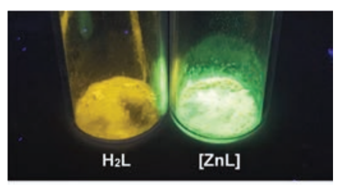


⇑ “Naked-Eye” fluorescence sensing of Zn^{2+} ions by a macrocyclic calix[4]arene ligand.

intermolecular offset face-to-face CH…π interactions (Figure 2). The zinc atom is six-coordinated in a distorted octahedral fashion, by two imino N and two phenolato O atoms from L and two cis-standing pyridine co-ligands. Note that the free imine functions point away from the center of the fluorophore thereby reducing the probability of a photo-induced electron transfer (PET) quenching mechanism. H_2L can be utilized for the sensitive optical detection of Zn^{2+} among a series of other biologically relevant metal ions (Co^{2+}, Ni^{2+}, Cu^{2+}, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cd^{2+}). In the presence of Na^+, K^+, Ca^{2+}, and Cd^{2+} the fluorescence properties of H^2L are not markedly altered, while Co^{2+}, Ni^{2+}, and Cu^{2+} quench, and Mg^{2+} and Zn^{2+} significantly augment the fluorescence of H_2L.







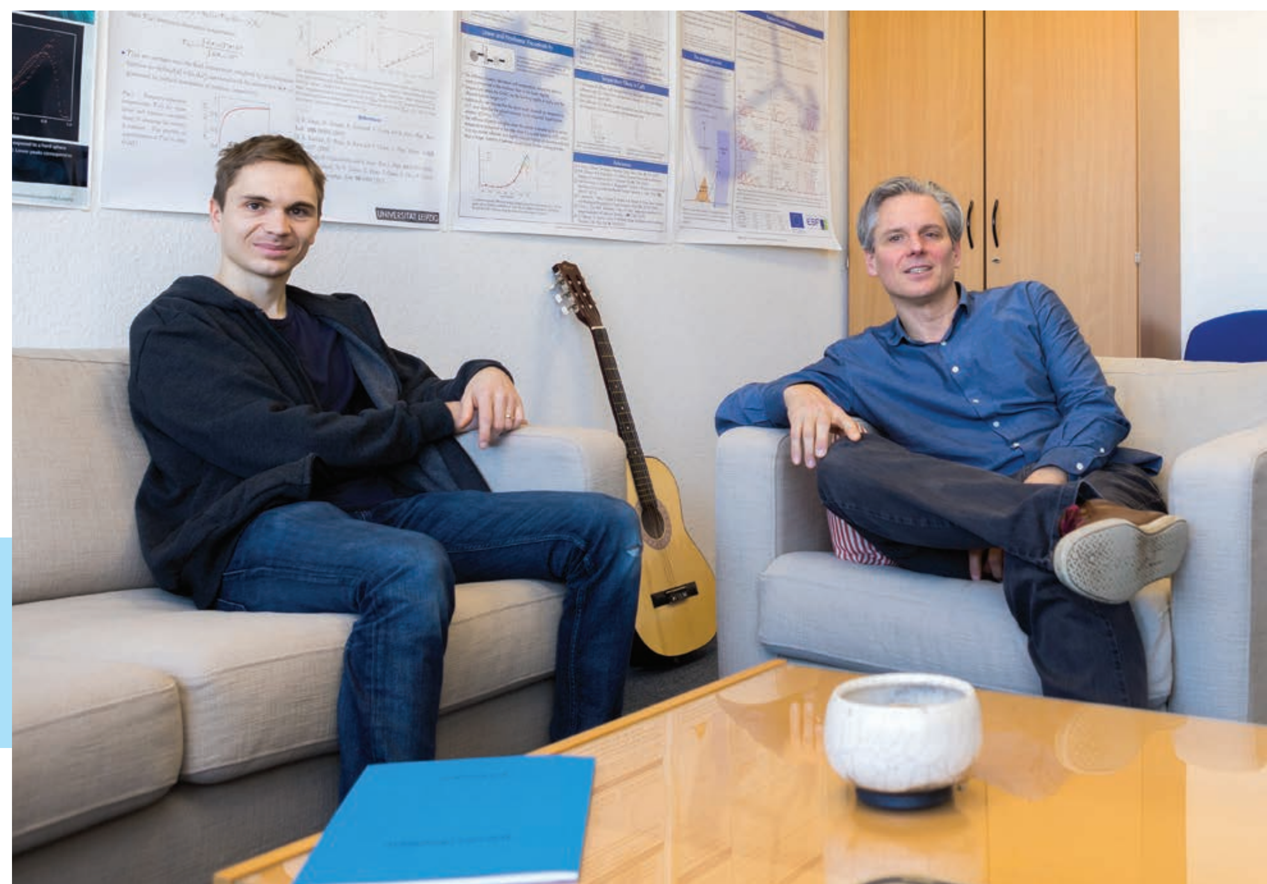
⇑ *Zn^{2+}-Ion Sensing by Fluorescent Schiff-Base Calix[4]arene Macrocycles*
S. Ullmann, R. Schnorr, M. Handke, C. Laube, B. Abel, J. Matysik, M. Findesien, R. Rüger, T. Heine, B. Kersting /Chem. Eur. J. (2017) **23** 3824-3827

Prof. Dr. Berthold Kersting
Institute of Inorganic Chemistry
http://www.uni-leipzig.de/~bkerst/
E-mail: b.kersting@uni-leipzig.de
Phone: +49 341 97-36143
Fax: +49 341 97-36199

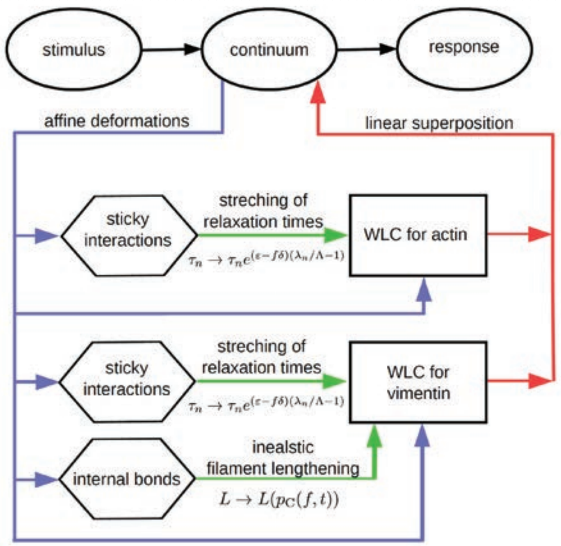
Bottom-up inelastic cell mechanics

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

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



combined systematically using interaction rules. A description on the level of the mesoscopic building blocks can than be related to a model on the continuum level employing integration and distribution rules. The developed models are currently used to interpret experimental data measured in various biophysics labs.



⇑ Schematic illustration of a model constructed by the inelastic bottom-up framework for cell mechanics to describe the linear and non-linear rheological properties of composite networks of semi exible polymers, based on the glassy worm-like chain model (GWLC). For the description of actin networks a GWLC is used, while for the vimentin networks the lengthening of single vimentin laments due forced opening of internal bonds as an additional inelastic effect is employed. The mesoscopic level is linked to the experimental level of bulk rheology via the assumption of affine deformations. The description of the composite network is obtained by a linear superposition of the descriptions of pure actin and pure vimentin networks.

Prof. Dr. Klaus Kroy
Institute for Theoretical Physics
https://home.uni-leipzig.de/~kroy/
E-mail: klaus.kroy@uni-leipzig.de
Phone: +49 341 97-32436
Fax: +49 341 97-32548

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

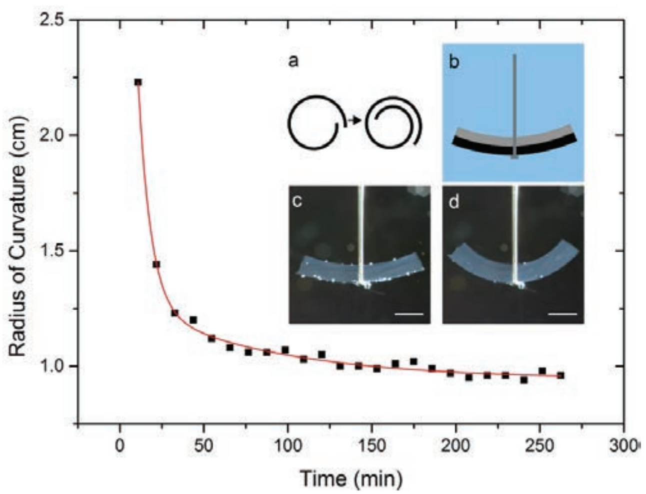
Prof. Dr. Stefan G. Mayr
M.Sc. Phys. Alina Bischoff, Dipl.-Phys. Anja Landgraf, Dipl.-Phys. Fritz Lehnert,
M.Sc. Phys. Stefanie Riedel, B.Sc. Eng. Emilia Wisotzki

Within the BuildMoNa Graduate School, our research work focuses on the development and modification of new functional materials for biomedical and related applications. Within the project exemplarily presented in the following, we concentrate on collagenous biopolymers especially on gelatin and collagen.

Modification of these biological hydrogels by using high energetic electron irradiation represents a promising technique to precisely tune structure, mechanics, thermal stability as well as stimuli responsiveness. In addition, swelling characteristics can be tailored towards hydration-sensitive actuatoric systems. Within the BuildMoNa Graduate School, a hydration sensitive gelatin bilayer was developed which shows a signifi-

cant deformation when in contact with water [6] as shown in Figure 1. This actuatoric effect can be obtained by the combination of two gelatin layers with distinct swelling ability achieved by different dose of irradiation. Within this project, also the influence of pH value and salt concentration of the hydration medium on the swelling of irradiated gelatin was investigated in order to further tune the deformation of the hydration sensitive gelatin bilayer.

In addition, small-angle X-ray scattering (SAXS) was used to investigate the network structures of gelatin hydrogels with increasing irradiation dose in contrast to gels of increasing physical entanglement [2]. From SAXS-obtained mesh sizes, the network shear modulus was predicted using several flexible and semi-flexible models, then compared to the macroscopically determined shear moduli. Overall, differences in the scaling behavior of the networks was apparent, highlighting fundamental differences in the entangled and chemically crosslinked gel networks.



⇑ Time resolved deformation (bending) of a water-sensing gelatin bilayer. The top layer consists of 4 wt% gelatin irradiated with 40 kGy. The bottom layer consists of 10 wt% gelatin irradiated with 5 kGy. The red line represents a two-phase exponential decay function. Inset: (a) Scheme of a stent demonstrator, (b) schematic drawing, (c) gelatin bilayer in water before deformation and (d) gelatin bilayer in water after deformation. Scale bars indicate 5 mm. Image from [6].

⇒ *Insights into growth of Fe-Pd ferromagnetic shape memory alloy thin films*
A. Bischoff, K. Hua, S. G. Mayr / Crystal Growth and Design (2017) **17** 2374

⇒ *Influence of high energy electron irradiation on the network structure of gelatin hydrogels as investigated by small-angle X-ray scattering (SAXS)*
E. I. Wisotzki, E. Fratini, P. Tempesti, S. G. Mayr / Phys. Chem. Chem. Phys (2017) **19** 12064

⇒ *Transmission electron microscopy on as-deposited and freestanding single crystalline Fe_7Pd_3 ferromagnetic shape memory alloy thin film*
A. Landgraf, A. Lotnyk, S. G. Mayr / Scripta Materialia (2017) **136** 97

⇒ *Acoustic emissions associated with stress-induced twin boundary mobility in Fe_7Pd_3 ferromagnetic shape memory alloys*
A. Bischoff, S. G. Mayr / Scripta Materialia (2017) **139** 162

⇒ *Binary Fe-Pd submicron structures fabricated through glancing angle deposition (GLAD) for bioapplications*
U. Allenstein, E. I Wisotzki, C. Gräfe, J. H. Clement, Y. Liu, J. Schroers, S. G. Mayr / Materials & Design (2017) **131** 366

⇒ *Programing stimuli-responsiveness of gelatin with electron beams: basic effects and development of a hydration-controlled biocompatible demonstrator*
S. Riedel, B. Heyart, K. S. Apel, S. G. Mayr / Sci. Rep. (2017) **7** 17436

⇒ *Nanoporous amorphous Ge–Si alloys – unraveling the physics behind ion beam induced morphogenesis*
F. Lehnert, S. G. Mayr / Phys. Chem. Chem. Phys. (2017) **19** 23461

⇒ *Topography evolution of germanium thin films synthesised by pulsed laser deposition*
P. Schumacher, S. G. Mayr, B. Rauschenbach / AIP advances (2017) **7** 045115

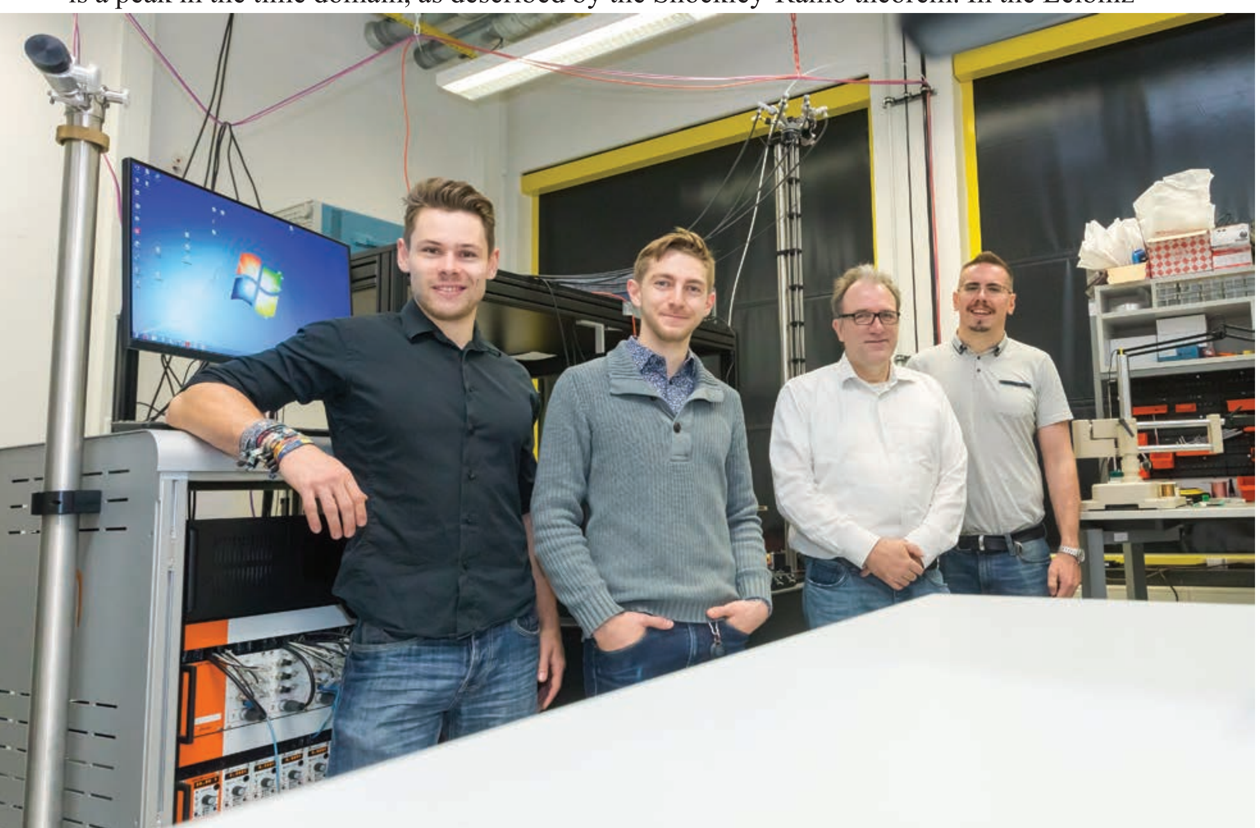
⇒ *Long-term Tissue Culture of Adult Brain and Spleen Slices on Nanostructured Scaffolds*
S. Kallendrusch, F. Merz, I. Bechmann, S. G. Mayr, M. Zink / Advanced Healthcare Materials (2017) 6 1601336

Prof. Dr. Stefan G. Mayr
Leibniz Institute of Surface Engineering (IOM) and Division of Surface Physics, Felix Bloch Institute for Solid State Physics, University of Leipzig
http://www.uni-leipzig.de/~agmayr/
E-mail: stefan.mayr@iom-leipzig.de
Phone: +49 341 235-3368
Fax: +49 341 235-2595

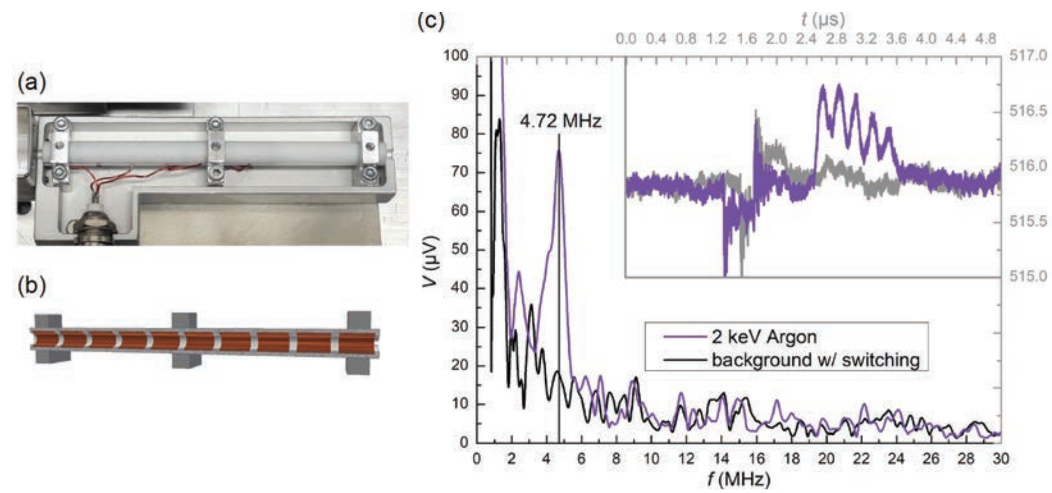
Single ion implantation for fabrication and absolute wide field magnetic imaging for application

Prof. Dr. Jan Meijer
M.Sc. Paul Räcke, Dipl.-Math. Roger John, M.Sc. Robert Staake, M.Sc. Sascha Becker

The concept of BuildMoNa makes it possible to combine manufacturing and application, e.g. to find new ways to create quantum systems for new applications such as wide field magnetic imaging.
To produce well defined quantum systems it is necessary to address exact one atom in a solid with high lateral resolution in all three dimensions. Focused ion beam implantation is able to address individual atoms in solids, but for quantum systems it is additionally necessary to count each individual ion. This sophisticated technique is called deterministic ion implantation and so far only highly complex ion traps with very specific atoms are able to perform this task in a suitable way. The BuildMoNa student Paul Räcke developed a new method for deterministic implantation called "ion fly by image charge detection". When a moving charge passes by a single electrode, the signal induced into that electrode is a peak in the time domain, as described by the Shockley-Ramo theorem. In the Leibniz

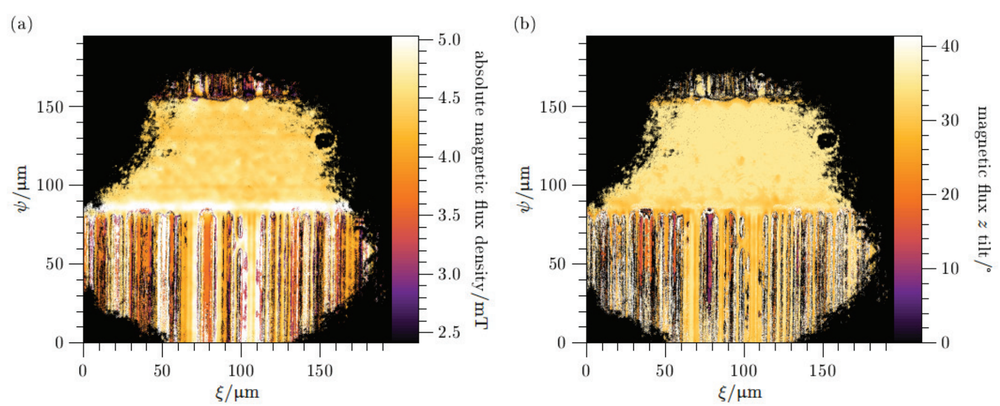


Joint Lab „Single Ion Implantation“ located at the IOM, Paul worked on methods for measuring and detecting small numbers of charges upon a single pass through an image charge detector (ICD).
The detector consists of a linear array of electrodes, so that a periodic signal is formed, which can be analysed in the frequency domain (compare Fig. 1 (a),(b)). The detection limit is determined by the signal-to-noise ratio, considering the image charge signal and the detector noise. The signal itself is proportional to the number of charges. Ion bunches and in future single highly charged ions are used for measurements to increase the SNR per measurement. In Fig. 1 (c), a typical measurement for a bunch of Argon ions is depicted. The time trace (inset, light scale) shows five clear peaks forming an approximate sinusoidal signal form between 2.4 and 3.8 MHz. In its Fourier transform (black scale) this is translated into a peak at the frequency that results from the ion velocity and the geometrical distance of the signal electrodes.
A well know quantum system can be produced by nitrogen implantation in diamond. This negatively charged nitrogen-vacancy centre in diamond, a nitrogen impurity with



Photograph of an image charge detector prototype. (b) Section of its 3D model, revealing the electrode geometry. (c) Time signal (upper right, blue line, grey scale) and its FFT spectrum (bottom left, blue line, black scale) of a 2 keV Argon bunch signal, shown together with the background spectrum (black/grey line) including switching interference, averaged over 100 acquisitions.

a neigbouring vacancy, can be used as an atomic scale magnetic quantum sensor due to having an electronic spin 1 ground state with phonon-assisted optical polarization and readout. Having [111] orientation, usage of ensembles of these close to the surface of a diamond that is fixed on a microwave resonator enables complete vectorial magnetic imaging of two-dimensional structures on the diamond surface. This is accomplished by recording fluorescence images of the back-illuminated diamond using a CMOS-camera while simultaneously sweeping the frequency of a microwave source irradiating the diamond on the resonator. The spectrum of every pixel is then fitted against an eight Lorentzian peak model that accounts for the two spin transitions of the four different orientations with temperature-sensitive zero-field splitting. The results thus provide lateral resolution at the Abbe-limit of ≈ 400nm , magnetic resolution of ≈ 150 μT and even temperature mapping, but with yet to be investigated accuracy. A measurement setup of this kind was set up by the BuildMoNa student Roger John in cooperation with Robert Staacke for the detection of various magnetic structures. To demonstrate correct operation, the results of the measurement of a floppy disk are given in figure 2. The magnetic resolution is intended to be enhanced by employing pulsed illumination and microwave irradiation techniques. Besides the high resolution, Roger and Robert demonstrated that the methods depends only on natural constants and is self-calibrating.



⇑ Image of the absolute value of the magnetic field on the surface of a floppy disk. The homogeneous area in the middle is part of the separation of the tracks, whereas the latter is visible as the vertical grid structure below and also above it. The irregular border is due to imperfect illumination. (b) Image of the tilt of the magnetic field with respect to the floppy disk surface normal, having quite high dynamic range.

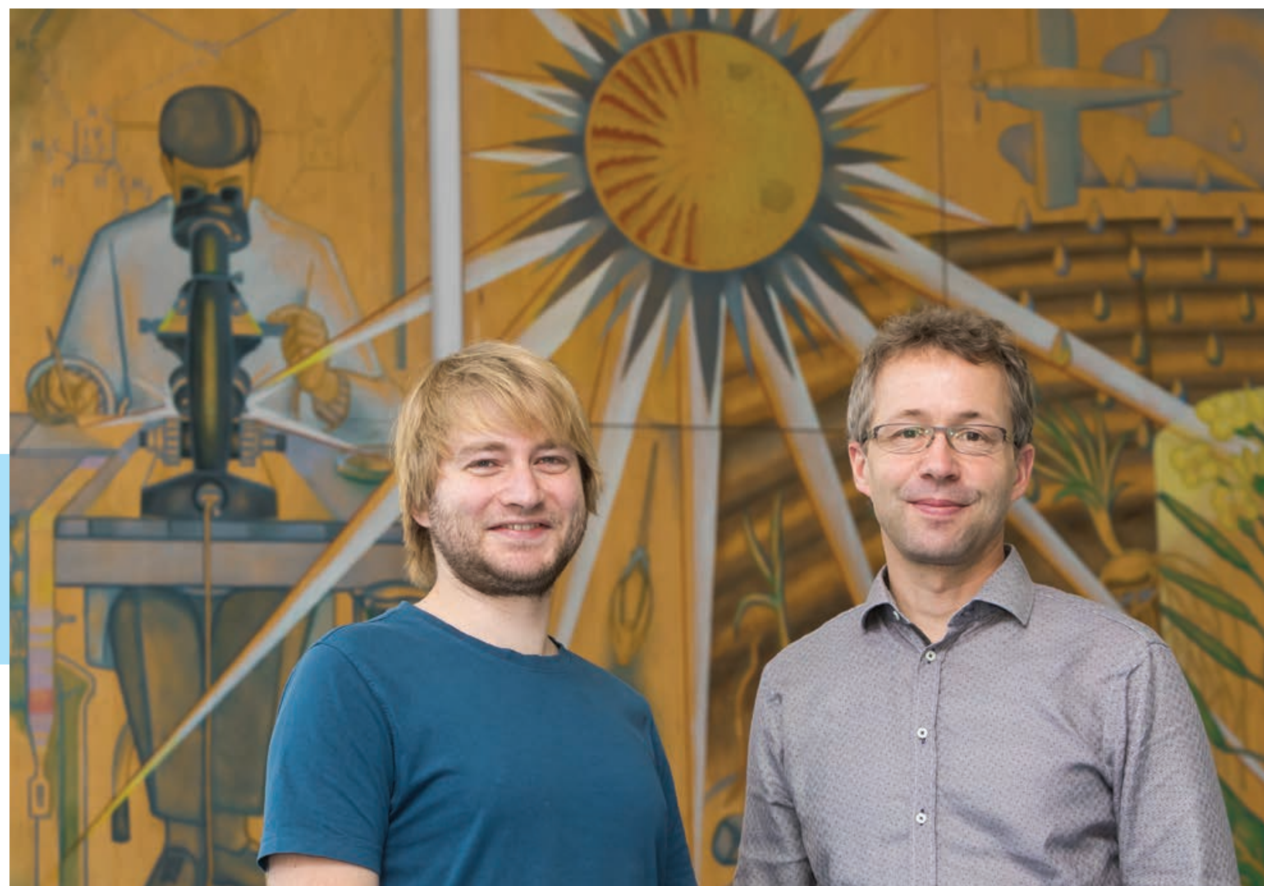
Prof. Dr. Jan Meijer
Felix-Bloch-Institut für Festkörperphysik
https://bloch.physgeo.uni-leipzig.de/nfp/
E-mail: jan.meijer@uni-leipzig.de
Phone: +49 341 97-36931
Fax: +49 341 97-36939

Soft colloidal microparticles as biomimetic sensors of low molecular weight analytes

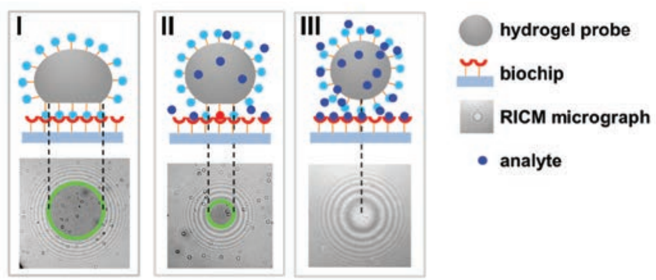
Prof. Dr. Tilo Pompe
M.Sc. David Rettke

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

D. Rettke specifically investigates biomimetic sensors to detect low molecular weight analytes in aqueous environments. The sensing system utilizes the elastic deformation of soft colloidal probes (hydrogel microparticles) as a result of the interfacial



interaction with an underlying chip surface. The associated contact area can be directly related to the adhesion energy, which is read out from optical microscopy based on reflection interference contrast patterns. By functionalization of soft colloidal probes with biospecific ligands they are capable of interacting with target molecules presented on a chip surface. Due to the reversible nature of this binding, competing analytes reduce the effective interaction of soft colloidal probes with the chip surface in dependence of the concentration leading to a quantitative read out. In applying this principle, compact and sensitive sensors for pesticides and other anthropogenic analytes.



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

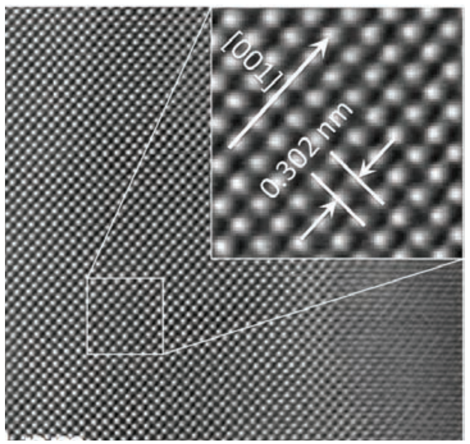
Prof. Dr. Tilo Pompe
Institute of Biochemistry, Leipzig University
https://biochemie.biphaps.uni-leipzig.de
E-mail: tilo.pompe@uni-leipzig.de
Phone: +49 341 97-36931
Fax: +49 341 97-36939

Thin films by low-energy ion beam and laser techniques

Prof. Dr. Dr. h.c. Bernd Rauschenbach
M.Sc. S. Liedtke-Grüner, M.Sc. X. Sun

With the rapid growth of global networking, big data centers and the portable devices application-driven data storage market, the memory industry ushered in a comprehensive opportunity for diverse developments. The ideal new type of memory is desired to be characterized by superior all-round capabilities, including non-volatility, long cycling life, small component size, low power consumption, fast read/write processes, multilevel storage, 3D integration and affordability of the final product. One of the most promising areas in this respect is the data storage technology based on phase-change materials (PCMs), which rely on the reversible transformation between the disordered amorphous and ordered crystalline states of PCMs induced by local heating/cooling either with laser pulses or electrical pulses. The phase transformation is accompanied by a significant change in optical reflectivity and electrical resistivity between these two

solid states. The research work is focused to explore the performance and mechanisms of PCMs with data storage applications in view, including such key features as thermal stability, signal to noise ratio, switching energy, data transfer rate, storage density and scalability. Related with this, in particular four mainly physical aspects, namely the crystallization kinetics, structure transformation, optical and electrical switching of $Ge_2Sb_2Te_5$, GeTe, and Sb_2Te_3 thin films prepared by pulse laser ablation have been investigated



⇐ Aberration-corrected HR-STEM images of a representative fs single laser pulse irradiated GST film viewed along the [001] zone axis. The inset shows a magnification of the marked regions.

⇒ *Glancing angle deposition of sculptured thin metal films at room temperature*
S. Liedtke, Ch. Grüner, A. Lotnyk and B. Rauschenbach / Nanotechnology (2017) **28** 385604

⇒ *Nanoscale bipolar electrical switching of $G_2Sb_2Te_5$ phase-change material thin films*
X. Sun, U. Ross, J.W. Gerlach, A. Lotnyk, B. Rauschenbach / Adv. Electr. Mater. (2017) 1700283

Prof. Dr. Dr. h.c. Bernd Rauschenbach
Leibniz Institute of Surface Modification and
Felix-Bloch-Institute for Solid State Physics
http://www.iom-leipzig.de
E-mail: bernd.rauschenbach@iom-leipzig.de
Phone: +49 341 235-2308
Fax: +49 341 235-2313

Non-Hermitian Hamiltonian for exceptional points of cavity modes

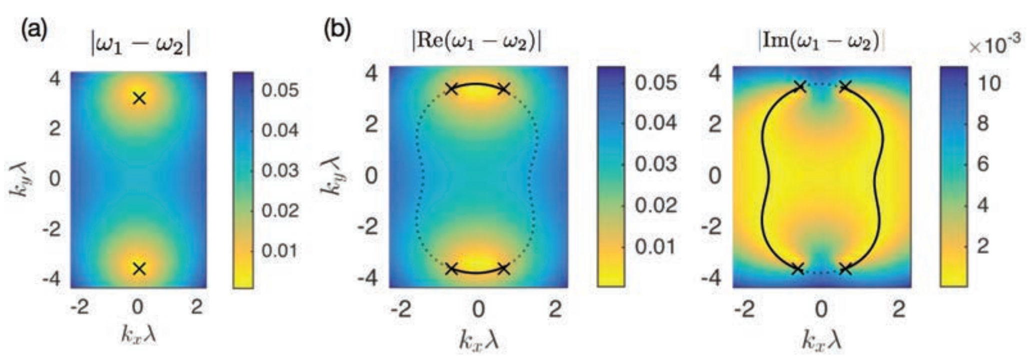
Prof. Dr. Bernd Rosenow
Dipl.-Phys. Alexander Janot, Dipl.-Math. Heinrich-Gregor Zirnstein

Topology, a branch of mathematics, has become an influential method in physics for finding new phases of matter. One of the first examples of a such a new phase is the topological insulator, which is a crystalline solid in which electrons move in such a way that the bulk of the system is insulating, but any surface is conducting. Example materials include Bi_2Se_3 and Bi_2Te_3. This unusual surface conductivity can only be understood in terms of quantum mechanics and the wave nature of electrons. But in recent years, it has been recognized that the topological methods originally developed for understanding electrons in a crystal do not require quantum mechanics and could also be applied to classical wave systems, in particular light in photonic crystals.

In this project, we want to apply topological methods to optical microcavities. The key difference between electrons in a crystal and light in a microcavity is that electrons stay inside the crystal because they are attracted by the ions in the crystal, whereas light can more easily escape from a cavity — light dissipates to the outside. Both the motion of electrons and the motion of light can be described by a mathematical object, the Hamiltonian. However, the fact that electrons do not leave the crystal implies that the corresponding Hamiltonian has a mathematical property called hermiticity, while the dissipation of

light means that the corresponding Hamiltonian must be non-Hermitian. To apply the topological methods originally developed for electronic systems, we first need to derive a non-Hermitian Hamiltonian for the optical microcavity, and then adjust the topological arguments to cope with its new, dissipative features.

Following this program, we have constructed a non-Hermitian model Hamiltonian for an optical microcavity which is simple enough to facilitate theoretical calculations and predictions. We consider the layered microcavity setup studied in a previous BuildMoNa project [*Exceptional points in anisotropic planar microcavities* S. Richter et al. / Phys. Rev. A (2017) **95**, 023836]. The defining feature of the model Hamiltonian is that it should correctly reproduce the resonance frequencies of the microcavity for different momenta; these can be calculated numerically by solving Maxwell's equations. We focus on a single pair of eigenfrequencies; each member of the pair corresponds to a polarization of light. The key idea is to construct the Hamiltonian in two steps: First, we augment the microcavity with two hypothetical perfect mirrors, thereby closing the cavity completely and forbidding dissipation. Then, we build on this auxiliary Hamiltonian and add non-Hermitian terms. The resulting new eigenvalues are complex numbers where the real part corresponds to an oscillation and the imaginary part describes the dissipative decay. Then, we build on this auxiliary Hamiltonian and add non-Hermitian terms. The resulting new eigenvalues are complex numbers where the real part corresponds to an oscillation and the imaginary part describes the dissipative decay. We compare these eigenvalues with the numerically calculated resonance frequencies for the open microcavity. Of special importance is the locus of momenta for which either the real or the imaginary part of the difference of the resonance frequencies vanish. First, this locus contains two pairs of exceptional points, which occur when the resonance frequencies become equal not just in either, but in both real and imaginary part. Such exceptional points generically occur whenever the auxiliary Hermitian Hamiltonian features Dirac points. Second, this locus closely follows a known shape, a Cassini oval; this information allows to determine which polynomials should be used in the non-Hermitian terms. Fitting coefficients gives excellent agreement between the model Hamiltonian and the numerical calculations.



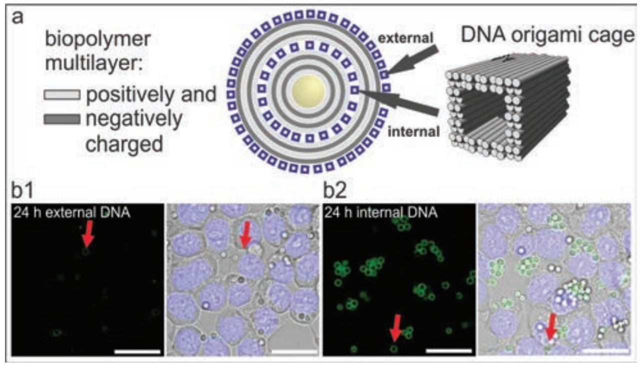
⇧ (a) Difference of the eigenfrequencies of the closed cavity with hypothetical perfect mirrors. The Dirac points are located where the difference vanishes (black crosses). (b) Difference of the resonance frequencies of the open cavity. The locus of vanishing real or imaginary part of the difference closely matches a Cassini oval (black lines). The two pairs of exceptional points are located where both parts vanish (black crosses).

Prof. Dr. Bernd Rosenow
Institute for Theoretical Physics
https://home.uni-leipzig.de/stp/
E-mail: rosenow@physik.uni-leipzig.de
Phone: +49 341 97-32468
Fax: +49 341 97-32469

A DNA-LbL hybrid system for drug delivery

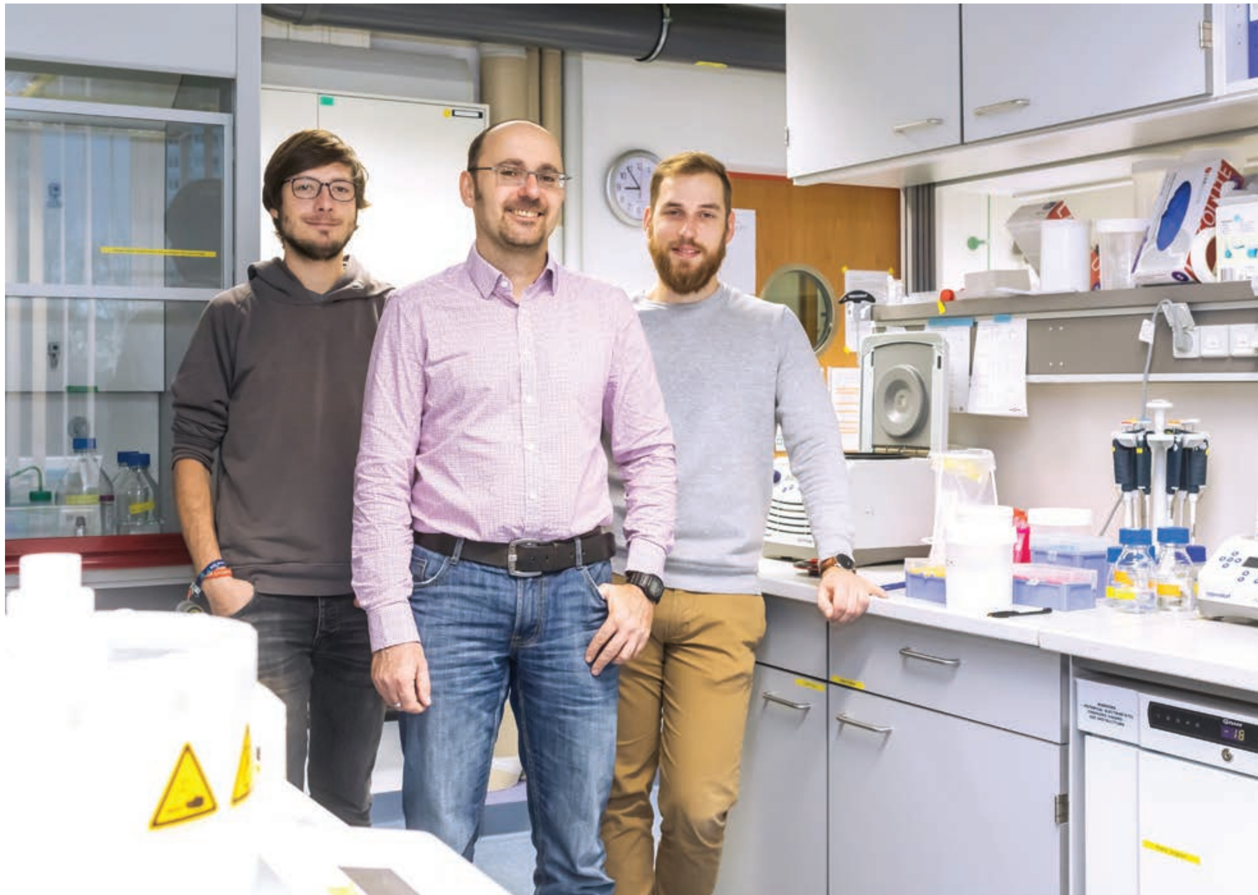
Prof. Dr. Ralf Seidel, PD Dr. Uta Reibetanz
M.Sc. Phys. Florian Engert

The DNA origami technique allows to fabricate complex three-dimensional DNA nanostructures in a programmable manner. In addition these structures can be made responsive to external stimuli. This makes such structures to highly promising candidates in drug delivery. However, DNA nanostructures are often instable under physiological conditions due to environmental conditions such as low pH or nucleases present in the extra- and intracellular environment. This research project focuses on integrating and protecting DNA origami nanocarriers within a super-ordinated Layer-by-Layer (LbL) microcarrier. The LbL microcarrier shall ensure a safe transport of the DNA structures to the particular cellular target and by surface modification provide a specific cellular uptake as well as guided intracellular processing. Overall such a hybrid system should combine the advantages of DNA nanocarriers as well as of the LbL microcarriers by enabling a responsive and individually tunable transport of drugs into desired cellular compartments.
Origami nanostructures are negatively charged and were thus applied in our investigations as a negative layer onto a previously assembled dextran sulfate (DXS) and poly-l-arginine (pARG) biopolymer multilayer. SiO2 particles (diameter 3µm) served as a template. The origami nanostructure could be assembled at variable amounts into any position of the LbL multilayer. The position turned out to be essential for the nanostructure stability: Due to the protective coverage with biopolymers, DNA nanostructures assembled as an internal layer preserved their structural integrity during intracellular transport. In contrast, when the DNA structures were assembled as an external layer, immediate disassembly in the cellular environment was observed. In vitro experiments in model environments (different pH conditions, salt and lysosomal enzyme concentrations) revealed that intra-cellular origami disassembly was due to enzymatic degradation in endolysosomal compartments.
Overall our investigations show that the established DNA-LbL hybrid system supports and enhances the targeted intracellular transport of DNA origami nanostructures into the cell interior.



⇧ DNA origami nanostructures assembled into the multilayer of an LbL designed microcarrier. In a) the coating schema is shown. B1) illustrates origami nanostructures positioned as an outer layer which leads to subsequent intracellular degradation after 24 h co-incubation with HEK 293T cells. In b2) origami nanostructures were assembled in an inner layer position with sustained intracellular integrity.

Prof. Dr. Ralf Seidel
Peter Debye Institute for Soft Matter Physics
https://debye.physgeo.uni-leipzig.de/mbp/
E-mail: ralf.seidel@uni-leipzig.de
Phone: +49 341 97-32501
Fax: +49 341 97-32599



Experiences

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

Prof. Dr. Harald Krautscheid

Research and teaching in natural sciences is still assigned to basic disciplines such as biology, chemistry and physics. While a great part of topical research concerns the border areas of these disciplines, e.g., biochemistry, biophysics, chemical biology or biophysical chemistry, the current research topics are becoming more and more specialized. Therefore, an important benefit of the graduate school BuildMoNa is that it consists of doctoral students and their supervisors of several faculties and research institutes bringing together experts from their various research fields and combining their expertise. This combination is an excellent prereqi site for developing new interdisciplinary research and setting up new interesting research projects. From its beginning, ten years ago, I realized how BuildMoNa catalyzes this formation of new research teams working successfully on novel interdisciplinary topics.
This possibility of crossing borders between the classical research disciplines is important for modern research as well as for the development of our doctoral students. In addition, BuildMoNa students benefit from the teaching program

Research and teaching in natural sciences is still assigned to basic disciplines such as biology, chemistry and physics. While a great part of topical research concerns the border areas of these disciplines, e.g., biochemistry, biophysics, chemical biology or biophysical chemistry, the current research topics are becoming more and more specialized. Therefore, an important benefit of the graduate school BuildMoNa is that it consists of doctoral students and their supervisors of several faculties and research institutes bringing together experts from their various research fields and combining their expertise. This combination is an excellent prereqi site for developing new interdisciplinary research and setting up new interesting research projects. From its beginning, ten years ago, I realized how BuildMoNa catalyzes this formation of new research teams working successfully on novel interdisciplinary topics.
This possibility of crossing borders between the classical research disciplines is important for modern research as well as for the development of our doctoral students. In addition, BuildMoNa students benefit from the teaching program that spreads from courses on "transferable skills" and basic moduls to advanced scientific moduls and minisymposia. BuildMoNa provides the opportunity for such two- or three-days workshops with invited national and international experts as guest lecturers focusing on selected topics. These seminars and discussions are not only great opportunities for our students, they are also extraordinarily interesting for the PIs and help to establish new scientific contacts. In the Annual BuildMoNa Conference, "ABC", the doctoral candidates take advantage of the possibility to present their own results. In oral or poster presentations they discuss their findings and conclusions with other BuildMoNa students, PIs and invited guest lecturers on a remarkably high level. In BuildMoNa's 10th year I very much hope that this successful graduate school will find adequate and reliable support also in the next 10 and more years.

Prof. Dr. Harald Krautscheid

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

M.Sc. Phys. Paul Räcke

Being a member of the graduate school BuildMoNa offers great chances for doctoral candidates. At the same time, it means that additional effort and time needs to be invested. PhD students work in different fields of physics, chemistry, biology and biochemistry. Getting in touch with researchers from different backgrounds can be inspiring and difficult at the same time, because everyone tends to speak their own language. But this is one of the great opportunities that a BuildMoNa membership offers. In the direct exchange between doctoral candidates, for example at the Annual BuildMoNa Conference, or via the participation in the scientific modules we not only broaden our horizon by learning about methods and research that we would otherwise not get in contact with, but also get a fresh look at our own work from an interdisciplinary perspective.

Besides the additional scientific education, transferable skills courses are an essential part of the compulsory program a PhD student has to complete to be awarded the BuildMoNa certificate. These courses are mainly offered by the Research Academy Leipzig (RAL). Participants come from all faculties of the University. Although many such skills are fairly universal and needed whether one studies medieval history, algae or semiconductor properties, not all offered courses are relevant to the natural scientist. Squeezing the additional workload into a doctoral candidate's schedule can be a challenge considering that the research project alone is usually stressful enough. Besides this, support from the graduate school is provided in the form of travel allowances for doctoral candidates. In this way, we are encouraged to actively participate in international conferences, summer schools, etc.

Internationally and also increasingly in Germany, the idea that every doctoral student should be member of a graduate school or structured PhD program seems to gain more popularity. The additional training in the form of soft skill and scientific modules is supposed to prepare students for either an academic career or make them more attractive for employers in the "real world" outside of academia. It will be interesting to see how this idea – regardless whether one agrees or disagrees with this approach – will shape the University of the Future.

Paul Räcke

M.Sc. Phys. Paul Räcke

Training

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

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

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

TRAINING CONCEPT

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

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

Scientific and methods modules

Chemical biology and biophysics of cancer (2017-A2)

04 - 6 October 2017,
written exam, 2 credit points, 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. J. Käs

Lecturers:

⇒ K. Alim, Max Planck Institute for Dynamics and Self-Organisation, Germany
Morphology Control by Active Fluid Flows

⇒ I. Bechmann, University of Leipzig, Germany
Slice Cultures as Tool to Study Cancers in Vitro

⇒ S. Diez, Technical University Dresden, Germany
Of Active Motors and Passive Crosslinker: Reconstituting Adaptive Microtubule Networks

⇒ B. Fabry, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany
Interactions of Natural Killer Cells with Cancer Cells in a 3-D Environment

⇒ C. Franz, Karlsruhe Institute of Technology, Germany
Mapping Cadherin-Dependent Cell Adhesion and Elasticity Changes in Tissue Explants during the Transition from Collective to Single-Cell Migration

⇒ E. Frey, Ludwig-Maximilians-University Munich, Germany
Multiscale Cell Motility: From Substrate Deformation to Collective Migration

⇒ R. Golestanian, University of Oxford, United Kingdom
Emergent Cancer-like Phenomenology in a Simple Model of Cells with Growth and Chemical Signalling

⇒ S. Grill, Technical University Dresden, Germany
Control of Mechanochemical Self-Organization during Cell Polarization

⇒ K.Gottschalk, University of Ulm, Germany
The Weakness of Senescent Fibroblasts

⇒ J. Guck, Technical University Dresden, Germany
Physical Aspects of Successful Cell Circulation and Migration

⇒ M. K. Jolly, Rice University, United States of America
Hybrid Epithelial/Mesenchymal Phenotype (E/M) - a "Metastatic Sweet Spot"

⇒ J. H. Kim, Harvard T. H. Chan School of Public Health, United States of America
Unjamming and Cell Shape Changes in Breast Cancer

⇒ U. Köhl, Hannover Medical School, Germany
From "CAR T Cells" to CAR Expressing NK Cells for Cancer Retargeting

⇒ J. Lammerding, Cornell University, United States of America
Cytoskeletal Intermediate Filaments - from Self-Assembly to Cell Mechancs

⇒ R. Merkel, Forschungszentrum Jülich, Germany
Physicochemical Properties of Basement Membranes Formed by a Cell Culture Model of Human Breast Glands

⇒ M. Plodinec, University of Basel, Switzerland
In Situ Mechanobiology of Epithelia in Health and Disease

⇒ K. Rippe, German Cancer Research Center Heidelberg, Germany
Establishing Nuclear Subcompartments and Chromatin Patterns to Regulate Gene Expression

⇒ J. Schwarz, Syracuse University, United States of America
Strain-Controlled Rigidity Transitions in Cells and the Role of the Cell Nucleus

⇒ P. Silberzan, Institute Curie, France
Collectively Emerging Nematic Order in Populations of Fibroblas

⇒ A.-S. Smith, Friedrich-Alexander University of Erlangen-Nuremberg, Germany

⇒ J. Spatz, Max Planck Institute for Medical Research and University of Heidelberg, Germany
Mechanotransduction in Collective Cell Migration

⇒ D. Sussman, Syracuse University, United States of America
Tissue Surface Tension in Simple Models of Dense Biological Tissue

⇒ A. Taiyab, McMaster University, Canada
Regulation of Actin Cytoskeleton during Epithelial to Mesenchymal Transition - The Ocular Lens Perspective

⇒ X. Trepat, IBEC Barcelona, Spain
Physical Forces Driving Migration, Division and Folding of Epithelial Sheets

⇒ K. Wolf, Radboud Institute for Molecular Life Science, The Netherlands
Control of Cancer Cell Invasion by Nuclear Deformability

⇒ T. Zech, University of Liverpool, United Kingdom
Matrix Adhesion Site Function in Polarised Invasive Migration

⇒ N. Zahir, National Cancer Institute, United States of America

Integrating Scales in Cancer Mechanobiology: The NCI Physical Sciences - Oncology Network

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, internalization of biomolecules into tumour cells, linkers for controlled release, etc.)
- ⇒ Personalised medicine and better tumour staging (single cell analysis, high throughput and content, genetic networks, tumour specificmtracers and their application by PET-imaging or fMRI-scanning, tumour cell biomechanics and adhesion)
- ⇒ Models of tumour growth (finite element-based models, differential adhesion hypothesis, glass-like behaviour)
- ⇒ Relapse (selective pressure and resistant tumour cells, dormant cancer cells, cancer stem cells)

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

Basic concepts in molecular spectroscopy (2017-B4)

16 / 17 March 2017,
written exam, 2 credit points, yearly recurrence with modification, 38 participants

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

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

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

Complex nanostructures – Topological matter and flat bands (2017-T3)

18 - 20 August 2017,
poster presentation 2 credit points, bi-yearly recurrence with modification

The module deepend the understanding of general interacting states in semimetals possessing exotic electronic dispersion like the flat band (dispersionless electron e nergy in k-space), such as materials with Dirac nodal lines (e.g. graphene/graphite), Weyl semimetals and systems close to a Lifshitz transition. Topics related to graphene/graphite, topological materials, topological and interface superconductivity and new states of matter was discussed.

Responsible Scientists:
Prof. Dr. P. Esquinazi, Prof. Dr. B. Rosenow

Lecturers:
Boris Aronzon, NRC Kurchatov Institute Moscow, Russia; Antonio Bianconi, Rome International Center for Materials Science Superstripes RICMASS, Italy; Valery Timofeevich Dolgopolov, Institute of Solid State Physics, Chernogolovka, Rus-

sia; Moritz Drescher Ruprecht-Karls- University Heidelberg, Germany; Pablo D. Esquinazi, University of Leipzig, Germany; Ion Cosma Fulga, IFW Dresden, Germany; Tero Heikkilä University of Jyväskylä, Finland; Timo Hyart University of Jyväskylä, Finland; Satoshi Ikegaya Hokkaido University, Sapporo, Japan; Ikuzo Kanazawa ,Tokyo Gakugei University, Japan; Victor A. Khodel, NRC Kurchatov Institute Moscow, Russia; Flore Kunst Stockholm University, Sweden; Vladislav Kurilovich, Moscow Institute of Physics and Technology, Russia; Tomas Löthman, Uppsala University, Sweden; Natália Menezes, Utrecht University, Netherlands; Jaakko Nissinen, Aalto University, Finland; Hiroyoshi Nobukane, Hokkaido University, Sapporo, Japan; Hee Chul Park, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Republic of Korea; Sebastiano Peotta (Aalto University, Finland; Warren Pickett, University of California Davis, USA; Rodrigo Andrés Vicencio Poblete, Universidad de Chile, Santiago de Chile, Chile; Nicolas Regnault, Princeton University, USA; Matteo Rizzi, Johannes Gutenberg-University, Mainz, Germany; Bernd Rosenow, University of Leipzig, Germany; Masatoshi Sato, Kyoto University, Japan; Vasily Shaginyan, Petersburg Nuclear Physics Institute, Russia; Alexey Soluyanov, ETH Zurich, Switzerland; Yukio Tanaka, Nagoya University, Japan; Päivi Törmä, Aalto University, Finland; Grigory Volovik, Aalto University, Finland and Landau Institute, Moscow, Russia; Georg Wolfgang Winkler, ETH Zurich, Switzerland; Maimaiti Wulayimu, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Republic of Korea

Contents:
⇒ Flat band in electronic systems
⇒ Flat band photonic lattices in one and two dimensions
⇒ Dipolar excitations
⇒ Two dimensional superconducting states
⇒ Josephson effect and Josephson junction arrays
⇒ Quantum Hall-superconductors
⇒ Majorana particles
⇒ Kosterlitz-Thouless transition
⇒ Honeycomb ribbons

Methods:
⇒ Scanning probe techniques (space-resolved magnetic microscopy)
⇒ Electrical Transport Techniques Synthesis
⇒ Preparation techniques of nanofilms
⇒ Si MOSFETs
⇒ Quantum Wells

From molecules to materials: Photocatalysis (2017-T4)

14 / 15 November 2017,
written exam, 2 credit points, bi-yearly recurrence with modification

This module linked molecular sciences and materials science, teached how materials with optimised photocatalytic activity are obtained, and provided an understanding of the properties and applications of these materials.

Responsible Scientists:
Prof. Dr. R. Gläser, Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins

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

Contents:
⇒ Materials from “hard” (synthetic molecules, crystalline nanostructures) building blocks and/or “soft” (polymers, biomolecules, whole cells and organisms) building blocks
⇒ Properties of these materials (magnetic, electronic, and optical properties, photocatalytic properties)
⇒ Applications (photocatalysis, immobilised catalysts, energy conversion including solar energy])
⇒ Theory

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

Scientific minisymposium

Transparent Conductive Oxides – Fundamentals and applications (2017-A3)

18 - 22 September 2017

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

⇒ Dr. Klaus Ellmer, Helmholtz-Zentrum Berlin, Germany

Thermophoresis for medicine and evolution

⇒ Dr. Joel B. Varley, Lawrence Livermore National Laboratory, Livermore, CA, USA
Insights into the conductivity of TCOs through hybrid functional calculations

⇒ Prof. Dr. Peter Deák, University of Bremen, Germany
Beyond-standard DFT defect calculations in the prospective TCO materials TiO_2 and Ga_2O_3

⇒ Prof. Dr. Takahisa Omata, IMRAM, Tohoku University, Japan
Wurtzite-type ternary I-III-O_2oxide semiconductors; new materials expanding the energy band gap range covered by oxide semiconductors

⇒ Dr. Encarnación G. Víllora, National Institute for Materials Science, Tsukuba, Japan
Halide vapor phase epitaxy of metastable α-and ε-Ga_2O_3

⇒ Prof. Dr. Armin Dadgar, Otto-von-Guericke-Universität Magdeburg, Germany
GaN, a transparent conductive nitride

⇒ Dr. Geoffroy Hautier, Université catholique de Louvain, Belgium
High-throughput computational search for new high mobility transparent (semi) conducting oxides

⇒ Prof. Dr.-Ing. Paul Erhart, Chalmers University of Technology, Gothenburg, Sweden
A unifying perspective on oxygen vacancies in wide band gap oxides

⇒ Prof. Dr. Lasse Vines University of Oslo, Norway
Self-compensation and the vacancy-dopant pair in highly Al-and Ga-doped ZnO

⇒ Dr. Jesús Zúñiga-Pérez, UCA, CRHEA-CNRS,Valbonne, France
ZnO-based polariton lasers: From heteroepitaxial to homoepitaxial optical microcavities

⇒ Dr. Chris Sturm, Universität Leipzig, Germany
Optics and tensor properties of anisotropic TCOs

⇒ Dr. Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany
Bulk and surface charge transport in semiconducting oxides

⇒ Alana Hyland, University of Canterbury, Christchurch/The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand
Persistent photoconductivity in ZnO-based ultraviolet photodetectors

⇒ Dr. Kevin D. Leedy, Air Force Research Laboratory, Ohio, USA
Conductivity control in homoepitaxial Si-doped β-Ga_2O_3 thin films by pulsed laser deposition

⇒ Prof. Dr. Judith L. MacManus-Driscoll, University of Cambridge, United Kingdom
A new paradigm for defect, strain and coupling in oxide epitaxial nanocomposite thin films for realising unprecedented functional properties

⇒ Prof. Dr. Marjorie Olmstead, University of Washington, Seattle, USA

Aluminum gallium oxide: A tunable solar-blind conductor

⇒ Prof. Dr. Andreas Klein, TU Darmstadt, Germany
Interfaces and grain boundaries of Cu_2O

⇒ Prof. Dr. Chris McConville, RMIT University Melbourne, Australia / University of Warwick, UK
Transparent conducting oxide semiconductors: Exploring their electronic structure

⇒ Prof. Dr. Alan Taylor (INFINITY), TWI Ltd., Cambridge, United Kingdom
Development of novel active binders for indium-free transparent conductive oxides

⇑ Participants of the scientific minisymposium: Transparent Conductive Oxides - Fundamentals and applications

Transferable skills workshops

Presentation Workshop

Dr. Frank Lorenz,
2 / 09 March 2017 in combination with the Annual BuildMoNa Conference,
9 participants

How to give successful oral presentations in the natural and related sciences? The workshop (held in English language throughout) aimed at an improvement of the presentation skills of doctoral candidates. Besides a short review of the basic foundations of uccessful 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. Santiago Gómez-Ruiz	*Departamento de Biología y Geología, Física y Química Inorgánica Móstoles, Madrid*	From Metal Complexes to Heterogeneous or Supported Systems:Applications of Hybrid Materials in Different Catalytic and Photocatalytic Reactions	09 March 2017	*Faculty of Chemistry and Mineralogy*
Prof. Dr. William F. Colmers	*University of Alberta*	Stress, Resilience and NPY	04 April 2017	*Faculty of Life Sciences*
Prof. Dr. Helma Wennemers	*ETH Zürich*	Controlling Supramolecular Assemblies with Peptides	06 April 2017	*Faculty of Chemistry and Mineralogy*

Annual BuildMoNa Conference

The fifth annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nanoobjects" (BuildMoNa) was held on 06 and 07 March 2017 at the Faculty of Physics and Earth Sciences. The following renowned guest speakers gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Claudia Felser, Max-Planck-Institut für Chemische Physik Dresden
Topology- from the materials perspective
⇒ Prof. Dr. Stefan Kaskel, Technische Universität Dresden
Metal-Organic Frameworks with Ultrahigh Porosity, Switchability and Functionality
⇒ Prof. Dr. Katharina Landfester, Max-Planck-Institut for Polymer Research Mainz
Molecular Design of Nanocapsuls
⇒ Prof. Dr. Elke Scheer, University of Konstanz
Atomic and Molecular Scale Functional Devices

⇑ Winners of the BuildMoNa Awards 2017 together with the Speaker and Vice-speaker of the Graduate School: Martin Glaser, Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins, Ria Schönauer, Prof. Dr. Marius Grundmann and Anup Adhikari (from left to right)

During the poster session, doctoral candidates presented their scientific topics and discussed them with the international guests, receiving further inspiration for their work at the Graduate School BuildMoNa. Furthermore, the BuildMoNa Awards were given to doctoral candidates to recognise their outstanding scientific achievements.

Ria Schönauer (Institute of Biochemistry) received the first prize for her work on Adrenomedullin 2.0 published in:
Adrenomedullin 2.0: Adjusting Key Levers for Metabolic Stability
R. Schönauer, S. Els-Heindl, J. P. Fischer, J. Köbberling, B. Riedl, A. G. Beck-Sickinger / J. Med. Chem. (2016) **59** (12) 5695-5705

Anup Adhikari (Insitute of Inorganic Chemistry) received the second prize for his work on Sodium Tetramesityltetraphosphanediide published in:
Unusual Reactivity of Sodium Tetramesityltetraphosphanediide Towards Cyclohexyl Isocyanide
A. Adhikari, M. B. Sárosi, T. Grell, P. Lönnecke and E. Hey-Hawkins / Chem. Europ. J. (2016) **22** 15664-15668

Martin Glaser (Institut for Experimental Physics I) received the third price for his research on DNA nanotube systems published in:
Self-assembly of hierarchically ordered structures in DNA nanotube systems
M. Glaser, J. Schnauß, T. Tschirner, S. Schmidt, M. Moebius-Winkler, D. Smith, J. A. Käs / New. J. Phys. (2016) **18** 055001

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference together with the Speaker and Vice-speaker of the Graduate School: Ayman Zaheer, Prof. Dr. Marius Grundmann, Jan-Patrick Fischer, Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins and Robert Karsthof (from left to right)

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

The first prize was awarded to Jan-Patrick Fischer for his presentation "Adrenomedullin - replacing the disulfide bond", the second to Robert Karsthof for his presentation "Interface engineering on NiO-ZnO-based UV solar cells" and the third to Muhammad Ayman Zaheer for his talk "In-situ characterisation of mixing dynamics in liquid-phase reactionsby ^{129}Xe NMR spectroscopy."

Participants of the Annual BuildMoNa Conference.

Funding of doctoral candidates

DFG Deutsche Forschungsgemeinschaft

DAAD

Europa fördert Sachsen. ESF Europäischer Sozialfonds

Bundesministerium für Bildung und Forschung

Freistaat Sachsen

Europa fördert Sachsen. EFRE Europäischer Fonds für regionale Entwicklung

Funktionalität Oxidischer Grenzflächen SFB 762

Marie Curie

Science without borders

SAB Sächsische AufbauBank

VolkswagenStiftung

Studienstiftung des deutschen Volkes

FCI Fonds der Chemischen Industrie

Universität Leipzig