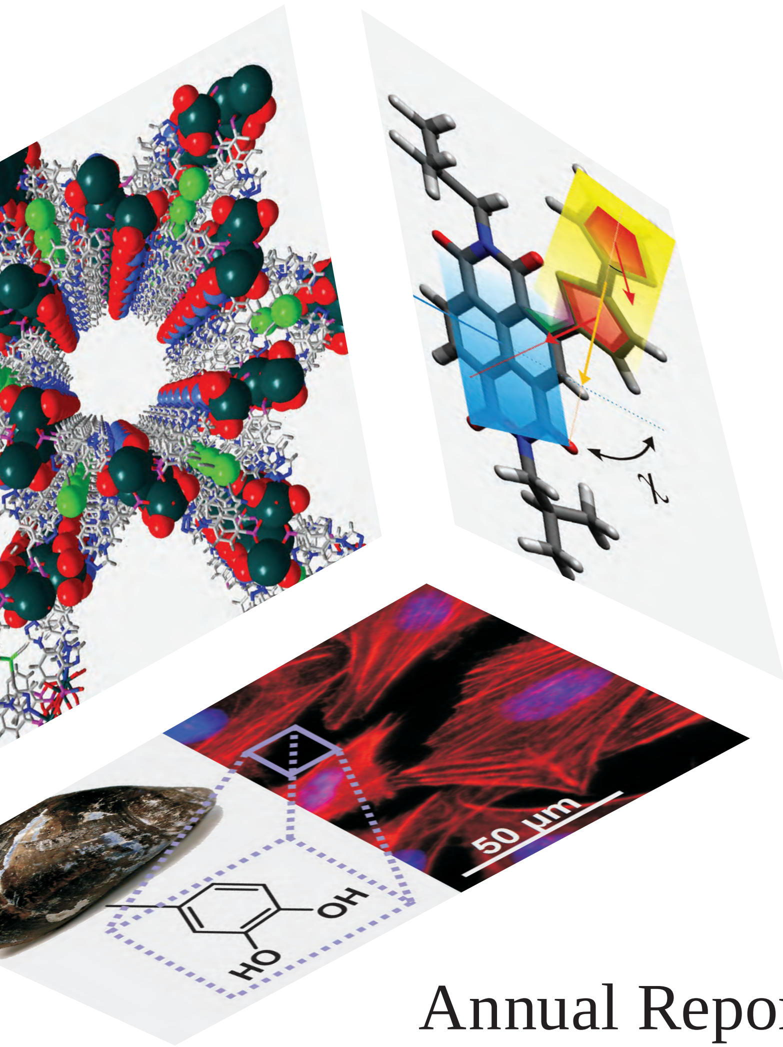
UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2014

UNIVERSITÄT LEIPZIG

Cover image:
⇒ *Left:* Fragment of the crystal structure of a phosphonate-based porous coordination polymer
⇒ *Right:* Subunit of the organic semiconducting copolymer P(NDI2OD T2)
⇒ *Bottom:* Blue mussel (Mytilus edulis) derived peptide

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Annual Report 2014

Founded as DFG Graduate School 185 in 2007

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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. B. Abel, Prof. Dr. A.G. Beck-Sickinger, Prof. Dr. F. Cichos,
Prof. Dr. P.D. Esquinazi, Prof. Dr. R. Gläser, Prof. Dr. M. Grundmann,
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Leipzig school of natural sciences – the seventh year of building with molecules and nano-objects

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

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

Since the establishment of the Graduate School in 2007, the number of doctoral candidates has continuously grown. At the end of 2014, 86 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 96 young scientists have already finished their doctoral studies. In 2014, 4 doctoral candidates were awarded a BuildMoNa scholarship, and 62 doctoral candidates were funded by third-party grants. Additionally, 21 doctoral candidates were funded by doctoral positions provided by the European Social Fund (ESF) of the European Union and the Free State of Saxony, and 18 doctoral candidates were involved in three new ESF-funded young researchers groups affiliated with the Graduate School.

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

Each year, one of the advanced modules is organised as an international minisymposium. In 2014, the minisymposium “Physics of Cancer” was organised by the research group of Prof. Josef Käs and brought together researchers from pioneering groups worldwide that are concerned with the investigation of the physical mechanisms underlying cancer progression. Science-related events included the second Annual BuildMoNa Conference, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School.

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

Prof. Dr. Evamarie Hey-Hawkins

Organisation and management

RESEARCH ACADEMY LEIPZIG ADVISORY BOARD

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Prof. Dr. Axel Mecklinger
Universität des Saarlandes

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RESEARCH ACADEMY LEIPZIG

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

BuildMoNa OFFICE

Scientific Manager
Dipl.-Phys. Andrea Kramer

Multilingual Secretaries
Isabel Holzke
Birgit Wendisch

STEERING COMMITTEE

Speaker of the Graduate School
Prof. Dr. Dr. h.c. Evamarie Hey-Hawkins

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Representative of Doctoral Candidates
Dipl.-Phys. Martin Göse

Deputy
M.Sc. Phys. André Heber

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Prof. Dr. Bernd Abel
Prof. Dr. Annette G. Beck-Sickinger
Prof. Dr. Frank Cichos
Prof. Dr. Daniel Huster
Prof. Dr. Frank-Dieter Kopinke
Prof. Dr. Harald Krautscheid
Prof. Dr. Felix Otto

SPOKESPERSONS OF THE DOCTORAL CANDIDATES

Faculty of Biosciences, Pharmacy and Psychology
M.Sc. Chem. David Boehme

Faculty of Chemistry and Mineralogy
M.Sc. Chem. Eng. Paul Boar
M.Sc. Chem. Andy Schmied

Faculty of Physics and Earth Sciences
M.Sc. Phys. André Heber
M.Sc. Phys. Johannes Zierenberg

Leibniz Institute of Surface Modification
M.Sc. Phys. Uta Allenstein

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

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. Dr. h.c. E. Hey-Hawkins as Research Academy Board member and by Martin Göse as representative of the doctoral candidates.

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

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

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

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

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

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Anup Kumar Adhikari	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis and reactivity of phosphorus-rich compounds*
M.Sc. Phys. Uta Allenstein	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Dynamic mechanical cell manipulation and characterisation using magnetostrain*
M.Sc. Chem. Michael Ansorge	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger/	*Biomimetic signalling gradients in reconstituted extracellular matrices*
Dipl.-Phys. Ariyan Arabi-Hashemi	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Ion beam assisted deposition of intelligent and adaptive surfaces*
M.Sc. Chem. Salma Begum	Prof. Dr. H. Krautscheid / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Metal-organic frameworks based on phosphonate linkers*
M.Sc. Phys. Francis Bern	Prof. Dr. P. Esquinazi / Prof. Dr. B. Kersting	*Coupling phenomena in multilayerd oxide nanostructures*
M.Sc. Phys. Alina Bischoff	Prof. Dr. S. Mayr / Prof. Dr. M. Grundmann	*Mechanical characterisation and training of ferromagnetic iron-palladium shape memory alloy thin films*
M.Sc. Chem. Eng. Paul Cosmin Boar	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phosphorus-based metallacycles for applications in catalysis*
M.Ed. Math./Phys. Johannes Bock	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Computer simulations of semiflexible polymers in disordered media*
M.Sc. Chem. David Boehme	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Cytotoxic neuropeptide Y-conjugates for the development of new therapeutical approaches of metastasing breast cancer*
M.Sc. Chem. Solveig Boehnke	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Novel carbaborane-containing building blocks for selective antitumour activity*
M.Sc. Phys. Michael Bonholzer	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Magneto-tunnel junctions with oxidic contacts*
Dipl.-Phys. Marco Braun	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Gold nanoparticle based thermophoretic nanofluids*
Dipl.-Phys. Jörg Buchwald	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Mechanical properties of surfaces at nanoscale*
Dipl.-Phys. Jakob Tómas Bullerjahn	Prof. Dr. K. Kroy / Prof. Dr. B. Abel	*How a polymer breaks a bond*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Antonio Buzharevski	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Synthesis, characterisation and evaluation of biologically active carborane derivatives of nonsteroidal anti-inflammatory drugs (NSAIDs) that are known COX inhibitors to improve COX-2 selectivity and reduce side effects*
Dipl.-Phys. Felix Daume	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Electrical properties and long-term stability of Cu(In,Ga)Se_2 solar cells on polyimide substrate*
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. Phys. Gianmaria Falasco	Prof. Dr. K. Kroy / Prof. Dr. F. Cichos	*Non-equilibrium dynamics of heated and self-propelled nanoparticles*
M.Sc. Phys. Annemarie Finzel	Prof. Dr. B. Rauschenbach / Prof. Dr. B. Abel	*Ion-beam assisted deposition of gallium nitride films*
M.Sc. Phys. Eike Lennart Fricke	Prof. Dr. M. Grundmann / Prof. Dr. B. Rauschenbach	*Nanostructured thin films and surfaces: Generalised ellipsometry and rigorous optical modeling*
Dipl.-Phys. Niklas Fricke	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Polymer conformations in disordered environments*
M.Sc. Phys. Nataliya Georgieva	Prof. Dr. J. Haase / Prof. Dr. B. Rosenow	*Magnetic resonance of topological insulators*
M.Sc. Chem. Anika Gladytz	Prof. Dr. B. Abel / Prof. Dr. A.G. Beck-Sickinger	*Nanospectroscopy near chemical and biological interfaces*
M.Sc. Chem. Thomas Gladytz	Prof. Dr. B. Abel / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Tracing chirality, reactivity and structures in space and time of smart molecules and materials near interfaces by XUVI soft X-ray photoelectron emission and absorption spectroscopy*
M.Sc. Phys. Martin Glaser	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	*Investigation of actin structures*
M.Sc. Chem. Florian Glasneck	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Novel calix[4]arene derivatives and their complexation behaviour towards f-elements*
M.Sc. Phys. Tom Golde	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Actin related contractile structures*
Dipl.-Phys. Martin-Patrick Göse	Prof. Dr. D. Huster / Prof. Dr. T. Pompe	*Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Toni Grell	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Preparation of phosphorus-rich metal phosphides on the basis of oligophosphanide complexes*
M.Sc. Chem. Yuting Guo	Prof. Dr. H. Harms / Prof. Dr. F.-D. Kopinke	*Nanoparticle interactions with microorganisms on the molecular level*
Dipl.-Phys. Chris Händel	Prof. Dr. J. Käs / Prof. Dr. B. Abel	*Chemical oscillations in cell membranes*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Principles of mechanosensitivity and durotaxis in mammalian cells*
M.Sc. Phys. André Heber	Prof. Dr. F. Cichos / Prof. Dr. M. Grundmann	*Spatially resolved investigations of thermal transport in micro- and nanostructures*
M.Sc. Chem. Thomas Heinze	Prof. Dr. R. Gläser / Prof. Dr. B. Kirchner	*Noble metal nanoparticles on ordered porous supports for the in-situ synthesis and conversion of* H_2O_2 *in supercritical carbon dioxide*
Dipl.-Phys. Marcel Hennes	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Synthesis and characterisation of magnetic core-shell nanoparticles*
M.Sc. Biochem. Sven Hofmann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of peptides*
M.Sc. Chem. Reinhard Hoy	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phospholane-based coordination cages for application in homogeneous catalysis*
M.Sc. Chem. Astrid Jäschke	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Synthetic approaches towards novel calix[4]arene based f-metal receptors*
Dipl.-Phys. Alexander Janot	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Quantum condensates-coherence, fluctuations and disorder*
Dipl.-Pharm. Cathleen Jendrny	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Design and development of peptides for therapeutic application*
M.Sc. Chem. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Heterogeneously catalysed liquid phase oxidation of hydrocarbons over metal-organic frameworks*
M.Sc. Phys. Michael Jurkutat	Prof. Dr. J. Haase / Prof. Dr. W. Janke	*Investigation of the electronic properties of high-temperature superconductors by means of NMR*
M.Sc. Phys. Robert Karsthof	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Transparent photovoltaic cells*
Dipl.-Phys. Fabian Klüpfel	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	*Transparent active multi-electrode arrays for the measurement of nerve cell signals*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Jonas Kohlrautz	Prof. Dr. J. Haase / Prof. Dr. P. Esquinazi	*Magnetic resonance under extreme condidtions*
Dipl.-Phys. Andrea Kramer	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	*How temperature affects cell mechanics*
M.Sc. Chem. Robert Kuhnert	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranes as phenyl mimetics in biologically active substances*
Dipl.-Phys. Anja Landgraf	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Magneto-mechanical characterisation and training of single crystalline FePd films for the purpose of designing a thin film membrane pump*
Dipl.-Phys. Marc Lämmel	Prof. Dr. K. Kroy / Prof. Dr. W. Janke	*Stiff biopolymer solutions and networks*
Dipl.-Phys. Fritz Lehnert	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Ion-aided synthesis and investigation of nanoporous materials*
M.Sc. Phys. Jürgen Lippoldt	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Stochastic analysis of plasma membrane fluctuations of neuronal growth cones*
Dipl.-Phys. Martin Marenz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Development of a coarse-graining procedure for polymer adsorption*
M.Sc. Chem. Michael Marx	Prof. Dr. R. Gläser / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Modifying metal nanoparticles by oxidative extraction into supercritical solution*
M.Sc. Phys. Tom Michalsky	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Light-matter interaction in systems of reduced dimensionality*
M.Sc. Phys. Erik Morawetz	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	*Optical deformability and tumour aggressiveness*
Dipl.-Phys. Andreas Müller	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	*Peptide friction in cell adhesion*
M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Metal-organic frameworks with chiral binaphthalene-based linkers*
M.Sc. Chem. Paul Neumann	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Switchable dendritic ferrocenyl phosphines*
M.Sc. Chem. Wilma Neumann	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Development of cyclooxygenase inhibitors as anti-tumour agents by conjugation with cisplatin analogues or incorporation of carbaboranes*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Mareen Pagel	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of surfaces for novel biomaterials*
Dipl.-Phys. Steve Pawlizak	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	*Interplay between compartmentalisation of cells and tumour spreading*
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*
Dipl.-Phys. Stefan Puttnins	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*The influence of inhomogeneities in Cu(In,Ga)Se_2 thin film solar cells*
M.Sc. Chem. Dennis Richter	Prof. Dr. R. Gläser / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Heterogeneous photocatalysis: water splitting with visible-light irradiation*
Dipl.-Chem. Stefan Richter	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Synthesis of transition-metal-based cytostatics for conjugation with tumour-selective peptides*
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Spin polarisation investigations on exciton-polaritons and their condensates*
M.Sc. Chem. Stefan Saretz	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranes for medical applications*
M.Sc. Phys. Marina Sarmanova	Prof. Dr. B. Rauschenbach / Prof. Dr. S. Mayr	*Measurements with nanometer resolution of mechanical properties of thin layers and structured surfaces by the contact resonance atomic force microscopy*
Dipl.-Phys. Friedrich-Leonhard Schein	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Dynamic properties of ZnO-based integrated circuits*
M.Sc. Phys. Philipp Schierz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Investigation of polymer aggregation by computer simulations*
M.Sc. Phys. Peter Schlupp	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Growth and optimisation of amorphous p- and n-type oxide semiconductors for electronic device applications*
M.Sc. Chem. Andy Schmied	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Phosphorus based nano-frames*
Dipl.-Phys. Jörg Schnauß	Prof. Dr. J. Käs / Prof. Dr. A.G. Beck-Sickinger	*Biomimetic actin networks*
Dipl.-Biol. Ria Anne-Rose Schönauer	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Chemical modification of peptide analogues*

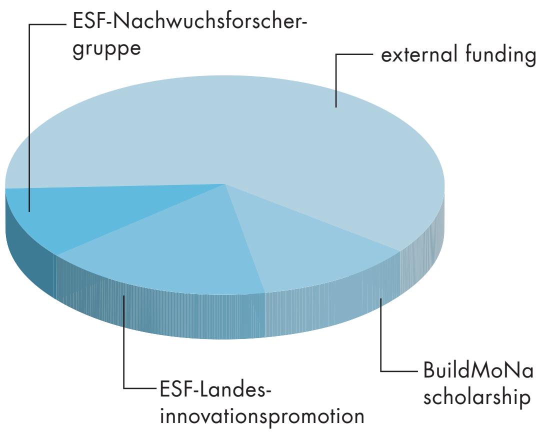
Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Carsten Schuldt	Prof. Dr. J. Käs / Prof. Dr. B. Abel	*Cellular force generation on the single molecule level*
M.Sc. Phys. Daniel Thomas Splith	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Investigation and optimisation of ß-Ga_2O_3 thin films and their application for electronic devices*
Dipl.-Phys. Tim Stangner	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Investigation of receptor/ligand interactions on the level of single contacts using high-resolution optical tweezers*
M.Sc. Chem. Karolin Stein	Prof. Dr. H. Krautscheid / Prof. Dr. B. Kersting	*1,2,4-triazolyl ligands for the synthesis of porous coordination polymers*
M.Sc. Phys. Xinxing Sun	Prof. Dr. B. Rauschenbach / Prof. Dr. S. Mayr	*Phase change materials*
M.Sc. Chem. Eng. Erik Thelander	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Synthesis of nanostructures using laser ablation*
Dipl.-Phys. Martin Thunert	Prof. Dr. M. Grundmann / Prof. Dr. B. Rosenow	*Bose-Einstein-Condensation and superfluids of exciton-polaritons in ZnO-based microresonators*
M.Sc. Phys. Martin Treffkorn	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	*Theoretical analysis of nanostructures for topolocgical quantum computing*
M.Sc. Chem. Steve Ullmann	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Extration of rare earths by means of preorganised calixarene*
M.Sc. Chem. Zhaoyang Wang	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	*Metal-organic frameworks based on linkers with hard and soft donor groups*
M.Sc. Phys. Marcel Wille	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Whispering Gallery modes: influence of the resonator shape on lasing properties*
B.Sc. Eng. Emilia Wisotzki	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Interaction of nanoparticles and polymers with biological matter for mechanical coupling*
M.Sc. Phys. Guillermo Zecua Ramirez	Prof. Dr. K. Kroy / Prof. Dr. T. Pompe	*Inelastic mechanics of the cytoskeleton and cell morphology*
M.Sc. Phys. Johannes Zierenberg	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Aggregation of polymers in crowded confinement with correlated disorder*

Alumni 2014

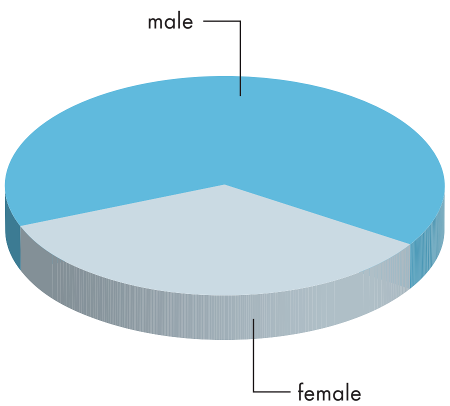
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Ana Isabel Ballestar Balbas	Prof. Dr. P. Esquinazi / Prof. Dr. T. Butz	*Superconductivity at graphite interfaces*
Dr. rer. nat. Kerstin Brachwitz	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Defect-induced conduction mechanisms and magnetic properties of spinel-type ferrites*
Dr. rer. nat. Martin Brehm	Prof. Dr. B. Kirchner / Prof. Dr. R. Gläser	*Analysing trajectories from molecular simulation*
Dr. rer. nat. Anatol Fritsch	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*From individual cells to tumour aggregates: Biomechanical and thermorheological studies*
Dr. rer. nat. Sina Gruschinski	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Carboxylate-functionalised chelate ligands as building blocks for the representation of exchange-coupled paramagnetic polynuclear complexes*
Dr. rer. nat. Marcel Handke	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	*MOFs: Structurally flexible coordination polymers with conformationally flexible ligand–ligand substitution and gate opening behaviour*
Dr. rer. nat. Tobias Kießling	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Thermorheology of living cells – The impact of temperature variations on cell mechanics*
Dr. rer. nat. Melanie Knorr	Prof. Dr. J. Käs	*Stochastic fluctuations in cell motility from leading edge to collective motion*
Dr. rer. nat. Christian Kranert	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Investigation of wide-bandgap semiconductors by UV Raman spectroscopy: resonance effects and material characterisation*
Dr. rer. nat. Anusree Viswanath Kuttatheyil	Prof. Dr. J. Haase / Prof. Dr. H. Krautscheid	*Multinuclear solid-state NMR spectroscopy of metal-organic frameworks characterisation based on organic ligands, metal centres and small molecule adsorption*
Dr. rer. nat. Veronika Mäde	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Pancreatic polypeptide analogs to modulate receptor function for therapeutic applications*
Dr. rer. nat. Tobias Möller	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. S. Berger	*P-chiral phosphines – new synthetic approaches*
Dr. rer. nat. Eva Perlt	Prof. Dr. B. Kirchner / Prof. Dr. B. Abel	*Floating orbital molecular dynamics*
Dr. rer. nat. Florian Schmidt	Prof. Dr. M. Grundmann / Prof. Dr. R. Gläser	*Depletion region spectroscopic methods for the characterisation of wide bandgap semiconductors*
Dr. rer. nat. Marko Stölzel	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Photoluminescence of excitons in polar ZnO/MgZnO quantum grave structures*
Dr. rer. nat. Dan Strehle	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Bundles of semi-flexible cytoskeletal filaments*
Dr. rer. nat. Martin Treß	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	*Broadband dielectric spectroscopy for the investigation of the molecular dynamics in nanometre-thick polymer layers*
Dr. rer. nat. Franziska Wetzel	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Biomechanical phenotyping of cells in tissue and determination of impact factors*
Dr. rer. nat. Patrick With	Prof. Dr. R. Gläser / Prof. Dr. Dr. h.c. E. Hey-Hawkins	*Preparation, physico-chemical characterisation and testing of supported metal (oxide) catalysts*

Statistics

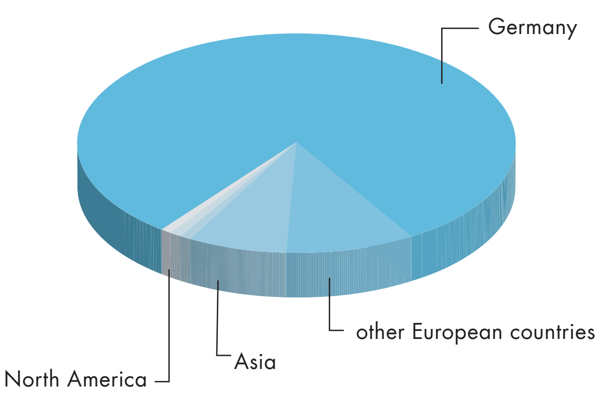
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:



Biophysical and macromolecular chemistry

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

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

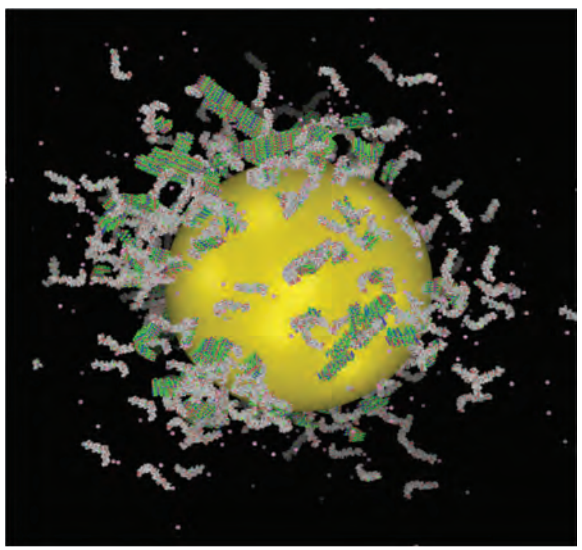
Within BuildMoNa we investigate amyloid aggregation and fibrillation with nanoscale imaging and spectroscopic techniques and we aimed at monitoring struc-

ures of aggregated proteins near interfaces of nanoparticles to resolve the question whether nanoparticles may induce Alzeimer's disease (A. Gladytz).

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

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

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



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

Prof. Dr. Bernd Abel
Wilhelm Ostwald Institute for Physical and Theoretical Chemistry
http://www.pc-uni-leipzig.de
E-mail: bernd.abel@uni-leipzig.de
Phone: +49 341 235-2715
Fax: +49 341 235-2317

Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger
M.Sc. Chem. David Boehme, M.Sc. Chem. Milos Erak, M.Sc. Biochem. Sven Hofmann, Dipl.-Pharm. Cathleen Jendrny, Dr. Veronika Mäde, M.Sc. Chem. Mareen Pagel, Dipl.-Biol. Ria Anne-Rose Schönauer

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

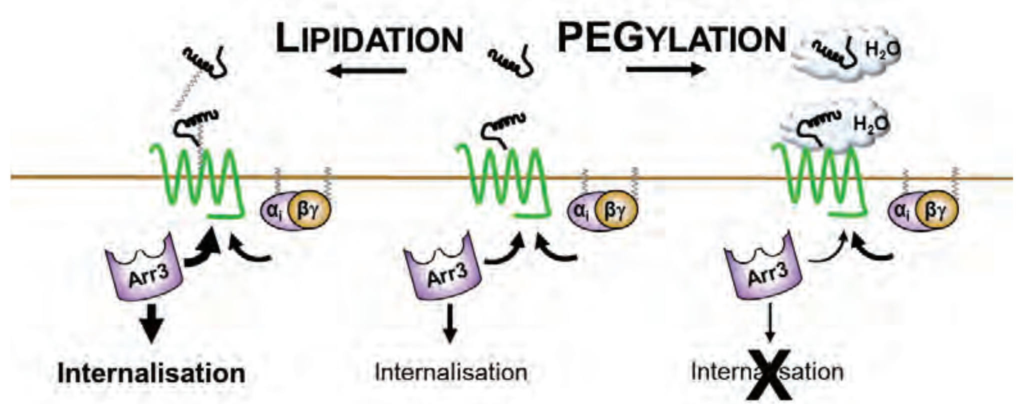
In 2014 Veronika Mäde finished her PhD. Veronika Mäde developed chemically modified analogues of pancreatic polypeptide and could find out that pegylation and palmitoylation lead to significant differences with respect to biological activity of peptide hormones. Furthermore she could modulate activity and selectivity by us-

ing different lipid moieties.

Sven Hofmann (M.Sc. Biochem.) and David Böhme (M.Sc. Chem.) work on the development of novel anti-tumour peptides by conjugation with carbaboranes or cytotoxic compounds. The peptides are used as shuttle systems to allow tumour specific uptake as the respective peptide receptors are overexpressed on tumour cells and internalise after agonist binding.

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

The field of biomaterial approaches was extremely successful in 2014. Mareen Pagel (Dipl.-Chem.) worked on chemically modified peptides and proteins to improve the properties of biomaterials. She has developed a novel biocompatible ligation method, the inverse Diels-Alder reaction, and successfully applied this to the derivatisation of inorganic surfaces. She could impressively show that cells prefer coated surfaces.



⇑ Pamitoylation favours arrestin-3 recruitment and internalisation of the ligand-receptor complex, whereas pegylation does not and leads to reduced internalisation. This was identified by Mäde et al. 2014 (V. Mäde, S. Babilon et al. / Angew. Chem. Int. Ed. (2014) **53** 10067).

⇒ *Slime Protein Profiling: A Non-invasive Tool for Species Identification in Onychophora (Velvet Worms)*
A. Baer, I. de Sena Oliveira, M. Steinhagen, A.G. Beck-Sickinger, G. Mayer / J. Zool. System. Evolut. Res. (2014) **52** 265

⇒ *Position and Length of Fatty Acids Strongly Affect Receptor Selectivity Pattern of Human Pancreatic Polypeptide Analogues*
V. Mäde, K. Bellmann-Sickert, A. Kaiser, J. Meiler, A.G. Beck-Sickinger / Chem. Med. Chem. (2014) **9** 2463

⇒ *Peptide Modifications Differentially Alter G Protein-coupled Receptor Internalization and Signaling Bias*
V. Mäde, S. Babilon, N. Jolly, L. Wanka, K. Bellmann-Sickert, L.E. Diaz Gimenez, K. Mörl, H.M. Cox, V.V. Gurevich, A.G. Beck-Sickinger / Angew. Chem. Int. Ed. Engl. (2014) **53** 10067

⇒ *Automated Solid-phase Peptide Synthesis to Obtain Therapeutic Peptides*
V. Mäde, S. Els-Heindl, A.G. Beck-Sickinger / Beilstein J. Org. Chem. (2014) **10** 1197

⇒ *Matrix Metalloproteinase 9 (MMP-9) Mediated Release of MMP-9 Resistant Stromal Cell-derived Factor 1α (SDF-1α) from Surface Modified Polymer Films*
M. Steinhagen, P.G. Hoffmeister, K. Nordsieck, R. Hötzel, L. Baumann, M.C. Hacker, M. Schulz-Siegmund, A.G. Beck-Sickinger / ACS Appl. Mater. Interfaces (2014) **6** 5891

Prof. Dr. Annette G. Beck-Sickinger
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

Single molecule trapping in dynamic temperature fields

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

The stable trapping of single molecules in liquids for an extended time of several hundred seconds is one of the long-standing challenges of single molecule spectroscopy. The observation of rare events, i.e. the misfolding of proteins to dysfunctional structures is limited by the possible observation time, which is typically only a few seconds. Long time observation becomes increasingly difficult as smaller objects diffuse more quickly according to the Stokes-Einstein relation. For this purpose new techniques employing homogeneous electric fields applied by small electrode structures appeared in the literature and provide a first glimpse on what type of novel experiments is possible. Current approaches allow the trapping of small organic chromophores. The molecular nano-photonics group has developed an experimental technique which is now going beyond the capabilities of the existing methods. The developed method relies on a spatio-temporal manipulation of the temperature. A small gold structure is heated optically to generate a highly localised temperature field. The resulting temperature gradient causes a thermophoretic drift typically directed away from the heat source.

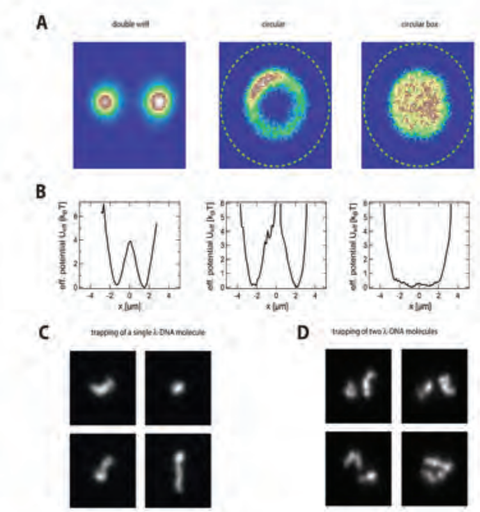
During the last year, we have been successful in:

a) Showing that temperature gradients of a few Kelvin per micrometer are sufficient to trap a single DNA molecule in water for time periods of more than 10 minutes giving access to even slow conformational fluctuations and chain statistics. The long time trapping is achieved by an optical feedback adjusting the position of the heat source in real-time.

b) Showing that the optical feedback can be modified to trap a well defined number of multiple molecules which gives unique possibilities for bimolecular interaction studies, i.e. for protein aggregation (see figure).

c) Showing that the optical feedback rules can be modified to obtain an almost arbitrary trapping potential (see figure).

These achievements now provide a toolbox which not only allows the study of single molecules and their interaction for biophysical studies, but also the means to explore fundamental aspects of the relation of information and work in thermal non-equilibrium.



⇐ **A** Heat map of particle positions for a 200 nm polystyrene particle in a thermophoretic feedback trap to create double, a circular and a circular box potential. **B** Corresponding potential cross-sections. **C, D** Snapshots from a single DNA molecule (left) and two single DNA molecules confined in the thermo-phoretic feedback trap.

⇒ *Metal Nanoparticle Based All-Optical Photothermal Light Modulator*
A. Heber, M. Selmke, F. Cichos / ACS Nano (2014) **8** 1893

⇒ *Photothermal Single Particle Microscopy Using a Single Laser Beam*
M. Selmke, A. Heber, M. Braun, F. Cichos / Applied Physics Letters (2014) **105** 013511

⇒ *Distortion of Power Law Blinking with Binning and Thresholding*
N. Amecke, A. Heber, F. Cichos / Journal of Chemical Physics (2014) **140** 114306

⇒ *Trapping of Single Nano-objects in Dynamic Temperature Fields*
M. Braun, A. Würger, F. Cichos / Phys. Chem. Chem. Phys. (2014) **16** 15207

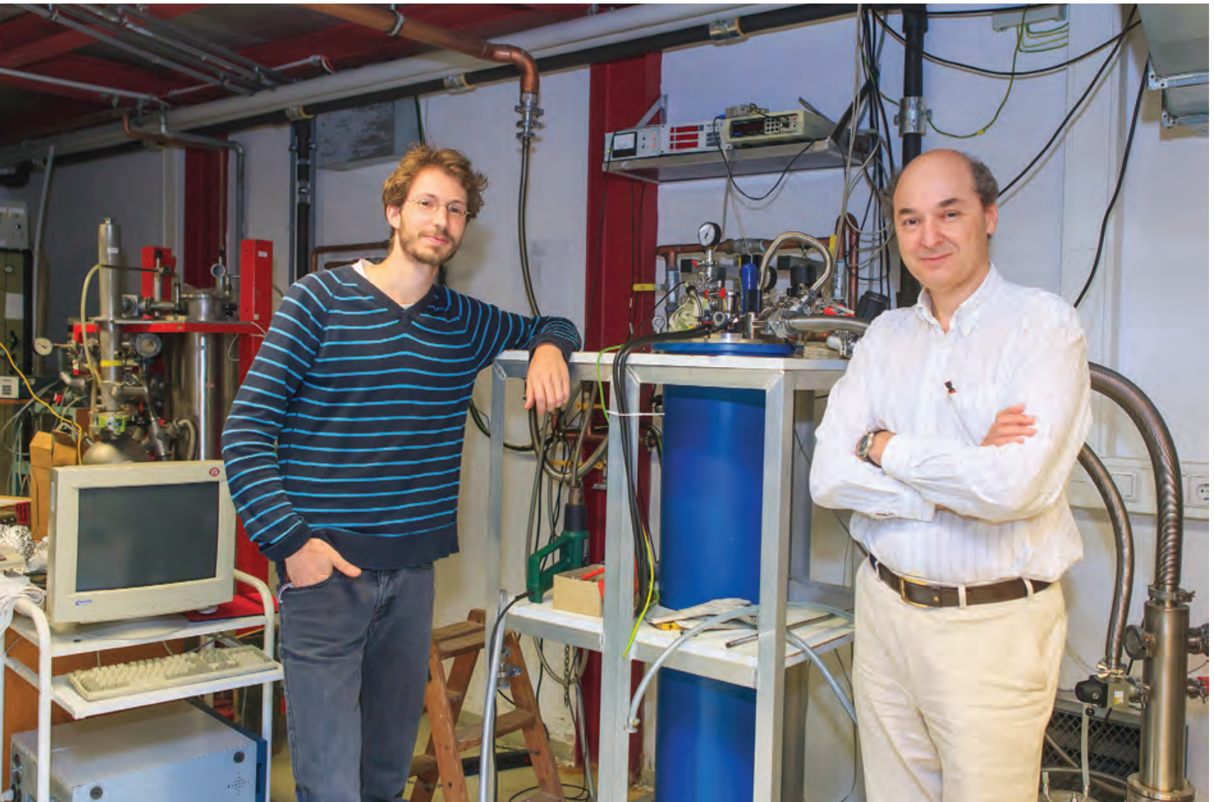
Prof. Dr. Frank Cichos
Institute for Experimental Physics I
http://www.uni-leipzig.de/~mona/
E-mail: cichos@physik.uni-leipzig.de
Phone: +49 341 97-32571
Fax: +49 341 97-32598

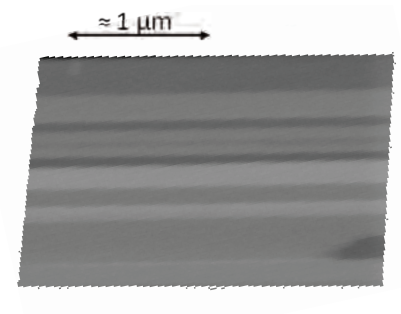
Superconductivity at graphite interfaces

Prof. Dr. Pablo D. Esquinazi
Dr. Ana Isabel Ballestar Balbas, M.Sc. Phys. Francis Bern

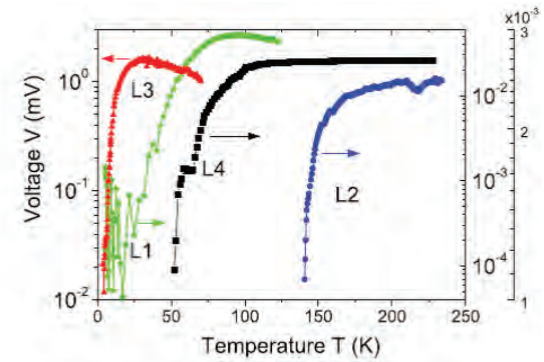
To understand the properties of the embedded interfaces in graphite, we have performed transport measurements contacting the edges of the embedded interfaces in different graphite samples. The TEM lamellae showed non-linear current-voltage characteristic curves, a drop of the voltage decreasing temperature, compatible with the existence of non-percolative superconducting regions weakly coupled by Josephson-coupling within graphene planes. The results are the first clear superconducting-like response through transport measurements in graphite that indicate the existence of superconductivity at graphite interfaces.

Local and non-local measurements were performed in pin-hole dominated mesoscopic multigraphene samples spin-valves. We found a strong local Hall effect that might hinder the spin injection into multigraphene, resulting in no spin signal in non-local measurements.





⇐ TEM picture of a graphite lamella with the electron beam parallel to the grahene layers. The different gray colors indicate graphite blocks with Bernal stacking order rotated different twist angles around the c-axis. This c-axis is normal to the graphene layers.



⇐ Temperature dependence of the voltage in a logarithmic scale for four samples measured with small input currents. A clear drop in the measured voltage is observed at 15 K < T < 150 K upon sample. For the sample L4, the region near the onset of voltage decrease is shown (second right y-axis)

⇒ *Multiferroic $BaTiO_3$–$BiFeO_3$ Composite Thin Films and Multilayers: Strain Engineering and Magnetoelectric Coupling*
M. Lorenz, V. Lazenka, P. Schwinkendorf, F. Bern, M. Ziese, H. Modarresi, A. Volodin, M.J . Van Bael, K. Temst, A. Vantomme, M. Grundmann / J. Phys. D: Appl. Phys. (2014) **47** 135303

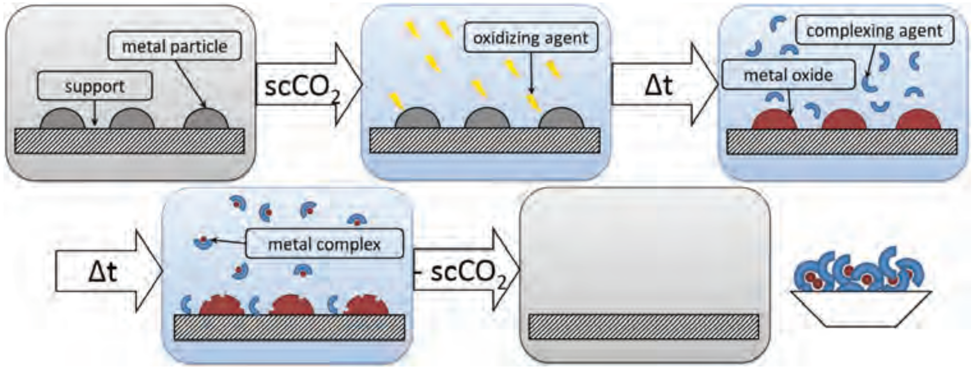
⇒ *Possible Superconductivity in Multi-Layer-Graphene by Application of a Gate Voltage*
A. Ballestar, P. Esquinazi, J. Barzola-Quiquia, S. Dusari, F. Bern, R.R. da Silva, Y. Kopelevich / Carbon (2014) **72** 312

Prof. Dr. Pablo D. Esquinazi
Institute for Experimental Physics II
http://http://www.uni-leipzig.de/~sum/
E-mail: esquin@physik.uni-leipzig.de
Phone: +49 341 97-32751
Fax: +49 341 97-32769

Complex nanomaterials for applied and innovative catalysis

Prof. Dr. Roger Gläser
M.Sc. Chem. Thomas Heinze, M.Sc. Chem. Ulrike Junghans, M.Sc. Chem. Michael Marx, M.Sc. Phys. Marcus Purfürst, M.Sc. Chem. Dennis Richter, Dr. Patrick With

Innovative catalytic systems continue to play a key role in heterogeneous catalysis. The research in our group is centred on nanoporous materials with defined porosity and tunable active components to investigate solutions to current challenges in catalysis, such as energy efficiency, stability, mass transfer and recycling. Following the principle approaches of the graduate school, we apply different strategies to synthesise novel materials for the use as catalysts and catalyst supports. One focus is on the immobilisation of multi-enzyme conjugates on hierarchically structured hexagonal mesoporous silicates. Also, the activity and stability of transition-metal containing metal-organic frameworks are studied in the liquid-phase oxidation of hydrocarbons under continuous-flow conditions. In terms of sustainable chemistry, a key research area is the recovery of metals from spent supported metal catalysts by supercritical fluid oxidative extraction. Moreover, the selective catalytic reduction of nitrogen oxides and the soot filtration and oxidation by diesel particulate filters is investigated as means of environmental protection. In the area of alternative fuels, we apply in-situ monitoring of reaction dynamics and transport of reactants during the transesterification of oils into biodiesel by multinuclear NMR techniques. Also, energy-related catalysis with the aim of photocatalytic water splitting for hydrogen production over modified porous carbon nitrides is another prominent research area.



⇑ Schematic presentation of supercritical fluid oxidative extraction (SFOE) for the recovery of metals from spent supported metal catalysts.

⇒ *Solid-Ionic Liquid Interfaces: Pore Filling Revisited*
T. Heinze, J.C. Zill, J. Matysik, W.-D. Einicke, R. Gläser, A. Stark / Phys. Chem. Chem. Phys. (2014) **16** 24359

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

Amorphous semiconductor diodes – A new paradigm

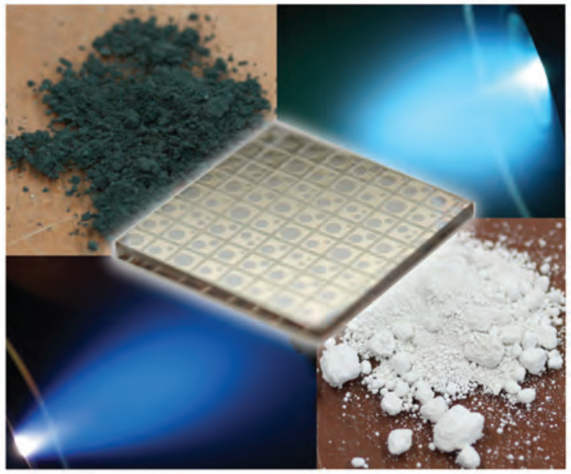
Prof. Dr. Marius Grundmann
M.Sc. Phys. Michael Bonholzer, Dr. Kerstin Brachwitz, Dipl.-Phys. Felix Daume, M.Sc. Phys. Eike Lennart Fricke, M.Sc. Phys. Robert Karsthof, Dipl.-Phys. Fabian Klüpfel, Dr. Christian Kranert, M.Sc. Phys. Tom Michalsky, Dipl.-Phys. Stefan Puttnins, M.Sc. Phys. Steffen Richter, Dipl.-Phys. Friedrich-Leonhard Schein, M.Sc. Phys. Peter Schlupp, Dr. Florian Schmidt, M.Sc. Phys. Daniel Thomas Splith, Dr. Marko Stölzel, Dipl.-Phys. Martin Thunert, M.Sc. Phys. Marcel Wille

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

Several BuildMoNa doctoral candidates in the Semiconductor Physics Group have achieved decisive progress in the use of such materials by building various electronic devices previously thought to be impossible. In particular the use of amorphous semiconductors and the deposition of thin films at room temperature enables the use of amorphous substrates, in particular cost-economic glass, and flexible polymeric substrates such as plastic foils for wearable electronics. These properties are explored in and supported through a new Horizon 2020 project ("LOMID") and DFG-funded projects.

Peter Schlupp adds a further twist to the story as he abandoned all materials that are overly toxic, rare and expensive by only resorting to metal oxides from abundant metals like tin, zinc and cobalt. He fabricated fully amorphous bipolar diodes from zinc-tin-oxide as the n-type materials and zinc-cobalt-oxide as the p-type material. Zinc-cobalt oxide was explored by Friedrich L. Schein who has in the meantime successfully finished his BuildMoNa curriculum and received his doctoral degree. All layers in the new diodes are deposited at room temperature and the starting materials are powders of the respective materials (see figure) with the optimised metal ratios (i.e. Zn/Sn and Zn/Co). The amazing result is that such pn-diodes easily outperform any previous reported approach, including even devices fabricated with sophisticated growth methods such as molecular beam epitaxy (MBE) and high temperature deposition and annealing [P. Schlupp, F.-L. Schein, H. von Wenckstern, M. Grundmann: *All Amorphous Oxide Bipolar Heterojunction Diodes from Abundant Metals* / Adv. Electr. Mater. (2015) **1** 1400023]. The only bipolar oxide diodes with better performance than Peter Schlupp's diodes come from other BuildMoNa students of our Leipzig team using more elaborate processing and higher deposition temperatures as reported in the 2013 BuildMoNa annual report.

Building on the great success of particularly our p-type amorphous oxides, BuildMoNa doctoral candidate Robert Karsthof has also explored amorphous nickel oxide as contact in bipolar diodes. He has found that NiO is equally useful as



⇑ Raw oxide powders for the fabrication of bipolar (Zn,Sn)O/(Zn,Co)O diodes (chip in the centre) and plasma plumes of pulsed laser deposition of these materials.

$ZnCo_2O_4$ with the added advantage of transparency [M. Grundmann, R. Karsthof, H. von Wenckstern: *The Recombination Current in Type-II Heterostructure Bipolar Diodes* / ACS Appl. Mat. & Interf. (2014) **6** 14785]. Robert has subsequently built transparent transistors using a NiO/ZnO gate electrode (JFETs) and also has achieved an UV (ultraviolet) solar radiation energy harvester (transparent solar cell) with a high efficiency of more than 20% in the UV region for the local power-up of fully transparent electronics.

⇒ *The Recombination Current in Type-II Heterostructure Bipolar Diodes*
M. Grundmann, R. Karsthof, H. von Wenckstern / ACS Applied Materials & Interfaces (2014) **6** 14785

⇒ *Improving the Optical Properties of Self-catalyzed GaN Microrods Towards Whispering Gallery Mode Lasing*
C. Tessarek, R. Röder, T. Michalsky, S. Geburt, H. Franke, R. Schmidt-Grund, M. Heilmann, B. Hoffmann, C. Ronning, M. Grundmann, S. Christiansen / ACS Photonics (2014) **1** 990

⇒ *Phonon-assisted Lasing in ZnO Microwires at Room Temperature*
T. Michalsky, M. Wille, C.P. Dietrich, R. Röder, C. Ronning, R. Schmidt-Grund, M. Grundmann / Applied Physics Letters (2014) **105** 211106

⇒ *Temperature Dependence of the Dielectric Function in the Spectral Range (0.5–8.5) eV of an* In_2O_3 *Thin Film*
R. Schmidt-Grund, H. Krauß, C. Kranert, M. Bonholzer, M. Grundmann / Applied Physics Letters (2014) **105** 111906

⇒ *Modeling the Electrical Transport in Epitaxial Undoped and Ni-, Cr-, and W-doped* TiO_2 *Anatase Thin Films*
M. Kneiß, M. Jenderka, K. Brachwitz, M. Lorenz, M. Grundmann / Applied Physics Letters (2014) **105** 062103

⇒ *Determination of the Spontaneous Polarization of Wurtzite (Mg,Zn)O*
M. Stölzel, A. Müller, G. Benndorf, M. Lorenz, M. Grundmann, C. Patzig, T. Höche / Applied Physics Letters (2014) **104** 192102

⇒ *Highly Rectifying p-*$ZnCo_2O_4$*/n-ZnO Heterojunction Diodes*
F.-L. Schein, M. Winter, T. Böntgen, H. von Wenckstern, M. Grundmann / Applied Physics Letters (2014) **104** 022104

⇒ *Schottky Contacts to* In_2O_3
H. von Wenckstern, D. Splith, F. Schmidt, M. Grundmann, O. Bierwagen, J.S. Speck / APL Materials (2014) **2** 046104

⇒ *Method of Choice for Fabrication of High-quality ZnO-based Schottky Diodes*
S. Müller, H. von Wenckstern, F. Schmidt, D. Splith, R. Heinold, M. Allen, M. Grundmann / Journal of Applied Physics (2014) **116** 194506

⇒ *Impact of Strain on Defects in (Mg,Zn)O Thin Films*
F. Schmidt, S. Müller, H. von Wenckstern, G. Benndorf, R. Pickenhain, M. Grundmann / Journal of Applied Physics (2014) **116** 103703

⇒ *Dielectric Function in the NIR-VUV Spectral Range of* $(In_xGa_{1-x})_2O_3$ *Thin Films*
R. Schmidt-Grund, C. Kranert, T. Böntgen, H. von Wenckstern, H. Krauß, M. Grundmann / Journal of Applied Physics (2014) **116** 053510

⇒ *Lattice Parameters and Raman-active Phonon Modes of* $(In_xGa_{1-x})_2O_3$ *for* $x < 0.4$
C. Kranert, J. Lenzner, M. Jenderka, M. Lorenz, H. von Wenckstern, R. Schmidt-Grund, M. Grundmann / Journal of Applied Physics (2014) **116** 013505

⇒ Ultrafast Dynamics of the Dielectric Functions of ZnO and BaTiO3 Thin Films after Intense Femtosecond Laser Excitation
S. Acharya, S. Chouthe, H. Graener, T. Böntgen, C. Sturm, R. Schmidt-Grund, M. Grundmann, G. Seifert / Journal of Applied Physics (2014) **115** 053508

⇒ *Multiferroic* $BaTiO_3$*-*$BiFeO_3$ *Composite Thin Films and Multilayers: Strain Engineering and Magnetoelectric Coupling*
M. Lorenz, V. Lazenka, P. Schwinkendorf, F. Bern, M. Ziese, H. Modarresi, A. Volodin, M. van Bael, K. Temst, A. Vantomme, M. Grundmann / Journal of Physics D: Applied Physics (2014) **47** 135303

⇒ *Highly Textured Fresnoite Thin Films Synthesized by Pulsed Laser Deposition with* CO_2 *Laser Direct Heating*
M. Lorenz, A. de Pablos-Martin, C. Patzig, M. Stölzel, K. Brachwitz, H. Hochmuth, M. Grundmann, T. Höche / Journal of Physics D: Applied Physics (2014) **47** 034013

⇒ *Conducting Behavior of Chalcopyrite-type* $CuGaS_2$ *Crystals Under Visible Light*
J.L. Cholula-Díaz, J. Barzola-Quiquia, H. Krautscheid, C. Kranert, T. Michalsky, P. Esquinazi, M. Grundmann / Physical Chemistry Chemical Physics (2014) **16** 21860

⇒ *Determination of the Mean and the Homogeneous Barrier Height of Cu Schottky Contacts on Heteroepitaxial* β*-*Ga_2O_3 *Thin Films Grown by Pulsed Laser Deposition*
D. Splith, S. Müller, F. Schmidt, H. von Wenckstern, J.J. van Rensburg, W.E. Meyer, M. Grundmann / physica status solidi (a) (2014) **211** 40

⇒ *Control of the Conductivity of Si-doped* β*-*Ga_2O_3 *Thin Films via Growth Temperature and Pressure*
S. Müller, H. von Wenckstern, D. Splith, F. Schmidt, M. Grundmann / physica status solidi (a) (2014) **211** 34

⇒ *Layer-by-Layer Growth of TiN by Pulsed Laser Deposition on in-situ Annealed (100) MgO Substrates*
M. Bonholzer, M. Lorenz, M. Grundmann / physica status solidi (a) (2014) **211** 2621

⇒ *Defect Studies on Ar-Implanted ZnO Thin Films*
F. Schmidt, S. Müller, R. Pickenhain, H. von Wenckstern, S. Geburt, C. Ronning, M. Grundmann / physica status solidi (b) (2014) **251** 937

⇒ *Raman Active Phonon Modes of Cubic* In_2O_3
C. Kranert, R. Schmidt-Grund, M. Grundmann / physica status solidi rapid research letters (2014) **8** 554

⇒ *Electronic Transitions and Dielectric Function Tensor of a* $YMnO_3$ *Single Crystal in the NIR–VUV Spectral Range*
R. Schmidt-Grund, S. Richter, S.G. Ebbinghaus, M. Lorenz, C. Bundesmann, M. Grundmann / RSC Advances (2014) **4** 33549

⇒ *Breakdown Characteristics of Flexible Cu(In,Ga)*Se_2 *Solar Cells*
S. Puttnins, S. Jander, A. Wehrmann, G. Benndorf, M. Stölzel, A. Müller, H. von Wenckstern, F. Daume, A. Rahm, M. Grundmann / Solar Energy Materials and Solar Cells (2014) **120** 506

⇒ *Low Rate Deep Level Transient Spectroscopy: A Powerful Tool for Defect Characterization in Wide Bandgap Semiconductors*
F. Schmidt, H. von Wenckstern, O. Breitenstein, R. Pickenhain, M. Grundmann / Solid-Stade Electronics (2014) **92** 40

⇒ *An Extended Drude Model for the in-situ Spectroscopic Ellipsometry Analysis of ZnO Thin Layers and Surface Modifications*
L. Fricke, T. Böntgen, J. Lorbeer, C. Bundesmann, R. Schmidt-Grund, M. Grundmann / Thin Solid Films (2014) **571** 437

⇒ *Several Approaches to Bipolar Oxide Diodes With High Rectification*
M. Grundmann, F.-L. Schein, R. Karsthof, P. Schlupp, H. von Wenckstern / Adv. Sci. Technol. (2014) **93** 252

⇒ *Optical Properties of and Optical Devices from ZnO-based Nanostructures*
M. Lorenz, M. Lange, C. Kranert, C.P. Dietrich, M. Grundmann / Zinc Oxide Nanostructures: Advances and Applications, M. Willander, ed. (Pan Stanford Publishing, Singapore, 2014) 43

Prof. Dr. Marius Grundmann
Institute for Experimental Physics II
http://www.uni-leipzig.de/~hlp/
E-mail: grundmann@physik.uni-leipzig.de
Phone: +49 341 97-32650
Fax: +49 341 97-32668

Investigation of the properties of modern materials with Magnetic Resonance

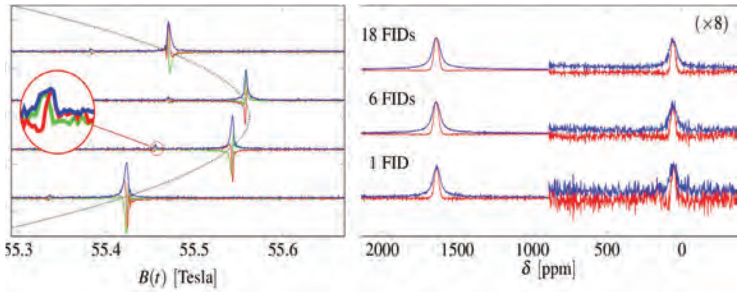
Prof. Dr. Jürgen Haase
M.Sc. Phys. Nataliya Georgieva, M.Sc. Phys. Michael Jurkutat, Dipl.-Phys. Jonas Kohlrautz, Dr. Anusree Viswanath Kuttatheyil

We are using the methods of Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR) to investigate the properties of materials, notably high-temperature superconductors, topological insulators, or porous materials like metal-organic frameworks (MOFs).

As the magnetic field strength is an important parameter for many systems, access to the highest fields possible is of great interest. These can only be obtained using pulsed magnets in dedicated facilities. We collaborate with the Dresden High Magnetic Field Laboratory to establish NMR at fields up to 70 T. Here, we develop methods to measure the NMR shift as well as relaxation under pulsed field conditions.

Topological insulators (TIs) are of interest in the condensed matter physics community. Using ^{77}Se NMR of the model compound Bi_2Se_3 we could characterise the special bulk electronic states of TIs. We discovered for the first time inequivalent Se sites and an uncommon indirect coupling. This enables us now to search for surface electronic states with NMR. For this purpose, nanocrystalline and microcrystalline powders having different surface-to-volume ratios have been produced and investigated. Significant differences in the NMR parameters of the two samples have been found (to be published).

The superconducting cuprates are still of great interest in condensed matter research. We investigated the shifts for several different doping levels of $HgBa_2CuO_4{}^{+}\backslash\Delta$ as a function of temperature and orientation. Here, we found that a multi-component description is needed to explain the observations, concluding the proof for the failure of a single fluid picture.



⇑ Knight shift measurements of metallic aluminum at about 56 Tesla. Linde type A zeolite (weak signal) is used to calibrate the shift scale (to be published).

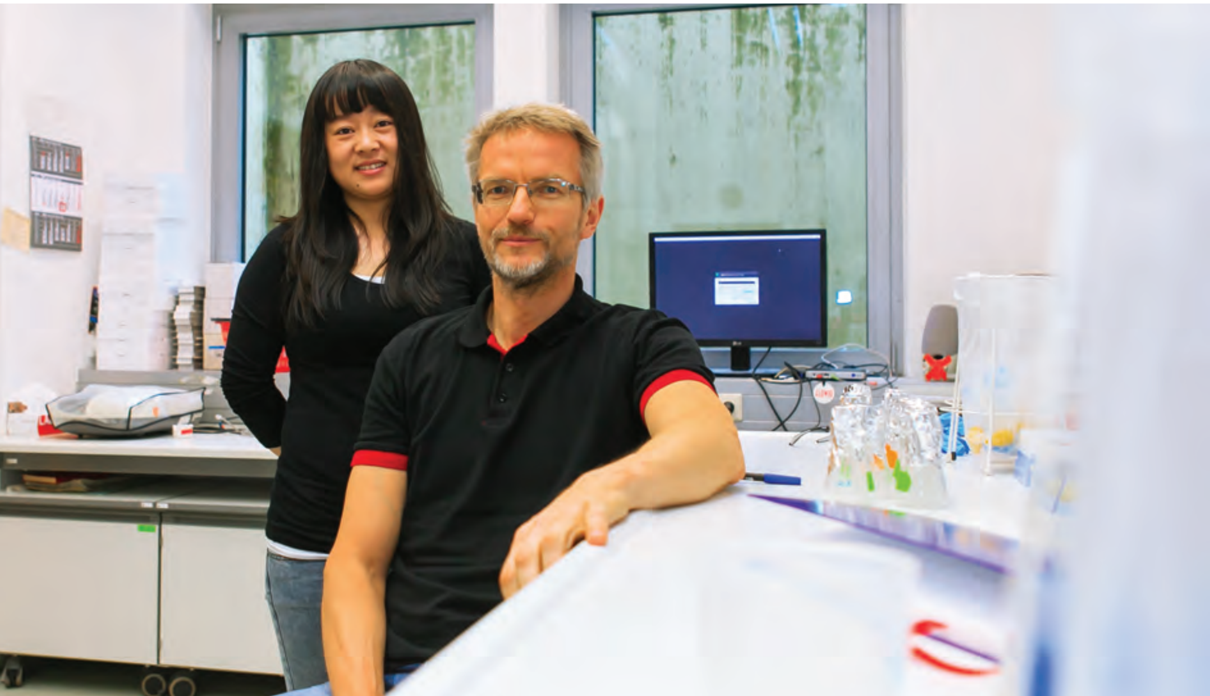
⇒ *Distribution of Electrons and Holes in Cuprate Superconductors as Determined from ^{17}O and ^{63}Cu Nuclear Magnetic Resonance*
M. Jurkutat, D. Rybicki, O.P. Sushkov, G.V.M. Williams, A. Erb, J. Haase / Phys. Rev. B (2014) **90** 140504

Prof. Dr. Jürgen Haase
Institute for Experimental Physics II
http://www.uni-leipzig.de/~mqf/
E-mail: j.haase@physik.uni-leipzig.de
Phone: +49 341 97-32601
Fax: +49 341 97-32649

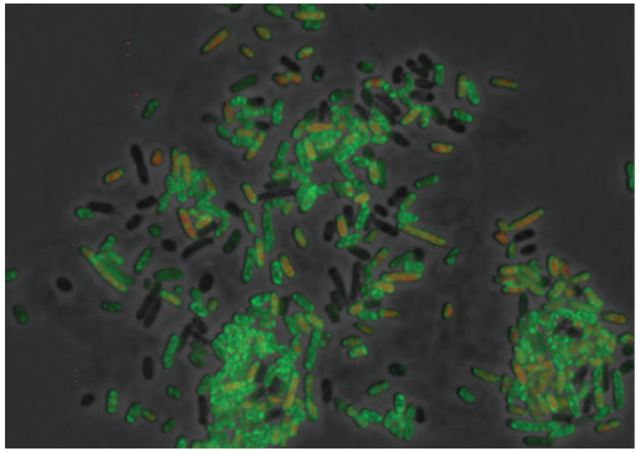
Nanoparticle interactions with micro-organisms on the molecular level

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

The small size of industrial nanoparticles results in a high surface to volume ratio, which is one reason for their high reactivity making them highly attractive for various technical applications and as ingredients in a constantly growing number of consumer products. Reactivity is, however, a Janus-faced characteristic as at the end of the product's lifetime it may result in undesired, detrimental effects in organisms and ecosystems. Our research at the Helmholtz Centre for Environmental Research addresses interactions of silver nanoparticles (which are purposely antibacterial) with microorganisms at the molecular level. We are particularly interested in the effects of silver nanoparticles on bacterially-based ecosystem services such as biodegradation and waste water treatment. Our present research focuses on nanoparticle effects on the physiology of two model bacteria (Pseudomonas putida KT2440 and Mycobacterium frederiksbergense LB501T), which are characterised by fundamentally different cell walls. The central method of our investigations is the flow cytometric analysis of bacterial populations, which allows to study the physiological status of high numbers of individuals at the single cell level and, after selective cell sorting, can be combined with -omics analyses (e.g. proteomics) to gain deeper insight into the underlying toxicity mechanisms.



In the first phase of the project, the flow cytometric methodology was tailored to the requirements, which consisted for instance in the choice and calibration of appropriate physiological stains. The figure shows cells of Pseudomonas putida stained with the lipophilic dye DIBAC4(3), which indicates silver toxicity-compromised cells by a reddish discoloration. The method was then applied for toxicity measurements as a function of nanoparticle concentration, size and pH. All three parameters exerted the expected influences on the physiology of the test organisms, with a higher susceptibility of the gram-postive Mycobacterium strain. The toxicity patterns point at an activity of silver dissolving from the nanoparticles, although presently effects of complete nanoparticles cannot be excluded. To be able to follow the fate of the nano-particles in future experiments, a method was developed which allowed the fluorescence labelling of silver nanoparticles.



⇑ Fluorescence microscopic image of a culture of Pseudomonas putida KT 2440. The reddish discoloration of cells indicates silver toxicity compromised individuals.

Prof. Dr. Hauke Harms
Centre for Environmental Research (UFZ)
https://www.ufz.de/index.php?de=13566
E-mail: hauke.harms@ufz.de
Phone: +49 341 235-1260
Fax: +49 341 235-1351

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

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

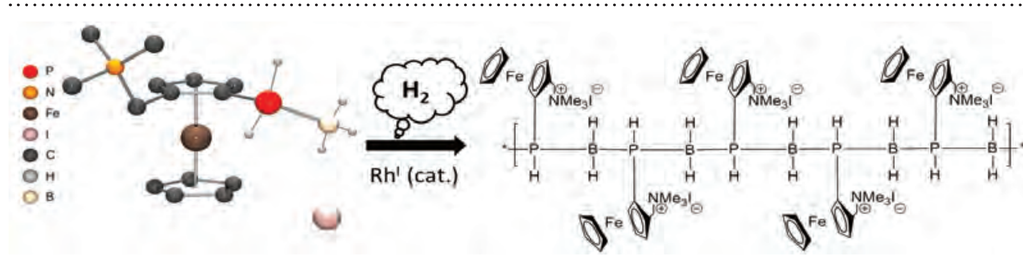
The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carbaborane clusters and antitumour drugs).

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

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

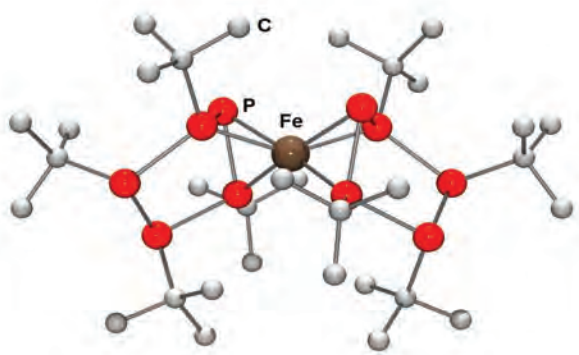
Another approach focusses on the use of selective phosphorus-based macrocycles, nano-frames (P. C. Boar, R. Hoy, A. Schmied), containers, or cavities (functionalised (*S*)-BINAP as linkers) in metal-organic frameworks (MOFs) with well-defined structure and porosity (J. A. Navarro). These compounds can be used as receptors for catalytically active transition metals, generating molecular nanosised 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.

From Molecules to Novel Materials:
Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of *functionalised building blocks* for organometallic or phosphorus-based polymers are: strained inorganic (T. Grell) or organic (T. Möller) phosphorus-based rings, alkylene- and arylene-bridged bis(phospholanes) (P. C. Boar, R. Hoy, A. Schmied) or (planar-chiral) ferrocene derivatives (P. Neumann, S. Pandey).



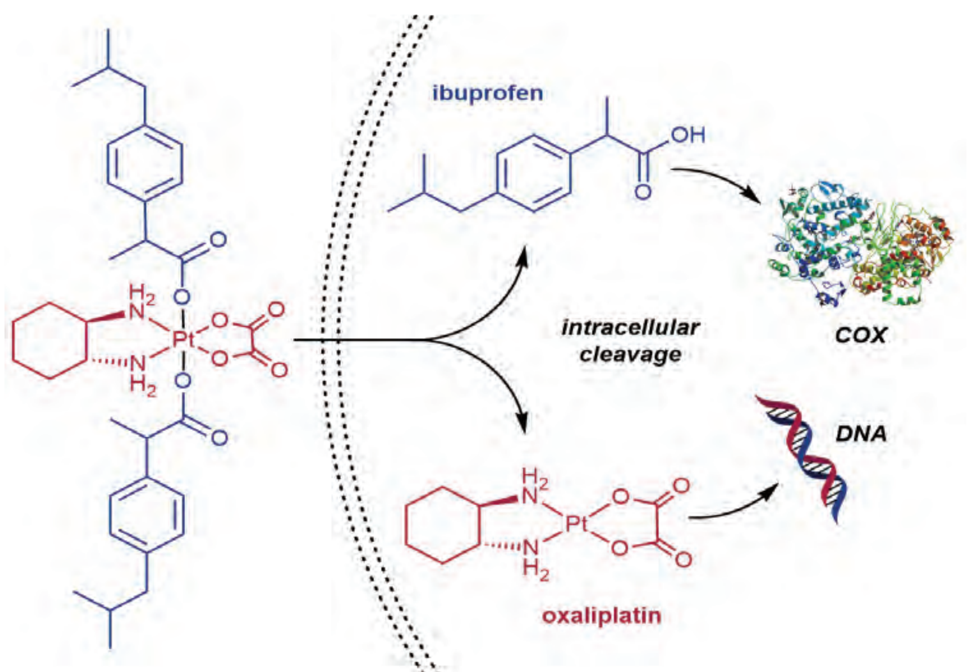
⇑ Molecular precursor for chiral polycationic inorganic polymers with redoxactive ferrocenyl groups.

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.



⇐ Molecular precursor (Fe{*cyclo*-$P_5{}^tBu_4$)$_2$}] for the synthesis of phosphorus-rich binary iron phosphides.

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



⇑ Platinum prodrugs ensure a concerted transport of cisplatin analogues and cyclooxygenase inhibitors into tumour cells.

Chemotherapy using platinum-based anti-tumour agents, such as cisplatin, is often associated with strong side effects and is further limited by resistance of tumour cells. To increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. NPY (S. Richter) or COX inhibitors (W. Neumann)).

⇒ *Aryl-Based Ferrocenyl Phosphine Ligands in the Rhodium(I)-Catalyzed Hydroformylation of Olefins*
M. Madalska, P. Lönnecke, E. Hey-Hawkins / Journal of Molecular Catalysis A: Chemical (2014) **137** 383

⇒ *Heterobimetallic Complexes with Ferrocenyl-substituted Phosphaheterocycles*
S. Stockmann, P. Lönnecke, S. Bauer, E. Hey-Hawkins / Journal of Organometallic Chemistry (2014) **751** 670

⇒ *Carbaborane-substituted 1,2,3-Triphospholanes and 1-Aza-2,5-diphospholane: New Synthetic Approaches*
A. Kreienbrink, S. Heinicke, T.T. Duong Pham, R. Frank, P. Lönnecke, E. Hey-Hawkins / Chemistry – A European Journal (2014) **20** 1434

⇒ *Synthesis, Structure and Luminescence Properties of a Three-Dimensional Heterobimetallic Chiral Metal–Organic Framework Based on Sodium(I), Lead(II) and (S)-5,5'-Bis(4-carboxyphenyl)-2,2'-bis(diphenylphosphinoyl)-1,1'-binaphthyl as Linker*
W.W. Lestari, P. Lönnecke, H. Cerqueira Streit, M. Handke, C. Wickleder, E. Hey-Hawkins / invited paper to special issue of European Journal of Inorganic Chemistry entitled "Advances in Phosphorus Chemistry"; European Journal of Inorganic Chemistry (2014) 1775

⇒ *Synthesis and Thermolysis of the Homoleptic Iron(II) Complex [Fe{cyclo-(Pt_5Bu_4)}$_2$]*
A. Kırcalı Akdag, P. Lönnecke, E. Hey-Hawkins / Zeitschrift für Anorganische und Allgemeine Chemie (2014) **640** 271

⇒ *Electrophile-Induced Nucleophilic Substitution in the nido-Dicarbaborate Anion nido-7,8-$C_2B_9H_{12}^-$ by Conjugated Heterodienes*
R. Frank, A. Adhikari, H. Auer, E. Hey-Hawkins / Chemistry – A European Journal (2014) **20** 1440

⇒ *Reduction of Hydroxy-functionalised Carbaboranyl Carboxylic Acids to Tertiary Alcohols by Organolithium Reagents*
W. Neumann, M. Hiller, P. Lönnecke, E. Hey-Hawkins / invited contribution, Special Issue Carboranes, Dalton Transactions (2014) **43** 4935, Inside Cover

⇒ *Phosphorus–Boron-Based Polymers Obtained by Dehydrocoupling of Ferrocenylphosphine–Borane Adducts*
S. Pandey, P. Lönnecke, E. Hey-Hawkins / European Journal of Inorganic Chemistry (2014) **2014** 2456

⇒ *Dehydrocrosscoupling: A Novel Synthetic Route to P–B–P–B Chains*
S. Pandey, P. Lönnecke, E. Hey-Hawkins / Inorganic Chemistry (2014) **53** 8242

⇒ *Selective Formation of Gold(I) Bis-phospholane Macrocycles, Polymeric Chains and Nano-tubes*
M. Streitberger, A. Schmied, E. Hey-Hawkins / Inorganic Chemistry (2014) **53** 6794

⇒ *P-chiral Phosphorus Heterocycles: A Straightforward Synthesis*
T. Möller, P. Wonneberger, N. Kretzschmar, E. Hey-Hawkins / Chemical Communications (2014) **50** 5826, Front Cover

⇒ *Conjugates of Cisplatin and Cyclooxygenase Inhibitors as Potent Antitumor Agents Overcoming Cisplatin Resistance*
W. Neumann, B.C. Crews, L.J. Marnett, E. Hey-Hawkins / ChemMedChem (2014) **9** 1150

⇒ *Organotantalum Phosphaketene and Phosphaazaallene Complexes*
A. Grundmann, M.B. Sárosi, P. Lönnecke, E. Hey-Hawkins / European Journal of Inorganic Chemistry (2014) 2997

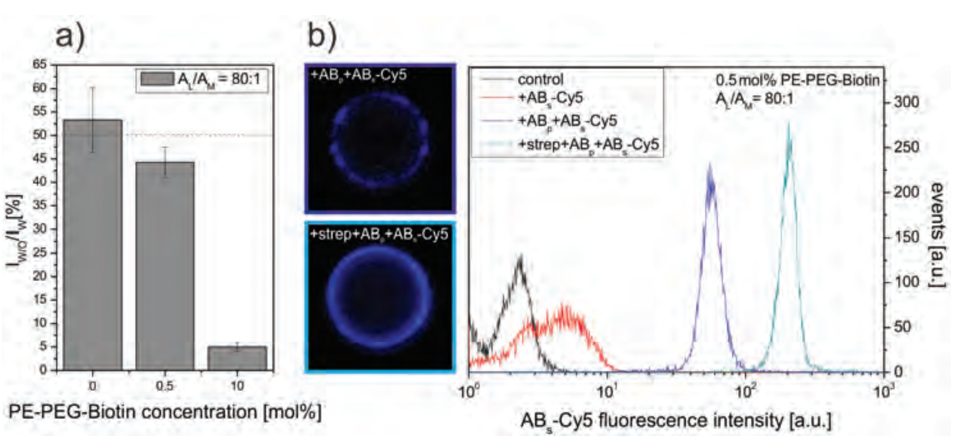
Prof. Dr. Dr. h.c. Evamarie Hey-Hawkins
Institute of Inorganic Chemistry
http://research.uni-leipzig.de/hh/
E-mail: hey@uni-leipzig.de
Phone: +49 341 97-36151
Fax: +49 341 97-39319

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

Prof. Dr. Daniel Huster
Dipl.-Phys. Martin-Patrick Göse

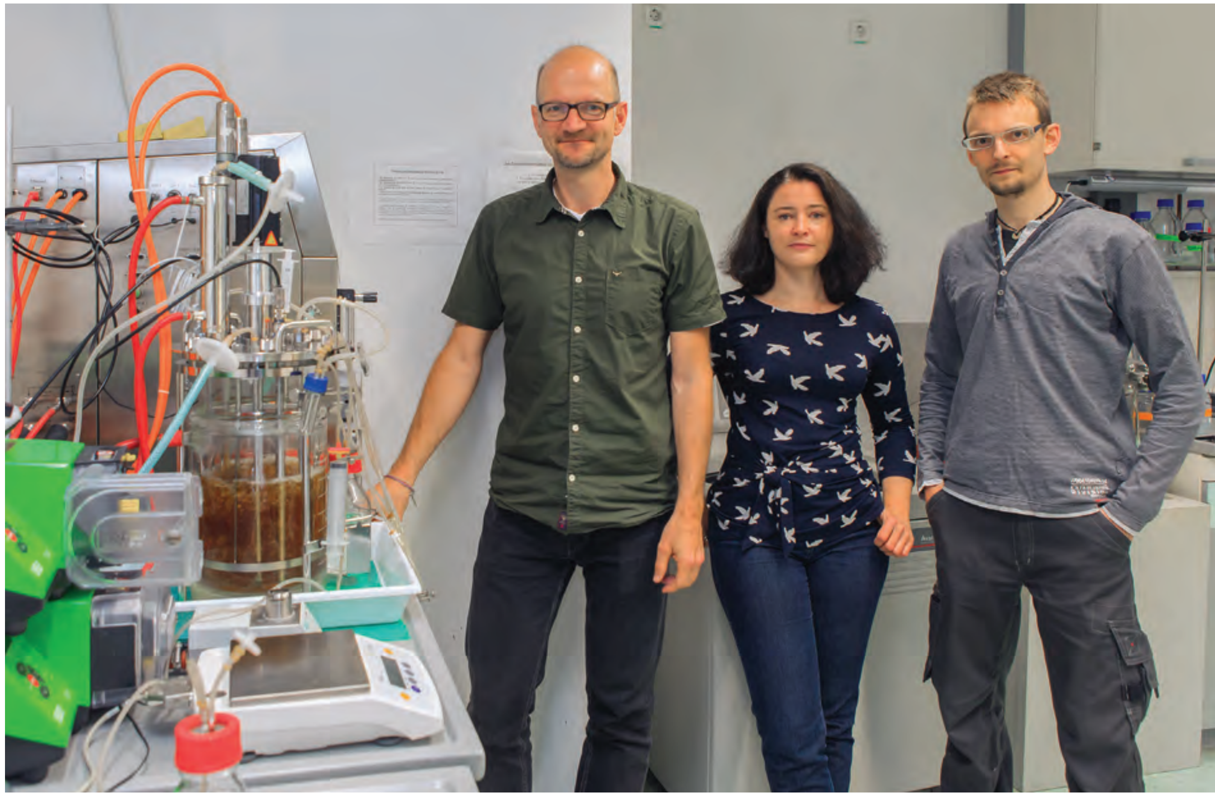
In designing structured polymer-based drug delivery systems such as based on Layer-by-Layer (LbL) self-assembly of biopolymers onto spherical templates, it's not only feasible to provide a protected transport of active agents but also to apply additional functional components e.g. for mimicking, targeting or enhancement of biocompatibility.

In his PhD work, Dipl.-Phys. Martin Göse is involved in the development and characterisation of a homogeneously formed supported lipid membrane assembled onto the surface of an LbL-biopolymer coated microcarrier. The investigations are taking polymer material, template size, insertion of an adapter molecule for the attachment of specific functional molecules and coating conditions into consideration. The focus is on the establishment of a LbL drug delivery system with a lipid membrane carrying a moiety for replaceable attachment of functional molecules such as antibodies or active agents without changing the inner structure.



a) Flow Cytometry investigations of remaining SiO_2-microcarrier fluorescence intensity (POPS/POPC 1:1, AL/AM of 80:1, 0.1 mol% PE-Fluorescein and 0 mol%, 0.5 mol% or 10 mol% PE-PEG-Biotin) after Trypan Blue penetration and fluorescein quenching. b) Flow Cytometry and Confocal Laser Scanning Microscopy investigations of specific antibody binding. Biotinylated antibodies were used and attached to the microcarrier surface via biotin/streptavidin binding.

Investigations show that best conditions are provided by using a 1:1 lipid mixture of POPS/POPC containing 0.5 mol% PE-PEG-Biotin and a ratio of liposome surface area to microcarrier surface area (AL/AM) of 80:1. Under those conditions, a homogeneous lipid membrane can be produced which is impenetrable even for very small molecules in the range of about 1 kDa, avoiding opsonisation. Via streptavidin, a multitude of biotinylated functional molecules could then be attached. The successful application of the biotin/streptavidin sandwich strategy is verified by a well-defined attachment of biotinylated antibodies, facilitating a specific interaction with addressed cells.

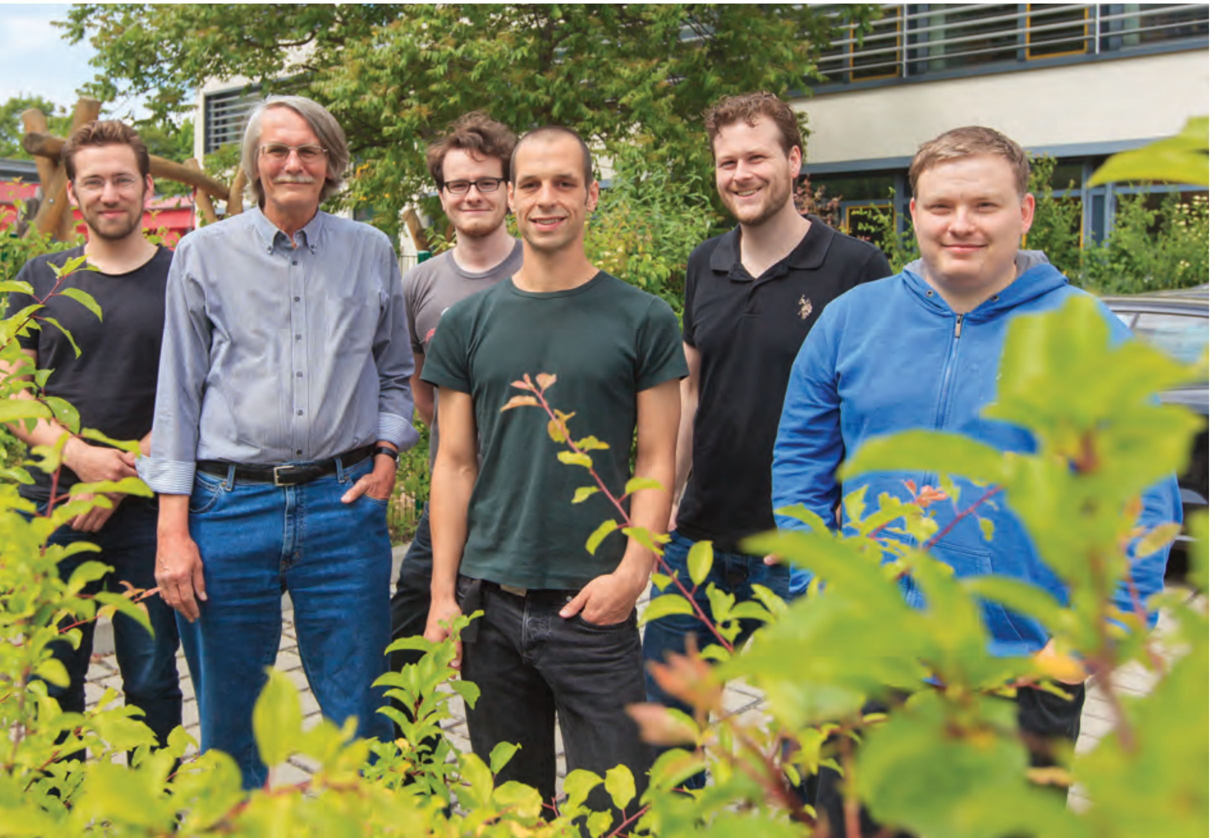


Prof. Dr. Daniel Huster
Institute of Medical Physics and Biophysics
http://www.uni-leipzig.de/~biophys/cms/index.php?id=200
E-mail: daniel.huster@medizin.uni-leipzig.de
Phone: +49 341 97-15701
Fax: +49 341 97-15709

Monte Carlo and molecular dynamics simulations of structure formation processes

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

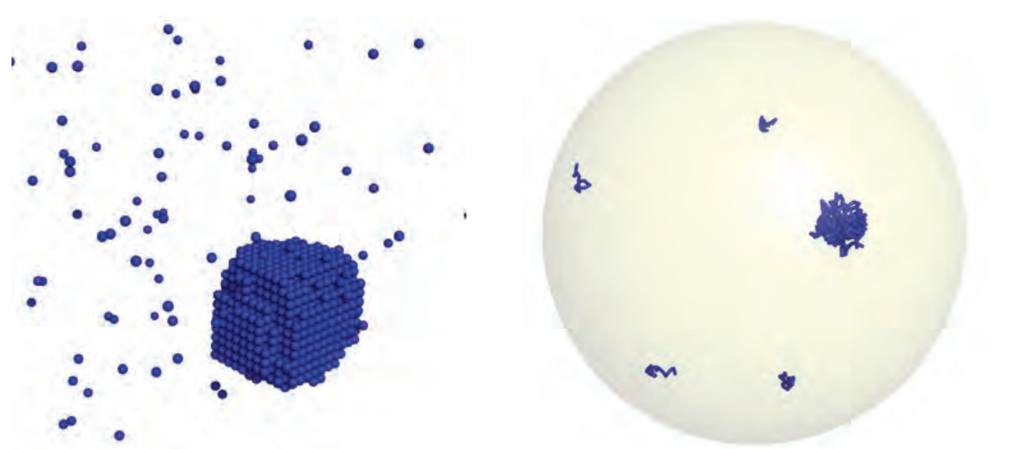
The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on several interrelated subprojects. In most projects, the employed methodology relies mainly on sophisticated Monte Carlo computer simulations based on multicanonical ensembles and parallel tempering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



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

(ii) Martin Marenz develops with the help of a few of his fellow PhD students a tool box ("framework") for multi-scale Monte Carlo computer simulations of mesoscopic and atomistic models of polymers in confined geometries such as a spherical cage or in interaction with a solid substrate. Extending our previous studies of a generic bead-stick model of flexible polymers to the case of semiflexible or stiff polymers, the adsorption propensity to substrates and structure formation processes under confinement are in the focus of his interests. In this work he discovered novel thermodynamically stable phases of knotted polymers.

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



left: Droplet phase of a lattice gas of particles close to the droplet evaporation/condensation transition. right: Ensemble of polymers enclosed in a spherical cavity. Varying the radius of the sphere allows one to study the influence of external confinement onto the physical properties of the polymer aggregation process.

(iv) Johannes Bock focused within the ESF/SAB Junior Research Group "Tools and Technologies for Rational Material Design" on the intriguing properties of polymers and proteins in disordered environments ("crowded cell problem") and thereby continues the work of Sebastian Schöbl by extending it to the three-dimensional case subject to additional confinement constraints.

(v) Philipp Schierz aimed within the ESF/SAB Junior Research Group "Emergent Phenomena of Atomistic and Molecular Aggregates" at efficient computer simulations of realistic polymer systems. To this end he investigates the advantages of computations performed on powerful graphics cards (GPUs) over the use of standard CPUs and carefully compares the performance of Molecular Dynamics (MD) and Monte Carlo (MC) implementations for this class of problems.

⇒ *Adsorption and Pattern Recognition of Polymers at Complex Surfaces with Attractive Stripe-like Motifs*
M. Möddel, W. Janke, M. Bachmann / Physical Review Letters (2014) **112** 148303

⇒ *Application of the Parallel Multicanonical Method to Lattice Gas Condensation*
J. Zierenberg, M. Wiedenmann, W. Janke / Journal of Physics: Conference Series (2014) **510** 012017

⇒ *Aggregation of Theta-Polymers in Spherical Confinement*
J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, W. Janke / Journal of Chemical Physics (2014) **141** 114908

⇒ *Polymers in Disordered Environments*
V. Blavatska, N. Fricke, W. Janke / Condensed Matter Physics (2014) **17** 33604

⇒ *Persistence-Length Renormalization of Polymers in a Crowded Environment of Hard Disks*
S. Schöbl, S. Sturm, W. Janke, K. Kroy / Physical Review Letters (2014) **113** 238302

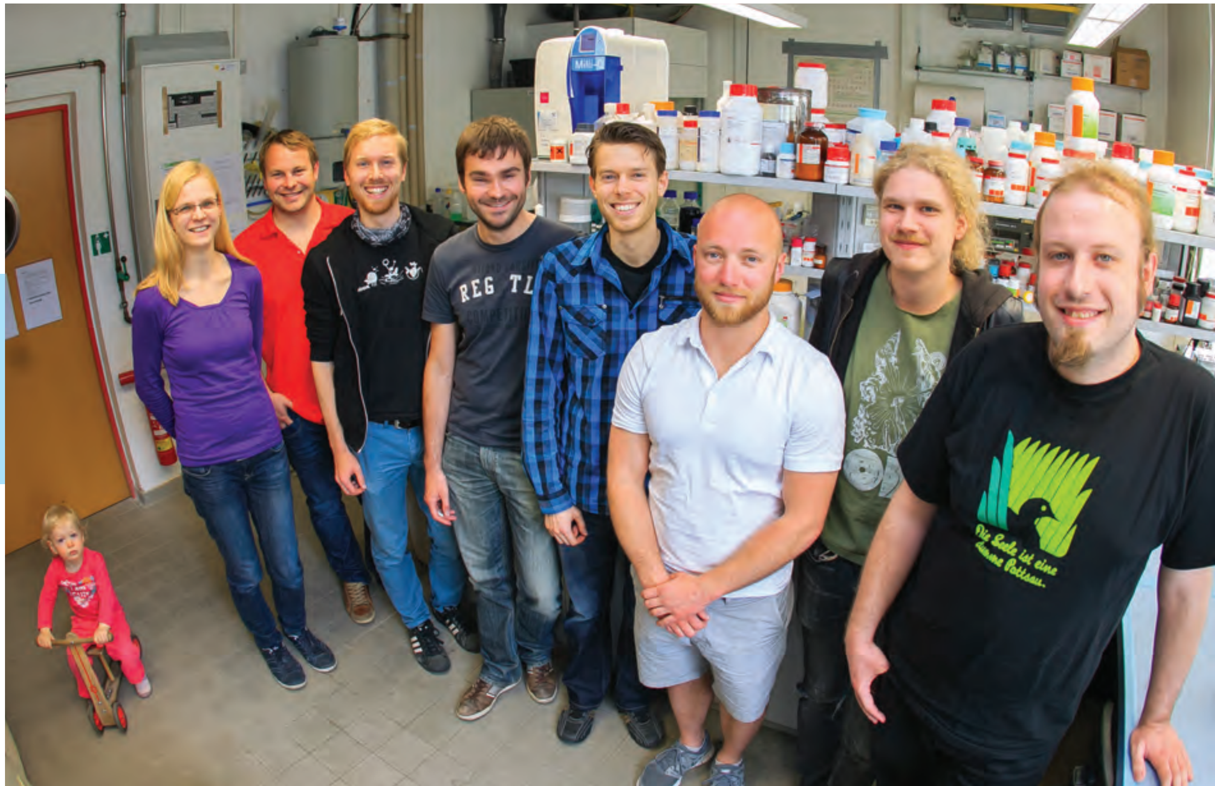
⇒ *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*
N. Fricke, W. Janke / Physical Review Letters (2014) **113** 255701

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 97-32421
Fax: +49 341 97-32450

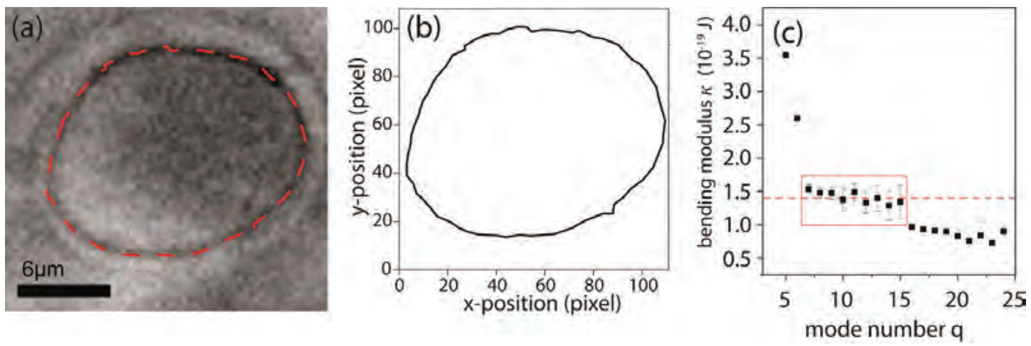
Cell membrane softening in human breast and cervical cancer cells

Prof. Dr. Josef Alfons Käs
Dr. Anatol Fritsch, M.Sc. Phys. Tom Golde, M.Sc. Phys. Martin Glaser, Dipl.-Phys. Chris Händel, Dipl.-Phys. Tina Händler, Dr. Tobias Kießling, Dr. Melanie Knorr, M.Sc. Phys. Jürgen Lippoldt, M.Sc. Phys. Erik Morawetz, Dipl.-Phys. Steve Pawlizak, Dipl.-Phys. Jörg Schnauß, Dipl.-Phys. Carsten Schuldt, Dr. Dan Strehle, Dr. Franziska Wetzel

Characterising mechanical properties of plasma membranes is an important step for understanding cellular behaviours like cell migration and invasion that are characteristic for cancer progression. Biomechanical properties of cytoskeleton have been intensively studied in cells and model systems. However, the role of membrane rigidity during cancer progression is not well understood and rigidity measurements exist only for vesicles composed of artificial lipids or erythrocytes. In this project, we studied thermal shape fluctuations of giant plasma membrane vesicles (GPMVs) produced from primary cells as well as cell lines by vesiculation or blebbing. GPMVs contain a larger variety of lipids and membrane proteins than any artificial



membrane and have to be regarded as more physiological model system. Based on a self-developed gradient-based edge detection algorithm, the bending rigidity was calculated by a Fourier analysis of thermal vesicle shape fluctuations. The experimental data show that membranes of cancer cells are significantly softer than those of their normal counterparts. This cell membrane softening could be attributed to a decrease of fluid raft forming lipids in malignant cells. Moreover, this finding indicates that cancer may directly influence the membrane composition and its mechanical properties.



Determination of the bending elastic modulus. (a) Phase contrast image of a GPMV obtained from isolated primary cells. (b) Contour of a GPMV extracted from a self-written edge detection algorithm. (c) Bending elastic modulus κ (rigidity) of a GPMV shown as function of the mode number q.

⇒ *Thermal Instability of Cell Nuclei*
E. Warmt, T.R. Kießling, R. Stange, A.W. Fritsch, M. Zink, J.A. Käs / New Journal of Physics (2014) **16** 073009

⇒ *Dynamic Membrane Structure Induces Temporal Pattern Formation*
J. Lippoldt, C. Händel, U. Dietrich, J.A. Käs / Biochimica et Biophysica Acta (BBA) – Biomembranes (2014) **1838** 2380

⇒ *Tailoring the Material Properties of Gelatin Hydrogels by High Energy Electron Irradiation*
E.I. Wisotzki, M. Hennes, C. Schuldt, F. Engert, W. Knolle, U. Decker, J.A. Käs, M. Zink, S.G. Mayr / Journal of Materials Chemistry B (2014) **2** 4297

⇒ *Active Contractions in Single Suspended Epithelial Cells*
M. Gyger, R. Stange, T. Kießling, A. Fritsch, K.B. Kostelnik, A.G. Beck-Sickinger, M. Zink, J.A. Käs / European Biophysics Journal (2014) **43** 11

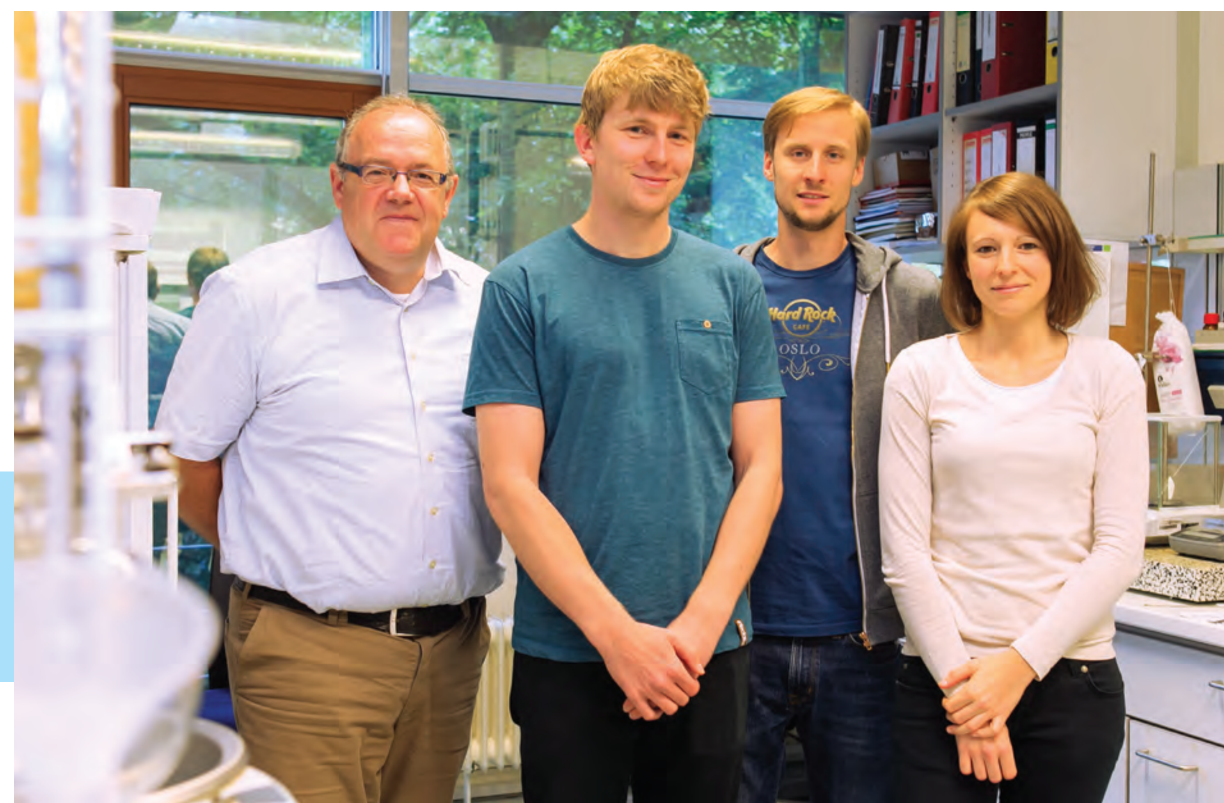
⇒ *Evaluation of Single Cell Biomechanics as Potential Marker for Oral Squamous Cell Carcinomas: A Pilot Study*
J. Runge, T.E. Reichert, A. Fritsch, J. Käs, J. Bertolini, T.W. Remmerbach / Oral Diseases (2014) **20** e120

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

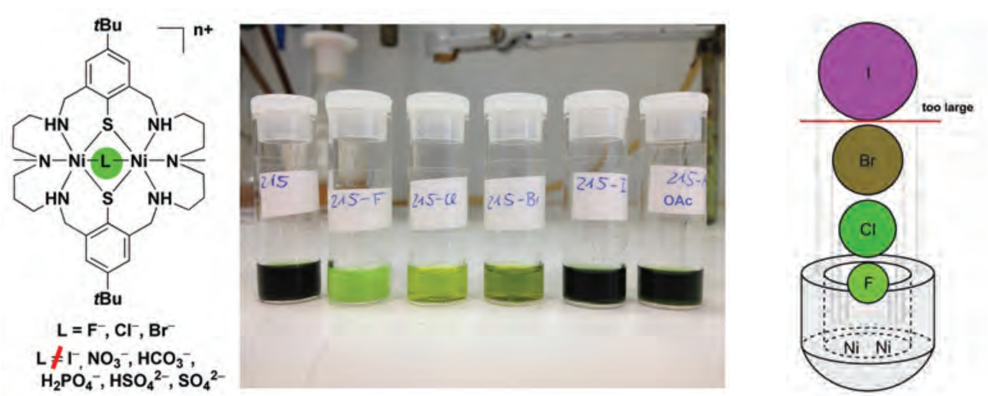
Coordination compounds in supramolecular chemistry and materials chemistry

Prof. Dr. Berthold Kersting
M.Sc. Chem. Florian Glasneck, Dr. Sina Gruschinski, M.Sc. Chem. Astrid Jäschke, M.Sc. Chem. Steve Ullmann

The design of artificial anion receptors is an attractive research area. Anions play important roles in many processes, both chemical and biological, and this makes their selective binding an area of great interest. Selective anion receptors can alter the reactivity of an anion, may assist in the separation of complex chemical mixtures, or act a phase transport reagents. One very successful approach to bind halide anions is chelation by Lewis acids, and several examples of multidentate Lewis-acids incorporating *d*-block and *p*-block metals have now been reported. The analogous chemistry of metallocavitands featuring an open binding site has been investigated far less frequently.



On these reasons, we have investigated the halide binding properties of the cavitand $[Ni_2(LMe_2H_4)]^{2+}$. The novel cavitand exhibits a chelating $N_3Ni(\mu\text{-}S)_2NiN_3$ moiety with two square-pyramidal $Ni^{II}N_3S_2$ units situated in an anion binding pocket of ~ 4 Å diameter formed by the organic backbone of the $(LMe_2H_4)^{2-}$ macrocycle. The receptor reacts with fluoride, chloride (in MeCN/MeOH), and bromide ions (in MeCN) to afford an isostructural series of halogenido-bridged complexes $[Ni_2(LMe_2H_4)(\mu\text{-}Hal)]^+$ (Hal = F^-, Cl^-, and Br^-). No reaction occurs with iodide or other polyatomic anions (ClO_4^-, NO_3^-, HCO_3^-, $H_2PO_4^-$, HSO_4^-, SO_4^{2-}). X-ray crystallographic analyses and computational studies reveal a significant increase of the intramolecular distance between two propylene groups at the cavity entrance upon going from F^- to I^- (for the DFT computed structure). In case of the receptor and fluorido-bridged complex, the corresponding distances are nearly identical. This indicates a high degree of pre-organisation of the $[Ni_2(LMe_2H_4)]^{2+}$ receptor and a size fit mismatch of the receptors binding cavity for anions larger than F^-.



⇑ Structure and anion binding by the cavitand $[Ni_2(LMe_2H_4)(\mu\text{-}Hal)]^+$.

⇒ *Encapsulation of the 4-Mercaptobenzoate Ligand by Macrocyclic Metal Complexes: Conversion of a Metallocavitand into a Metalloligand*
J. Lach, A. Jeremies, D. Breite, B. Abel, B. Mahns, M. Knupfer, V. Matulis, O.A. Ivashkevich, B. Kersting / Inorganic Chemistry (2014) **53** 10825

⇒ *Adsorption of Diiodine by Macrocyclic Polyaza-Dithiophenolato Complexes*
M. Golecki, N. Beyer, G. Steinfeld, V. Lozan, S. Voitekhovich, M. Sehabi, J. Möllmer, H.-J. Krüger, B. Kersting / Angewandte Chemie (2014) **126** 10107

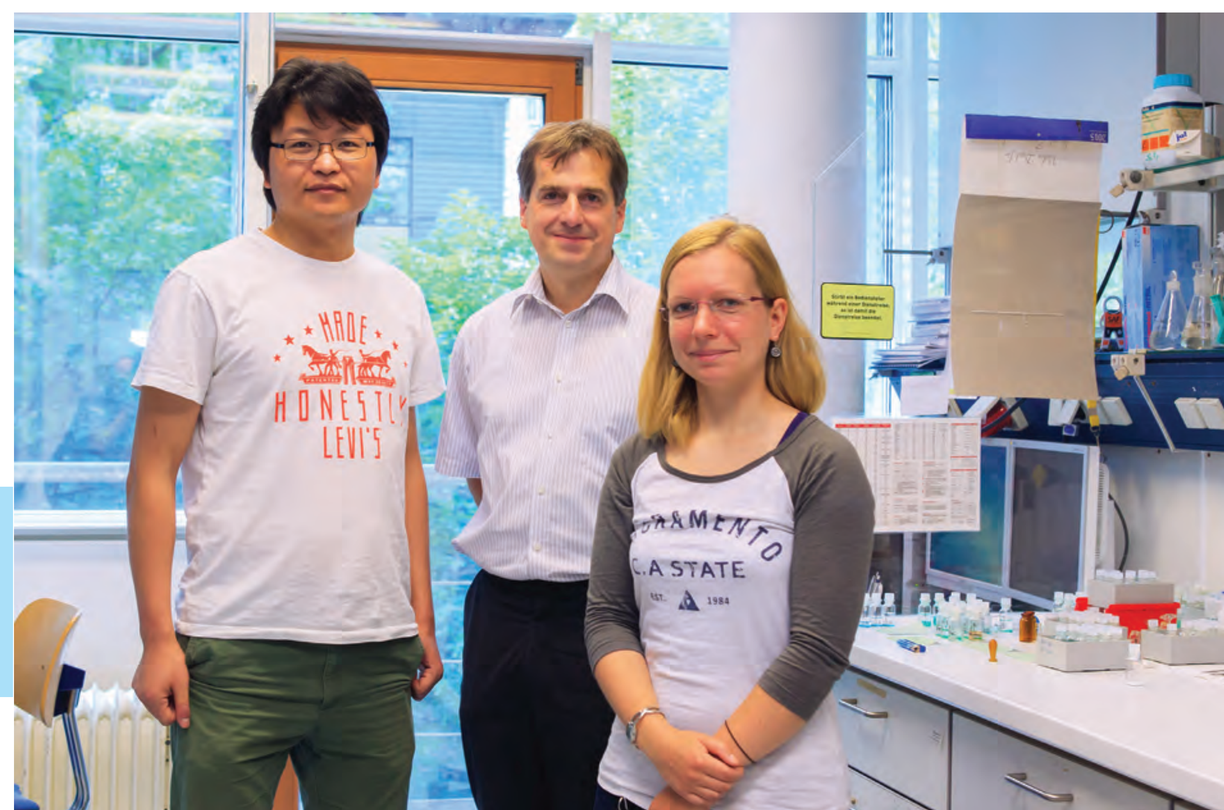
Prof. Dr. Berthold Kersting
Institute of Inorganic Chemistry
http://www.uni-leipzig.de/~bkerst/
E-mail: b.kersting@uni-leipzig.de
Phone: +49 341 97-36143
Fax: +49 341 97-36199

Proton conduction in a phosphonate based porous coordination polymer

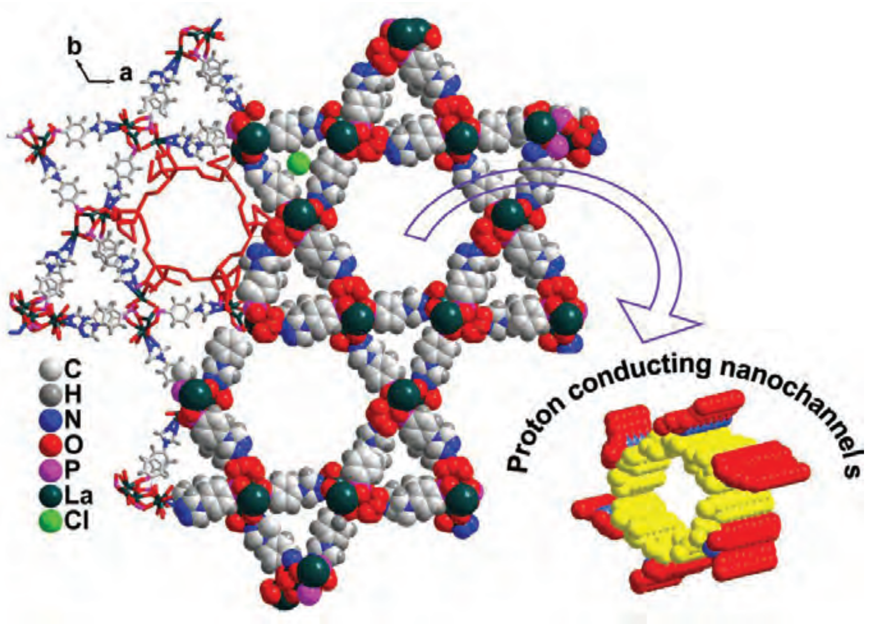
Prof. Dr. Harald Krautscheid
M.Sc. Chem. Salma Begum, Dr. Marcel Handke, M.Sc. Chem. Karolin Stein, M.Sc. Chem. Zhaoyang Wang

Porous coordination polymers, so-called MOFs (Metal-Organic Frameworks) have been investigated in the last years because of their rich structural chemistry and potential applications in gas storage and separation, catalysis, as sensors or for drug delivery. In addition, proton conductivity can be achieved by generating charge carriers in a hydrophilic pore structure. Water mediated proton conducting materials operating around 100 °C are important for applications such as membranes in fuel cells. Their development remains challenging because the extended structures of existing materials usually deteriorate at high temperatures.

$[La_3L_4(H_2O)_6]Cl{\cdot}xH_2O$, a novel MOF with triazolylphenylphosphonate (L^{2-}) linkers, crystallises in a hexagonal three-dimensional structure with highly hydrophilic, linear channels. The regular pores (1.9 nm in diameter) are among the largest in phosphonate frameworks reported to date. Water molecules are arranged



as one dimensional chains along the vertices of the hexagonal nanochannels. The water stable, porous structure can be reversibly hydrated and dehydrated. According to impedance spectroscopy measurements the proton conductivity is gradually increasing with increasing temperature and relative humidity, even at temperatures up to 110 °C. MAS and PFG NMR confirm the dynamic nature of the incorporated water molecules. The diffusivities determined by PFG NMR and IR microscopy are found close to that of liquid water. The proton conductivity is proposed to occur by the vehicle mechanism.



⇑ Fragment of the crystal structure of $[La_3L_4(H_2O)_6]Cl \cdot xH_2O$. The arrow directs to the enlarged 1D channels (1.9 nm in diameter) filled with non-coordinated (yellow) and coordinated (red) water molecules; phosphonate free oxygen atoms are shown in light blue.

⇒ *Water Mediated Proton Conduction in a Robust Triazolyl Phosphonate MOF with Hydrophilic Nanochannels*
S. Begum, Z. Wang, A. Donnadio, F. Costantino, M. Casciola, R. Valiullin, C. Chmelik, M. Bertmer, J. Kärger, J. Haase, H. Krautscheid / Chemistry – A European Journal (2014) **20** 8862

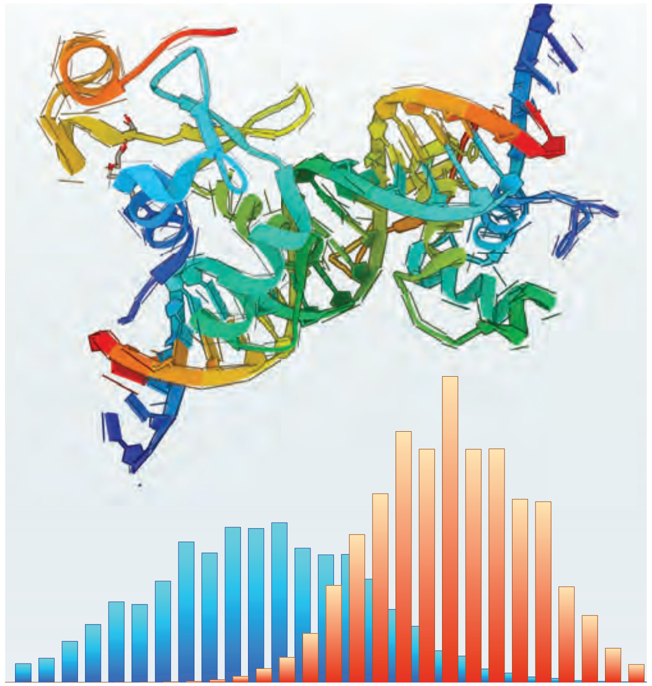
⇒ *Microimaging of Transient Guest Profiles to Monitor Mass Transfer in Nanoporous Materials*
J. Kärger, T. Binder, C. Chmelik, F. Hibbe, H. Krautscheid, R. Krishna, J. Weitkamp / Nature Mater. (2014) **13** 333

Prof. Dr. Harald Krautscheid
Institute of Inorganic Chemistry
http://www.uni-leipzig.de/~chemiehk/
E-mail: krautscheid@rz.uni-leipzig.de
Phone: +49 341 97-36172
Fax: +49 341 97-36199

Non-isothermal Brownian motion and rapid force spectroscopy

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

In our previous work, we showed that the complex non-equilibrium hydrodynamics of a laser-heated nanoparticle can be reduced to an isothermal equilibrium description with an effective temperature. Starting from a microscopic description of the particle's erratic motion, we have now expanded this concept to a whole "temperature spectrum". Depending on how the frequency of thermal excitation compares to the solvent's ability to transport dissipated heat from the particle, the effective temperatures associated with the particle's rotation and translation can vary drastically. This formalism resolves previous controversies regarding hot Brownian motion, e.g. that the kinetic effective temperature of a heated particle differs from its positional one.



⇑ By repeatedly exposing the bond to external forces, a series of unbinding events are produced that can shed light on the underlying energy landscape when analysed with an appropriate theory.

In an interdisciplinary project relevant for single-molecule biochemistry and biophysics, we investigated escape processes that can be used to model the forcible breaking of weak, non-covalent bonds in single molecule experiments. Conventional theories of such bond dissociations rely on the bond being quasi-statically pulled apart, which is well justified for current experimental setups, but fails to cover the high loading rates amenable to full-scale molecular dynamics simulations and, possibly, future high-speed force spectroscopy assays. We extended these theories to rapid force spectroscopy protocols by explicitly resolving the non-equilibrium internal bond dynamics. Our analytical predictions are exact for fast loading protocols and reduce to established quasi-static results in the limit of slow external loading.

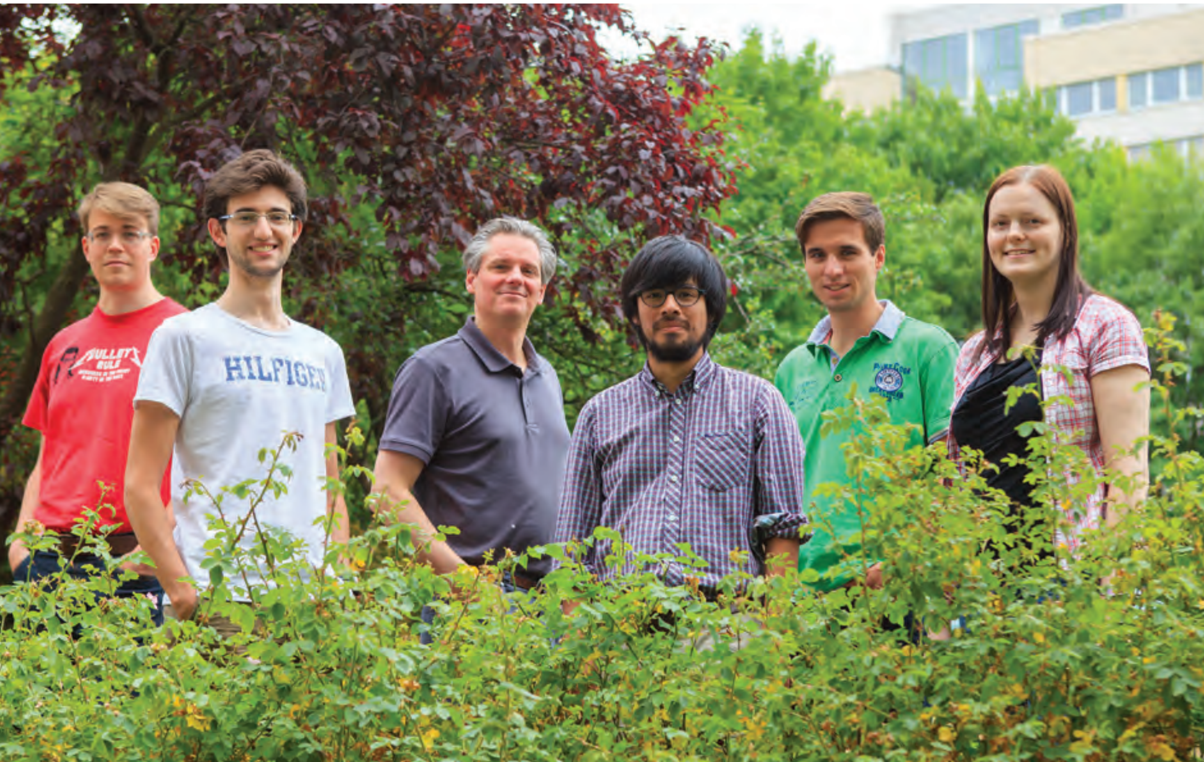
⇒ *Effective Temperatures of Hot Brownian Motion*
G. Falasco, M.V. Gnann, D. Rings, K. Kroy / Physical Review E (2014) **90** 032131

⇒ *Theory of Rapid Force Spectroscopy*
J.T. Bullerjahn, S. Sturm, K. Kroy / Nature Communications (2014) **5** 4463

⇒ *Intramolecular Relaxation in Dynamic Force Spectroscopy*
S. Sturm, J.T. Bullerjahn, K. Kroy / EPJ Special Topics (2014) **223** 3129

⇒ *Polarization of Active Janus Particles*
T. Bickel, G. Zecua, A. Würger / Phys. Rev. E (2014) **89** 050303(R)

Prof. Dr. Klaus Kroy
Institute for Theoretical Physics
http://www.physik.uni-leipzig.de/~kroy/
E-mail: klaus.kroy@uni-leipzig.de
Phone: +49 341 97-32436
Fax: +49 341 97-32439

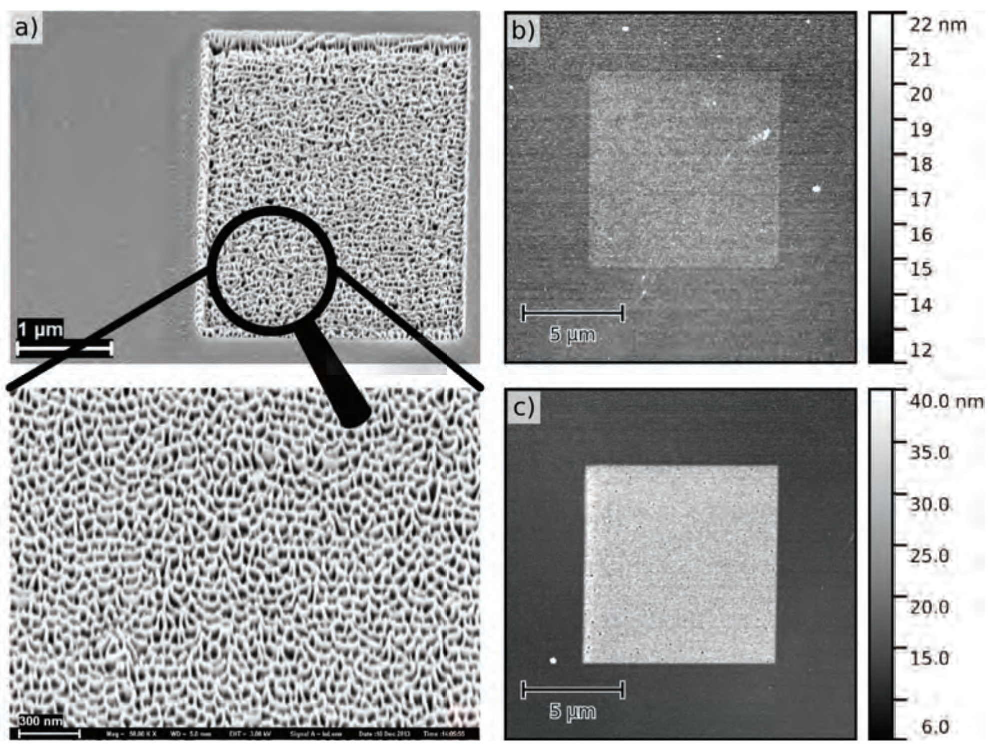


New functional materials for biomedical applications and material physics at the nanoscale

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

Functional materials offer a wide range of applications. Thus they are the main research topic in our group with emphasis on biomedical and regenerative energy applications. State-of-the-art synthesis and characterisation techniques as well as computer modelling are employed to reach a detailed understanding of the underlying physical concepts and processes. Within BuildMoNa, the following topics are currently addressed: bimetallic magnetic nanoparticles, ion irradiation induced nanoporous structures, irradiation tailored biocompatible hydrogels, inorganic-organic interfaces and hybrid systems, and ferromagnetic shape memory alloys (FSMA). Hereafter selected topics will be discussed more in-depth.

Nanoporous structures are of constant interest for research due to their manifold application areas, which include percolation and adsorption filters, heat exchangers, catalysts, membranes, prostheses, coatings, and drug delivery systems. In addition ion irradiation is a versatile tool to tailor material properties due to its various parameters, such as ion species, ion energy, ion fluence and angle of incidence. While some applications make use of nanoporous structures already today, the underlying physics is not yet fully understood. Thus the germanium-silicon-system has been investigated in order to have a simple two-component alloy model system. For this system, a strong dependence of nanoporous structure development on the alloy composition was found. That is, for silicon ratios above 22 at% (i.e., 10 wt%) a nanoporous structure is not observable for room temperature irradiation. Below that silicon content, a pronounced nanoporous structure, as well as a pronounced surface swelling, was observed. Moreover the threshold fluence needed to achieve a porous structure development, increases more than one order of magnitude with increasing silicon content. Although germanium and silicon show similar behaviour when forming a crystal (e.g., same crystal structure), the behaviour upon ion irradiation is distinctively different, which makes the germanium-silicon-system an ideal candidate for investigations of the principle processes involved in nanoporous structure development.



Ion irradiation induced nanoporous structures in GeSi-alloys. a) SEM micrograph of a nanoporous structure for an irradiated area in comparison to its pristine surroundings. b)+c) AFM micrographs showing increased surface swelling with increasing fluence for b) $9 \cdot 10^{14}$ cm^{-2} and c) $9 \cdot 10^{15}$ cm^{-2}.

FSMAs have been shown to yield strains of 5–10% upon application of moderate external magnetic fields and can therefore be considered as promising candidates for the development of miniaturised actuators or pumps. Our research focuses on Fe_7Pd_3, featuring high conductivity, high ductility, and biocompatibility. Essential for future applications is the detailed understanding of twin boundary mobility. With in-situ stress-strain experiments, combined with SEM measurements, the austenite-martensite phase transformation was observed and twin boundary movement was investigated in detail. Molecular dynamics modelling accompanied the experimental studies in order to get a better insight into the atomistic processes involved.

The FSMA Fe_7Pd_3 was further functionalised with respect to biomedical applications using an organic lysine-based coating. For the coating process, a RF-plasma deposition technique was implemented to achieve a strongly cross-linked, closed, robust, and biocompatible polymer thin film. In order to investigate the processes occurring during plasma induced polymerisation of lysine, density functional theory calculations were employed. It was shown that the carbon-carbon bonds of the lysine molecule are weakest and are thus broken first by the plasma treatment. As a result, the plasma energy was chosen carefully to ensure that the carboxyl and amino groups remain functional. Furthermore, the biocompatibility of the synthesised poly-lysine films was verified by the growth of NIH3T3 fibroblast cells on coated FSMA samples.

⇒ *Nanometer-resolved Mechanical Properties Around GaN Crystal Surface Steps*
J. Buchwald, M. Sarmanova, B. Rauschenbach, S.G. Mayr / Beilstein Journal of Nanotechnology (2014) **5** 2164

⇒ *Interfacing Hard and Living Matter: Plasma-assembled Proteins on Inorganic Functional Materials for Enhanced Coupling to Cells and Tissue*
U. Allenstein, F. Szillat, A. Weidt, M. Zink, S.G. Mayr / Journal of Materials Chemistry B (2014) **2** 7739

⇒ *Epitaxy from the Liquid Phase: Tuning Metastable Phases in Fe–Pd Thin Films by Laser-assisted Rapid Solidification on Substrates*
A. Arabi-Hashemi, M. Ehrhardt, P. Lorenz, D. Hirsch, K. Zimmer, S.G. Mayr / Journal of Physics D: Applied Physics (2014) **47** 415302

⇒ *Tailoring the Material Properties of Gelatin Hydrogels by High Energy Electron Irradiation*
E.I. Wisotzki, M. Hennes, C. Schlundt, F. Engert, W. Knolle, U. Decker, J.A. Käs, M. Zink, S.G. Mayr / Journal of Materials Chemistry B (2014) **2** 4297

⇒ *Nanoscale-resolved Elasticity: Contact Mechanics for Quantitative Contact Resonance Atomic Force Microscopy*
A.M. Jakob, J. Buchwald, B. Rauschenbach, S.G. Mayr / Nanoscale (2014) **6** 6898

⇒ *Plasma-assisted Synthesis and High-resolution Characterization of Anisotropic Elemental and Bimetallic Core–shell Magnetic Nanoparticles*
M. Hennes, A. Lotnyk, S.G. Mayr / Beilstein Journal of Nanotechnology (2014) **5** 466

Prof. Dr. Stefan G. Mayr
Leibniz Institute of Surface Modification,
Translational Centre for Regenerative Medicine and
Institute for Experimental Physics II
http://www.uni-leipzig.de/~agmayr/
E-mail: stefan.mayr@iom-leipzig.de
Phone: +49 341 235-3368
Fax: +49 341 235-2595

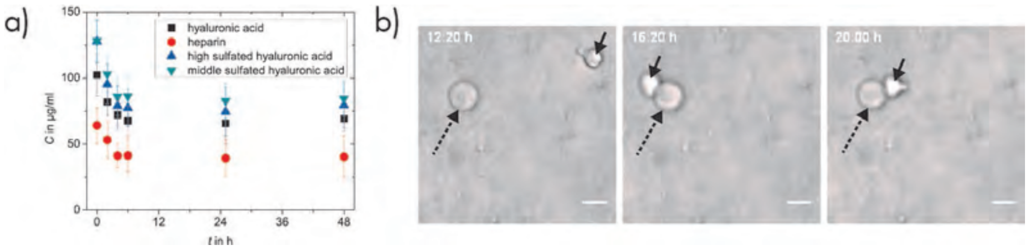
Engineering biomimetic microenvironments for *in vitro* cell studies

Prof. Dr. Tilo Pompe
M.Sc. Chem. Michael Ansorge, Dipl.-Phys. Andreas Müller

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

In this context M. Ansorge builds and characterises micrometer sized gradients of soluble mediators of hematopoietic stem cells as well as fibroblasts and macrophages during wound healing. He constructs polymeric microparticles with various glycosaminoglycan functionalisations exhibiting a controlled and slow release of signalling molecules like SDF-1, IL-10, and TGF-β1, which allow to establish microscale gradients in 2D and 3D cell culture scaffolds. The systems are used to study local, single cell behaviour within these gradients in terms of migration, proliferation and differentiation.

A. Müller uses synthetic hydrogel layers to model the impact of materials stiffness, ligand affinity and spatial constraints on cell adhesion. The latter are introduced by micropatterning the top of the polymer coated hydrogels, as spatial constraints were recently shown to impact the intracellular structure of the actin cytoskeleton.



⇑ a) Release rate of IL-10 over 48 hours can be tuned by the glycosaminoglycan (GAG) functionalisation of microparticles in dependence on the degree of sulfation of the used GAG. b) Directed chemotactic migration of a hematopoietic stem cell (solid arrow) within a gradient of the chemokine SDF-1 released from a microparticle (dashed arrow) investigated by long-term video microscopy (scale bar: 20 µm).

⇒ *Cytoskeletal Transition in Patterned Cells Correlates with Interfacial Energy Model*
A. Müller, J. Meyer, T. Paumer, T. Pompe / Soft Matter (2014) **10** 2444

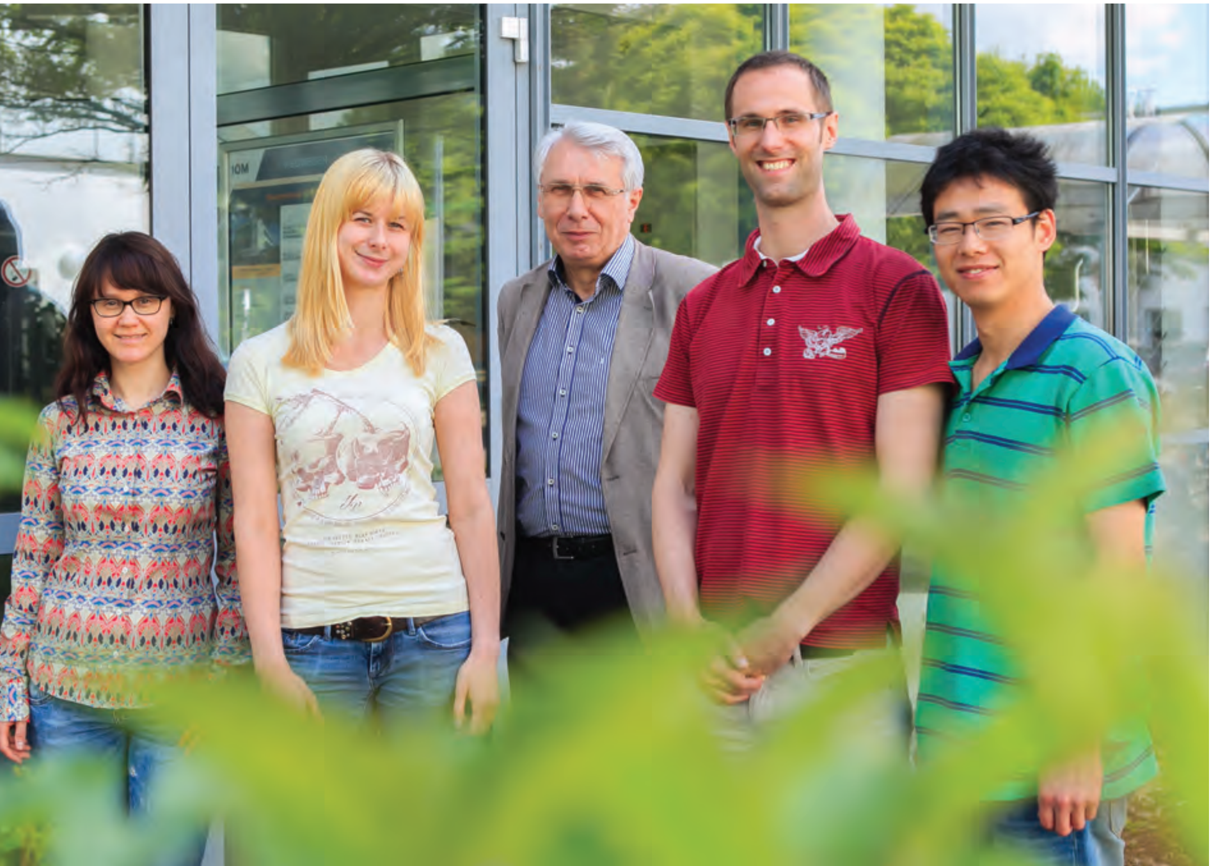
⇒ *Mimicking the Hematopoietic Stem Cell Niche by Biomaterials*
E. Müller, M. Ansorge, C. Werner, T. Pompe / In Bioinspired Materials for Biomedical Engineering, edited by A.B. Brennan, C.M. Kirschner, John Wiley & Sons (2014) 309

Prof. Dr. Tilo Pompe
Institute of Biochemistry
http://www.biochemie.uni-leipzig.de/agpompe/home.php
E-mail: tilo.pompe@uni-leipzig.de
Phone: +49 341 97-36931
Fax: +49 341 97-36939

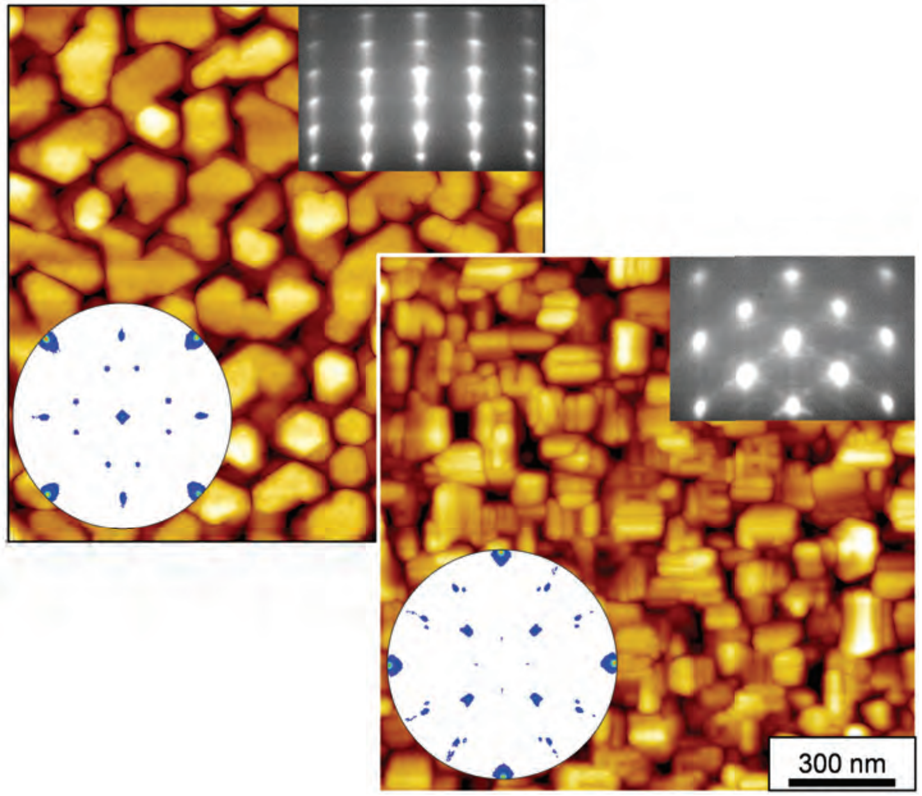
Ion and laser beam induced thin films and nanostructures

Prof. Dr. Dr. h.c. Bernd Rauschenbach
M.Sc. Phys. Annemarie Finzel, M.Sc. Phys. Marina Sarmanova, M.Sc. Phys. Xinxing Sun, M.Sc. Chem. Eng. Erik Thelander

The studies were focused on the deposition and characterisation of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium. For this purpose, ion and laser beam techniques were used to influence the nucleation and growth as well as the structural, optical and electrical properties of the films as a consequence of atomic rearrangement. These atomic rearrangements were induced by a low-energy bombardment or by pulsed laser irradiation. The main key aspects of this research were the epitaxial growth of gallium nitride (GaN) thin films and phase change materials (GST) on new substrates, like Si(111) or BaF2(111).



For the applications of GaN (e.g. as LEDs, LDs) it is necessary to grow GaN of high quality and purity. In order to match these requirements, the GaN thin films here were grown by ion beam assisted molecular beam epitaxy (IBA-MBE) using hyperthermal nitrogen ions for the growth process. As substrate material Si(111) and Si(100) was chosen, because Si is well established in the manufacturing of electronic devices. Furthermore, Si is cost-effective and readily available. Despite the high lattice and thermal mismatch between GaN and Si and many more difficulties, it was possible to grow GaN thin films epitaxially on Si. Various methods were used for topographical and structural analysis of the thin films, like reflection high energy electron diffraction (RHEED), atomic force microscopy (AFM), X-ray diffraction (XRD) and photoluminescence (PL) spectroscopy. The GaN thin films exhibited three dimensional growth of the hexagonal phase on Si(111) with a c-axis orientation and of the cubic phase on Si(100) with (200) orientation. In the PL measurements (not shown here), the near bandgap luminescence of the hexagonal and cubic GaN was observed with only a weak yellow luminescence.



⇑ AFM topography images and RHEED patterns of a hexagonal GaN thin film deposited on Si(111) (left) and of a cubic GaN thin film deposited on Si(100) (right). XRD in-plane pole figure measurements (z-GaN{200} (left) and z-GaN{220} (right), also containing contributions from Si{311}) of a cubic GaN thin film deposited on Si(100).

⇒ *SERS Biosensor Using Metallic Nano-Sculptured Thin Films for the Detection of Endocrine Disrupting Compound Biomarker Vitellogenin*
S.K. Srivastava, A. Shalabney, I. Khalaila, Ch. Grüner, A. Finzel, B. Rauschenbach, I. Abdulhalim / Small (2014) **10** 3579

⇒ *Direct Imaging of Crystal Structure and Defects in Metastable $Ge_2Sb_2Te_5$ by Quantitative Aberration Corrected STEM*
U. Roß. A.Lotnyk, E. Thelander, B. Rauschenbach / Appl. Phys. Lett. (2014) **104** 121904

⇒ *Epitaxial Growth of Ge-Sb-Te Films on KCl by High Deposition Rate Pulsed Laser Deposition*
E. Thelander, J.W. Gerlach, U. Roß. F. Frost, B. Rauschenbach / J. Appl. Phys. (2014) **115** 213504

⇒ *Nanoscale-Resolved Elasticity: Contact Mechanics for Quantitative Contact Resonance Atomic Force Microscopy*
A.M. Jakob, J. Buchwald, B. Rauschenbach, S.G. Mayr / Nanoscale (2014) **6** 6898

⇒ *High-Fluence Hyperthermal Ion Irradiation of Gallium Nitride Surfaces at Elevated Temperatures*
A. Finzel, J.W. Gerlach, J. Lorbeer, F. Frost. B. Rauschenbach / Appl. Surf. Sci. (2014) **317** 811

⇒ *Nanosecond Laser-Induced Phase Transitions in PLD-deposited GeTe Films*
X. Sun, E. Thelander, P. Lorenz, J.W. Gerlach, U. Decker, B. Rauschenbach / J. Appl. Phys. (2014) **116** 133501

⇒ *Low-Temperature Epitaxy of Ge-Sb-Te Films on BaF_2 (111) by Pulsed Laser Deposition*
E. Thelander, J.W. Gerlach, U. Ross, A. Lotnyk, B. Rauschenbach / Appl. Phys. Lett. (2014) **105** 221908

⇒ *Nanometer-Resolved Mechanical Properties around Crystal Surface Steps*
J. Buchwald, M. Sarmanova, B. Rauschenbach, S.G. Mayr / Beilstein J. of Nanotechnology (2014) **5** 2164

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

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

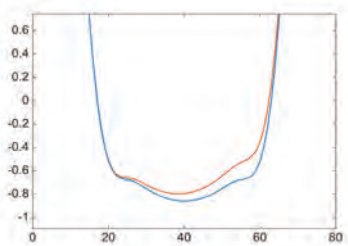
Prof. Dr. Bernd Rosenow
Dipl.-Phys. Alexander Janot, M.Sc. Phys. Martin Treffkorn

Research in the group is focused on the analysis of quantum condensates, their low-energy excitations, and on topological quantum systems. Examples for quantum condensates are superconductors and exciton-polariton condensates. The common characteristic of such condensates is the existence of a macroscopic wave function, which describes the collective quantum dynamics of the system. This allows for a variety of novel fascinating phenomena, e.g. condensation at a finite momentum and experimentally controllable superflow. An exciton-polariton condensate, in contrast to a common condensate, is a non-equilibrium macroscopic state and allows to study the physics of a condensed non-equilibrium steady state. Quantum Hall systems on the other hand are a well known example for topologically ordered

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

Subsequently to our former work, we analysed a polariton condensate in a disordered environment. In order to compare with experiment we considered a finite region of excitation and investigated the far field emission pattern. In line with our previous results, we find that the non-equilibrium polariton condensate is strongly affected by disorder; disorder induces fluctuations in the far field emission pattern which remain strong even at high densities. This prediction is supported by comparison to measurements in a ZnO micro-cavity [Institute for Experimental Physics II, Universität Leipzig].

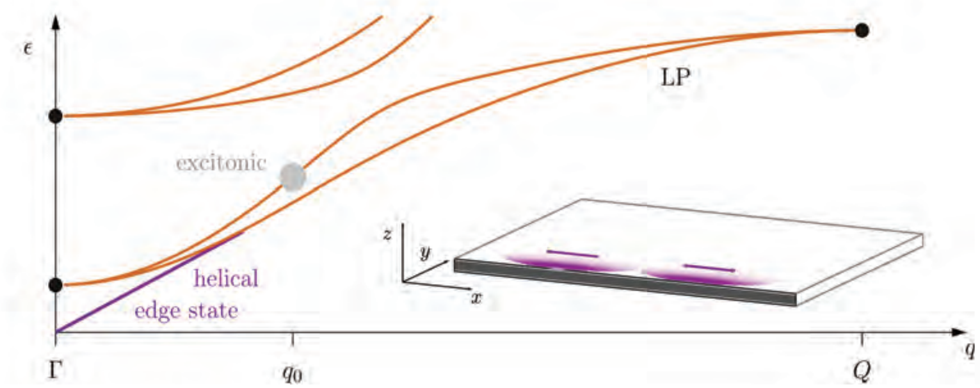
Furthermore, we focused on the topological properties of a solid-state system due to the interaction of light and matter, and for this purpose considered topological polaritons in a hybrid system of a two-dimensional quantum spin Hall insulator embedded into an optical cavity. In particular, we identified the topological index and hallmarks for topological polaritons in a quantum spin Hall cavity. We predicted helical polaritonic edge states, which are topologically protected by non-vanishing Chern numbers. These Chern numbers are equivalent to the number of wrappings of the polarisation vector of the bulk polaritons around the Bloch sphere. Applying an external Zeeman field allows an experimental extraction of this topological invariant. In summary, we make precise prediction on how topological polaritons in a time reversal invariant setup can be observed, and demonstrate that a topologically nontrivial quantum spin Hall insulator coupled to cavity photons is a candidate.



⇐ Equilibrium (blue curve) vs. non-equilibrium (red curve) potential for electrons inside a two dimensional electron gas, confined by a gate potential, with a perpendicular magnetic field of 2 T. Coulomb interaction between the electrons leads to the formation of broad compressible (flat) and incompressible (steap) strips. A bias of 0.1\hbar\Ω_c is applied to one of the edge channels to obtain the non-equilibrium potential.

The low energy excitations of the quantum Hall condensate at filling factor 5/2 are believed to be quasiparticles with non-abelian statistics, an exotic generalisation of bosonic and fermionic statistics. Currently, experimental efforts are under way to proof the existence of these particles through interference experiments in submicron scale devices. Important building blocks of such interferometers are quantum point contacts, which allow tunneling between counter-propagating edge states. The result of this tunneling is plateaus in the conductance as a function of gate voltage or magnetic field. The model of edge states passing through or being reflected at the quantum point contact is well accepted, but little is known about details, such as exact position and width of individual edge states inside the point contact. Recent experiments managed to image the quantum Hall edge states by scanning gate microscopy. With this technique, one can analyse the detailed structure of edge states.

We construct a self-consistent potential of a gate induced quantum point contact taking into account Coulomb interactions between electrons at finite temperature. Considering a picture of interacting electrons improves the results dramatically as compared to the results obtained with the often-used harmonic saddle-point potential. Interactions lead to an alternating pattern of compressible and incompressible strips within the 2D electron gas. Within compressible strips, the potential is pinned to the corresponding Landau level energy, while it varies strongly across incompressible strips. Consequently the edge channels in the interacting picture are much wider than the ones in a non-interacting picture. Being able to calculate a self-consistent potential, we focused on the non-equilibrium physics of quantum point contacts. A bias is applied across the system and we calculate non-equilibrium potentials and electron densities using a non-equilibrium Greens function technique. The next step will be the calculation of non-equilibrium currents and the exact current distribution inside the 2D electron gas.



⇑ Signatures of topologically nontrivial polaritons in a quantum spin Hall cavity: (i) Along a closed line q_0 in momentum space around the γ-point the polariton wave function is purely excitonic. (ii) Helical edge states emerge at the boundary of a finite sample with dispersion below the lower polariton (LP) branch.

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

Experiences

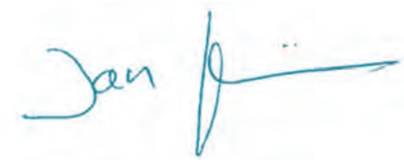
BuildMoNa's seventh year – a principal investigator's view

Prof. Dr. Jan Meijer

The established Graduate School BuildMoNa in Leipzig combines chemical, biochemical and physical scientific institutions with the aim to transfer the knowledge and infrastructure of the different disciplines. BuildMoNa therefore underlines the strong life-science community in Leipzig and leads to fruitful synergetic effects. This success is shining far beyond the borders of Saxony.

Basically the strong interdisciplinary character of the graduate school allows the doctoral candidates to profit by learning new scientific backgrounds and getting a different view of their own fields; but also the PIs profited and can combine the interdisciplinary knowledge in order to create new ideas. However, as for every successful institution, the main important parts are their members and the persons who make the continuously living platform of scientific exchange possible. The speaker Prof. Dr. Hey-Hawkins guarantees the friendly and open atmosphere that captures all areas and every member. As a newcomer I feel directly integrated and her open and curious mind allows a fast and easy start.

Beside the exchange of knowledge an additional advantage is the possibility to get a fast and easy admission to the equipment that could help to solve a specific question. Of course due to its limited financial support the graduate school has to concentrate on its basic duties. I am convinced that BuildMoNa will further play an important part in the education of young scientists of our university, for their future career in industry or academia.



Prof. Dr. Jan Meijer

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

M.Sc. Phys. André Heber

The interdisciplinary Graduate School BuildMoNa offers great opportunities for young scientists from the disciplines physics, chemistry and biochemistry who study and design molecules, nano-objects as well as nano-structures in their research. The Graduate School also fills gaps from the undergraduate studies where the education is concentrated on a particular discipline.

A large part of the doctoral education takes place in scientific modules. The modules are usually small workshops for which experts from a field of research are invited. From the workshops principal investigators and doctoral candidates benefit at the same time. The doctoral candidates get insights into different scientific topics that broaden their views and provide new ideas for their research. The senior scientists can advance the area of research by discussing recent results, developing new hypotheses and start new collaborations. The informal part of the workshops is well suited to make personal contact with well-established scientists from abroad, which is not easily possible at international conferences.

The examination procedure of the modules is strongly discussed within the doctoral candidates. We find that the frequent use of written exams does not always agree with the objective of BuildMoNa. The tests usually query factual knowledge and do not encourage the detailed occupation with the topic or certain aspects of it that are relevant for the individual doctoral researcher. I would personally prefer oral exams or reports on the scientific module.

The part in which BuildMoNa has excelled is the integration of the doctoral candidates who are not just participants of the modules and the Annual BuildMoNa Conference but also influence the topics and propose lecturers. The Annual BuildMoNa Conference is great for the interdisciplinary scientific and personal exchange within the doctoral candidates and the principal investigators. As a member of the Steering Committee I always had the feeling that BuildMoNa is focussed on the interests of the doctoral candidates. I strongly encourage the principal investigators to continue the excellent work of the Graduate School BuildMoNa and to recruit new doctoral candidates for BuildMoNa. In my opinion BuildMoNa is a good example for a structured doctoral programme within the Research Academy Leipzig.

M.Sc. Phys. André Heber

Training

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

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

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

TRAINING CONCEPT

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

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

Scientific and methods modules

Basic concepts in chemistry (2014-B1)

27 / 28 March 2014,
written exam, 2 credit points, yearly recurrence, 18 participants

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

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

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

Basic concepts in biochemistry (2014-B2)

17 / 18 March 2014,
written exam, 2 credit points, yearly recurrence, 18 participants

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

Responsible Scientist:
Prof. Dr. H. Harms

Lecturers:
Dipl.-Biochem. M. Bosse, Universität Leipzig, Germany; Dr. A. Chatzinotas, UFZ, Leipzig, Germany; Prof. Dr. H. Harms, UFZ, Leipzig, Germany; Dr. F. Harnisch, UFZ, Leipzig, Germany; Dr. U. Krug, Universität Leipzig. Germany; M.Sc. Biochem. G. Künze, Universität Leipzig, Germany; Dr. P. Schmidt, Universität Leipzig, Germany; Dr. L. Wick, UFZ, Leipzig, Germany

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

Basic concepts in physics (2014-B3)

07 / 14 / 15 May 2014,
written exam, 2 credit points, yearly recurrence, 6 participants

Doctoral researchers without a physics background were brought up to a level necessary to understand the thematic and advanced modules (T1–T6, A3, A2). The doctoral researchers gained insight into the physical principles of materials, the size-dependence of properties, strength- and length dependence of interaction energies, Brownian motion, quantum mechanics and molecular dynamics. They were exposed to fundamental concepts of statistical physics and thermodynamics. Moreover, they gained a feeling for the quantitative analysis that is the basis of physical thinking.

Responsible Scientists/Lecturers:
Prof. Dr. F. Cichos, Prof. Dr. P. Esquinazi, Prof. Dr. W. Janke

Contents:
⇒ Fundamentals of matter
⇒ Solid-state physics (charge transport, band structure, Bloch oscillation, point contacts, tunnelling, magnetotransport)
⇒ Diffusion (Brownian motion, mass transport, random motion, ballistic motion, dissipation)
⇒ Hydrodynamics
⇒ Nanoconfinement (electrons, photons, phonons, structured dielectric media/ photonic crystals, plasmons, metallic nanostructures)
⇒ Optics (ray optics, nonlinear optics)
⇒ Computer simulations (molecular dynamics, Markov chain Monte Carlo methods)
⇒ Polymer physics (entropic forces, viscoelasticity, polymer dynamics)

Basic concepts in molecular spectroscopy (2014-B4)

21 / 22 July 2014,
written exam, 2 credit points, yearly recurrence, 29 participants

This module introduced the basic concepts in molecular spectroscopy, i.e. infrared (IR), (surface enhanced) Raman- with imaging options and broadband dielectric spectroscopy (BDS), nuclear magnetic resonance spectroscopy, optical microscopy, superresolution microscopy and single molecule fluorescence detection.

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

Contents:
⇒ Quantum mechanical foundation of infrared spectroscopy
⇒ Experimental principles of Fourier transform infrared spectroscopy
⇒ Principle of broadband dielectric spectroscopy
⇒ Modern applications of broadband dielectric spectroscopy
⇒ Discussion of the chemical shift Hamiltonian with isotropic and anisotropic parts in NMR spectroscopy
⇒ Influence of sample orientation and molecular dynamics on the NMR signals
⇒ Magic angle spinning
⇒ Requirements for single molecule fluorescence detection at low and room temperature
⇒ Optical microscopy
⇒ Schemes as well as microscopic detection beyond the diffraction limit

Smart molecules: Building on the nanoscale with nucleic acids (2014-T1)

01 / 02 September 2014,
written exam, 2 credit points, bi-yearly recurrence with modification, 15 participants

The module aimed to provide participants with some understanding of the basic principles of DNA-based self-assembly nanobiotechnology, the functionalisation of biological surfaces, i.e. lipid and biological membranes, and the interaction of DNA with metal ions.

Responsible Scientists:
Prof. Dr. E. Hey-Hawkins, Prof. Dr. D. Huster

Lecturers:
Dr. A. Arbuzova, HU Berlin, Germany; Prof. Dr. D. Huster, Universität Leipzig, Germany; Prof. Dr. J. Liebscher, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania; Jessica Lorenz, Fraunhofer Institute, Leipzig, Germany; Prof. Dr. J. Müller, University of Münster, Germany; Prof. Dr. R. Seidel, University of Münster, Germany

Contents:
⇒ Chemical synthesis of lipid modified nucleosides and oligonucleotides
⇒ Membrane partitioning of lipophilic DNA, oligomer formation, Watson-Crick base pairing
⇒ Domain-specific portioning of DNA oligonucleotides
⇒ DNA origami
⇒ Interaction of DNA with metal ions
⇒ Application of DNA constructs in cell therapy

Methods:
⇒ Synthesis
⇒ Confocal fluorescence imaging
⇒ Fluorescence spectroscopy
⇒ NMR spectroscopy (both in solution and in the solid state)
⇒ Differential scanning calorimetry
⇒ Microscopy

From molecules to materials: Transparent conductive oxides – fundamentals and applications (2014-T4)

29 September – 02 October 2014,
written exam, 2 credit points, bi-yearly recurrence with modification, 26 participants

The material class of transparent conductive materials has been discovered 1907 by Karl W. Baedeker in Leipzig. This module focused on modern transparent functional materials, from their basic material physics to applications.

Responsible Scientists:
Prof. Dr. M. Grundmann

Lecturers:
Prof. Dr. M. Allen, University of Canterbury, New Zealand; Prof. Dr. F. Bechstedt, Friedrich-Schiller-Universität Jena, Germany; Dr. A. Bikowski, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany; Prof. Dr. L.J. Brillson, Ohio State University, USA; Dr. K.T. Butler, University of Bath, UK; Prof. Dr. C. Elsässer, Fraunhofer IWM, Freiburg, Germany; Prof. Dr. E. Fortunato, University of Lisbon, Portugal; Dr. Z. Galazka, Institut für Kristallzüchtung, Berlin, Germany; Prof. Dr. A. Hoffmann, TU Berlin, Germany; Prof. Dr. K.H. Kim, Seoul National University, Republic of Korea; Dr. S. Lany, NREL, USA; PD Dr. E.V. Lavrov, TU Dresden, Germany; Dr. D.C. Look, Wright State University, USA; Prof. Dr. W. Mader, Universität Bonn, Germany; Prof. Dr. B.K. Meyer, Justus Liebig Universität Gießen, Germany; Dr. L. Piper, Binghamton University, USA; Prof. Dr. B. Szyszka, TU Berlin, Germany; Prof. Dr. J.F. Wager, Oregon State University, USA

Contents:
- ⇒ Theory of oxide electronic materials
- ⇒ Growth of bulk semiconducting oxides
- ⇒ Amorphous oxide thin films
- ⇒ Metal-like n-type TCOs
- ⇒ p-type oxides
- ⇒ Point defects in oxides
- ⇒ Oxide devices

Methods:
- ⇒ Thin film deposition
- ⇒ Optical and electrical characterisation
- ⇒ Device processing

Hybrid systems: Functional biomolecules at (solid) materials interfaces (2014-T6)

22 / 23 May 2014,
written exam, 2 credit points, bi-yearly recurrence with modification, 17 participants

This module taught the principles in preparation and application of hybrid systems, including immobilisation of biomolecules and cells and prerequisites for materials to attach biomolecules, as well as possible future applications in biomedicine, biotechnology and informatics. Moreover, it introduced the knowledge to produce solid-state devices that can be interfaced with soft matter.

Responsible Scientist:
Prof. Dr. T. Pompe

Lecturers:
Prof. Dr. C. Duschl, Fraunhofer Institute for Biomedical Engineering, Potsdam, Germany; Dr. H. Hähl, Saarland University, Saarbrücken, Germany; Prof. Dr. M. Salmeron-Sanchez, University of Glasgow, UK; Dr. S. Schmidt, Universität Leipzig, Germany; Dr. C. Sperling, Leibniz Institute of Polymer Research, Dresden, Germany; Dr. T. Weikl, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Contents:
- ⇒ Hybrids of synthetic and biological compounds (combinations of synthetic molecules and peptides, advantages of synthetic and biological building blocks)
- ⇒ Hybrid compatible proteins (protein expression by methods that allow modification and introduction of non-proteinogenic amino acids, intein and impact system, modification of tRNA and genetic code expansion, selective chemical modification, cellfree protein production, pegylation)
- ⇒ Biocompatibility, toxicity and biodegradation
- ⇒ Chemical aspects (generation of polymers, surface modification, nanoscaffolds, preparation of building blocks, smart materials)
- ⇒ Hybrid compounds (preparation, analysis, ligation strategies, immobilisation)
- ⇒ Applications (biomedical science, biosensors)
- ⇒ Biological cells on chips (bioimpedance, electrodes and MOSFETs for cells, neuronal networks, cardiac tissue)
- ⇒ Smart cell substrates (switchable polymers, nanopores, nanostructures, nanocontact printing)

Methods:
⇒ Methods for proteins and peptides (techniques for modified proteins, side-chain protection strategies in peptide synthesis, cell-based assays to study toxicity, biostability and inflammation)
⇒ Analytics (biocompatible mass spectrometry [MALDI-TOF, ESI-Q3], AFM, solid-state NMR, solution NMR, fluorescence microscopy, confocal microscopy, SPR)
⇒ Neuronal cells (isolation, culture, patch clamp)
⇒ Fabrication of solid-state devices (building nanostructures, ZnO-based devices)

Quantum coherent structures (2014-A3)

06 / 07 October 2014,
written exam, 2 credit points, yearly recurrence with modification, 15 participants

This module dealt with coherent quantum states which occur in so-called mesoscopic systems, i.e. condensed matter systems intermediate between the atomic scale and the macroscopic world. While macroscopic objects are described by average properties derived from its constituent materials and usually obey the laws of classical mechanics, a mesoscopic object is affected by fluctuations around the average, and is subject to quantum mechanics. For example, in contrast to the conductance on the macroscopic level which increases continuously with the diameter of a wire, at the mesoscopic level, the conductance is quantised – the increase occurs in discrete steps. On the fundamental level, interference processes and the quantum Hall effects are part of mesoscopic physics. From a more applied point of view, mesoscopic physics is very relevant for the ongoing miniaturisation of transistors and other electronic devices, which in the future will operate using quantum mechanical principles and in this way support solid state quantum information processing. The fundamentals of the field and several examples will be considered.

Responsible Scientists:
Prof. Dr. B. Rosenow

Lecturers:
Prof. Dr. Y. Gefen, Weizmann Institute of Science, Israel; Dr. A. Romito, FU Berlin, Germany

Contents:
⇒ Coherent transport
⇒ Conductance quantisation
⇒ Quantum dots
⇒ Nonequilibrium (shot) noise
⇒ Anyons and fractional statistics
⇒ Electronic and anyonic interferometers
⇒ Dephasing and decoherence
⇒ Quantum measurement
⇒ Solid state qubits
⇒ Solid state quantum information processing

Methods:
⇒ Theoretical methods of modern solid state physics

Scientific minisymposium

Physics of cancer (2014-A2)

02–05 October 2014

The fifth BuildMoNa Minisymposium was organised by the research group of Prof. Dr. J. Käs. It brought together researchers from the worldwide pioneering groups that are concerned with the investigation of the physical mechanisms underlying cancer progression. The speakers were:

⇒ Patricia Bassereau, Institut Curie, France: *Pulling with Filopodia: High Forces on Weak Connections*
⇒ Joel Beaudouin, German Cancer Research Center & BioQuant, Germany: *Mechanism of CD95 Clustering and Activation at the Single Cell Level*
⇒ Timo Betz, Institut Curie, France: *The Mechanics of Invasion: How Contraction Sets the Stage for Invasive Migration*
⇒ Daria Bonazzi, Institut Jacques Monod, France: *Actin-based Transport adapts Polar Cap Size to Local Curvature*
⇒ Jasna Brujic, New York University, USA: *Mimicking Tissues with Densely Packed Lipid Droplets*
⇒ Giovanni Cappello, Institut Curie, France: *Applying Controlled Mechanical Pressure on Tumour Cells Aggregates*
⇒ Dino Di Carlo, University of California, Los Angeles, USA: *Measuring Cell Mechanics for Medicine*

- Prof. Dr. Ben Fabry, University of Erlangen-Nuremberg, Germany: *Tumour Cell Migration is a Superstatistical Process*
- Prof. Dr. Claudia Fischbach-Teschl, Cornell University, USA: *Tissue Engineering Approaches and their Relevance to Studying Tumour–Stroma Interactions*
- Daniel Fletcher, University of California, Berkeley, USA: *Mechanical Constraints and Cancer*
- Karin Forsberg Nilsson, Uppsala University, Sweden: *Modeling Glioma and Targeting the Glioma Niche*
- Kristian Franze, University of Cambridge, UK: *Mechanotransduction in Developing Cell Systems*
- Annica K. B. Gad, Karolinska Institutet, Sweden: *Oncogenic Cell Transformation Changes the Nanoscale Organisation of Adhesions, Vimentin Filaments and Cell Stiffness*
- Dr. Rhoda J. Hawkins, University of Sheffield, UK: *Modelling Cell Motility using Active Gel Theory*
- David M. Helfman, KAIST, South Korea: *Oncogenic Signalling and the Cytoskeleton*
- Sylvie Hénon, Université Paris Diderot, France: *Role of Serum Response Factor in the Mechanotransduction of Myoblasts*
- Prof. Dr. Michael Höckel, Universität Leizig, Germany: *Association between Embryonic Development and Locoregional Cancer Progression*
- Prof. Dr. Paul Janmey, University of Pennsylvania, USA: *Mechanical Sensing by Normal and Transformed Cells*
- Prof. Dr. Josef A. Käs, Universität Leipzig, Germany: *The Cytoskeleton Significantly Impacts Invasive Behaviour of Biological Cells*
- Franziska Lautenschläger, Saarland University, Germany: *Micromechanical Tools to Study the Role of Vimentin in Cells*
- Lance L. Munn, Massachusetts General Hospital & Harvard Medical School, USA: *Biomechanical Processes and Topological Dynamics in Tumours*
- Inke Näthke, University of Dundee, UK: *Early Changes in Tissue Organisation and Structure in Colorectal Cancer*
- Timothy Newman, University of Dundee, UK: *Quantifying Metastasis using Rare Events*
- Dr. Matthieu Piel, Institut Curie, France: *Cell Migration in Confining Spaces: Pushing off the Walls and Squeezing through Small Holes*
- Jacques Prost, Institut Curie, France: *Analysis of a few in vitro Experiments*
- Cynthia Reinhart-King, Cornell University, USA: *Individual and Collective Metastatic Cell Migration Behaviours*
- Prof. Dr. Ana-Suncana Smith, University of Erlangen-Nuremberg, Germany: *Toward the Understanding of the Growth of Model Epithelial Tissues*
- Melda Tozluoglu, University College London, UK: *Plasticity of Cancer Cell Migration: Extracellular Matrix enables the Optimisation of Blebbing, Adhesions, and Spreading*
- Krystyn J. van Vliet, Massachusetts Institute of Technology, USA: *Chemomechanics of Cell Migration and Activation in the Cancer Microenvironment*
- Raphaël Voituriez, Pierre-and-Marie-Curie University, France: *Active Gels, Cell Motility and Cell Trajectories*
- Angelika M. Vollmar, LMU Munich, Germany: *Biophysical Characterisation of the Myxobacterial Compound Soraphen A: An Innovative Option to Fight Invasive Cancer*
- Dr. Franziska Wetzel, Institut d'Optique Graduate School, France: *Caveolae-mediated Mechanotransduction in Single Cells and Imaging of Confined Spheroids*

Transferable skills workshops

Presentation workshop

Dr. Frank Lorenz, Rhetoric Excellence,
27 February / 6 March 2014 in combination with the Annual BuildMoNa Conference,
7 participants

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

Grant proposal writing

RaumZeit e.K.,
19 / 20 May 2014, in cooperation with the Research Academy Leipzig, 12 participants

The workshop covered the complete proposal process:
⇒ Identification of the right funding scheme
⇒ Assessment of the framework defined by the funding scheme
⇒ Mapping the research idea to the framework to achieve a high relevance
⇒ Setting up a concept for the project
⇒ Identification of necessary expertise and resources
⇒ Structuring the proposal
⇒ Visualisation
⇒ Formulation of the different parts of the proposal with regard to the framework and the evaluation criteria
⇒ Coordination of the proposal writing and submission process

Doctorate and then what?! Workshop on career planning for doctoral candidates in the sciences

Uni support,
05 / 06 June 2014, in cooperation with the Research Academy Leipzig, 10 participants

The decision to pursue a particular career has a great impact on one's further personal development. With this is mind, it is crucial to make a carefully considered and well-founded decision for an individually tailored career.

This workshop provided a variety of information about career paths within and outside of academia and explains the special rules of each professional field. Participants had an opportunity to assess their current situation in detail as a basis for further planning their professional profile.

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Andre Skirtach	*Ghent University, Belgium*	Polyelectrolyte multilayer capsules and films: towards single cell manipulation	07 January 2014	*Faculty of Biosciences, Pharmacy and Psychology*
Professor Dr. Rory Waterman	*University of Vermont, USA*	Zirconium-catalysed heterofunctionalisation	24 April 2014	*Faculty of Chemistry and Mineralogy*
Dr. Peter Georgiev	*Sofia University, Bulgaria*	Neutron scattering studies of hydrogen in materials for gas storage and catalysis	14 May 2014	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Marius Andruh	*University of Bucharest, Romania*	Heterotrispin complexes and 3d-4f clusters. Synthetic strategies, magnetic and photophysical properties	28 May 2014	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Lawrence J. Marnett	*Vanderbilt University, USA*	Cyclooxygenase-2 oxidation of endocannabinoids: New biological mediators and therapeutic opportunities	20 June 2014	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Kenton H. Whitmire	*RICE University, USA*	Using molecular single source precursors for the preparation of advanced materials: Strategies, limitations and successes	09 July 2014	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Munetaka Akita	*Tokyo Institute of Technology, Japan*	Photoredox catalysis: Inorganic-based organic synthesis promoted by visible light	15 October 2014	*Faculty of Chemistry and Mineralogy*
Dr. Lee J. Higham	*Newcastle University, UK*	Surprises in primary phosphine chemistry and their applications in catalysis and disease imaging	22 October 2014	*Faculty of Chemistry and Mineralogy*

Annual BuildMoNa Conference

The second annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held on 3 and 4 March 2014 at the Helmholtz Centre for Environmental Research (UFZ) and at the Faculty of Chemistry and Mineralogy. The following renowned guest speakers from science gave talks on current topics of BuildMoNa:

⇒ Prof. Dr. Manfred Helm, Helmholtz-Zentrum Dresden-Rossendorf, Germany: *Terahertz spectroscopy of nanostructures with a free electron laser*
⇒ Prof. Dr. Rudolf Merkel, Forschungszentrum Jülich, Germany: *Biophysical experiments on cellular mechanobiology*
⇒ Prof. Dr. Eva Rentschler, Johannes Gutenberg Universität Mainz, Germany: *The bottom-up approach towards magnetic materials*
⇒ Prof. Dr. Klaus Roth, Freie Universität Berlin, Germany: *Weird crystallisations and Sir William's beard*

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

⇐ Participants of the Annual BuildMoNa Conference

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

Martin Treß (Institute for Experimental Physics I) received the first prize for his work on the molecular dynamics of single polymer chains, published in:
Glassy Dynamics in Condensed Isolated Polymer Chains
M. Tress et al. / Science (2013) **341** 1371

Marco Braun (Institute for Experimental Physics I) received the second prize for his work on a novel method for the confinement and manipulation of single nano-objects in solution, published in:
Optically Controlled Thermophoretic Trapping of Single Nano-Objects
M. Braun and F. Cichos / ACS Nano (2013) **7** 11200

Wilma Neumann (Institute of Inorganic Chemistry) was awarded the third prize for her publications

Reduction of Hydroxy-functionalised Carbaboranyl Carboxylic Acids to Tertiary Alcohols by Organolithium Reagents
W. Neumann et al. / Dalton Trans. (2014) **43** 4935
and
2-Carbaborane-3-phenyl-1H-indoles – Synthesis via McMurry Reaction and Cyclooxygenase (COX) Inhibition Activity
M. Laube, W. Neumann et al. / ChemMedChem (2013) **8** 329

15 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.

⇑ Winners of the BuildMoNa Awards 2014: Martin Treß (left), Marco Braun, Wilma Neumann

For the 7 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 Uta Allenstein for her presentation “Functionalisation of FePd ferromagnetic shape memory alloys for biomedical applications – An experimental and theoretical survey”, the second to Andrea Kramer for her presentation “Melting of pectin gels” and the third to Cathleen Jendrny for “Characterisation of serpin-derived peptides by enzymatic cleavage to design KLK7 inhibitors”.

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference: Uta Allenstein, Andrea Kramer, Cathleen Jendrny (from right to left)

Funding of doctoral candidates

DFG

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Europäischer Sozialfonds

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