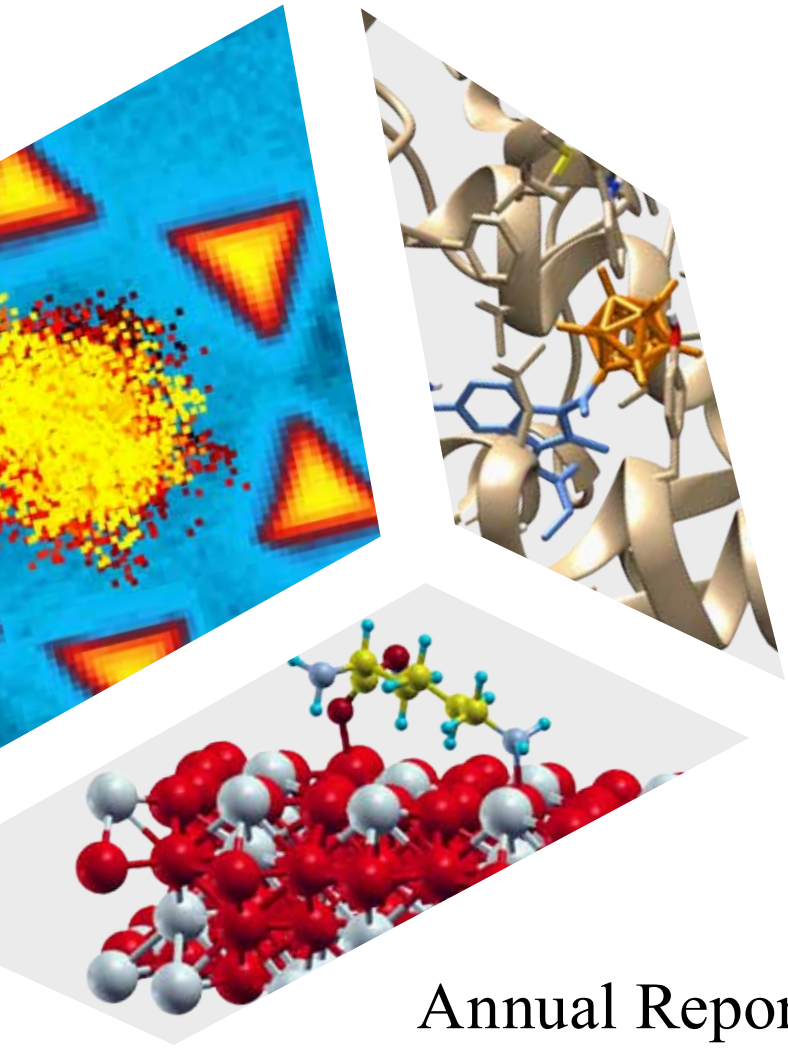
UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2013

Cover image:
- *Left:* Thermophoretic trapping of a 200 nm polystyrene sphere by a laser heated gold nano-structure
- *Right:* Carbaborane derivatives as pharmacophores: Molecular modelling of indoborin in the active site of COX-2
- *Bottom:* Biomolecule lysine binding to the ferromagnetic shape memory alloy iron-palladium

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Annual Report 2013

Founded as DFG Graduate School 185 in 2007

- Publisher: Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa)
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- Editor: Dipl.-Phys. Andrea Kramer
- Photographers: Swen Reichhold, Sebastian Willnow, Jan Woitas, Benjamin Bigl, Christian Hüller
- Design & Layout: Tim Klinger, Franziska Becker, Leipzig, meantrafik.com
- Production: Merkur Druck- & Kopierzentrum GmbH & Co. KG, Leipzig

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

Preface Prof. Dr. 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 2013, 103 doctoral candidates have been enrolled as members of BuildMoNa and 77 young scientists have already finished their doctoral studies. In 2013, 11 doctoral candidates were awarded a BuildMoNa scholarship, and 80 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 14 doctoral candidates were involved in three new ESF-funded young researchers groups affiliated with the graduate school.

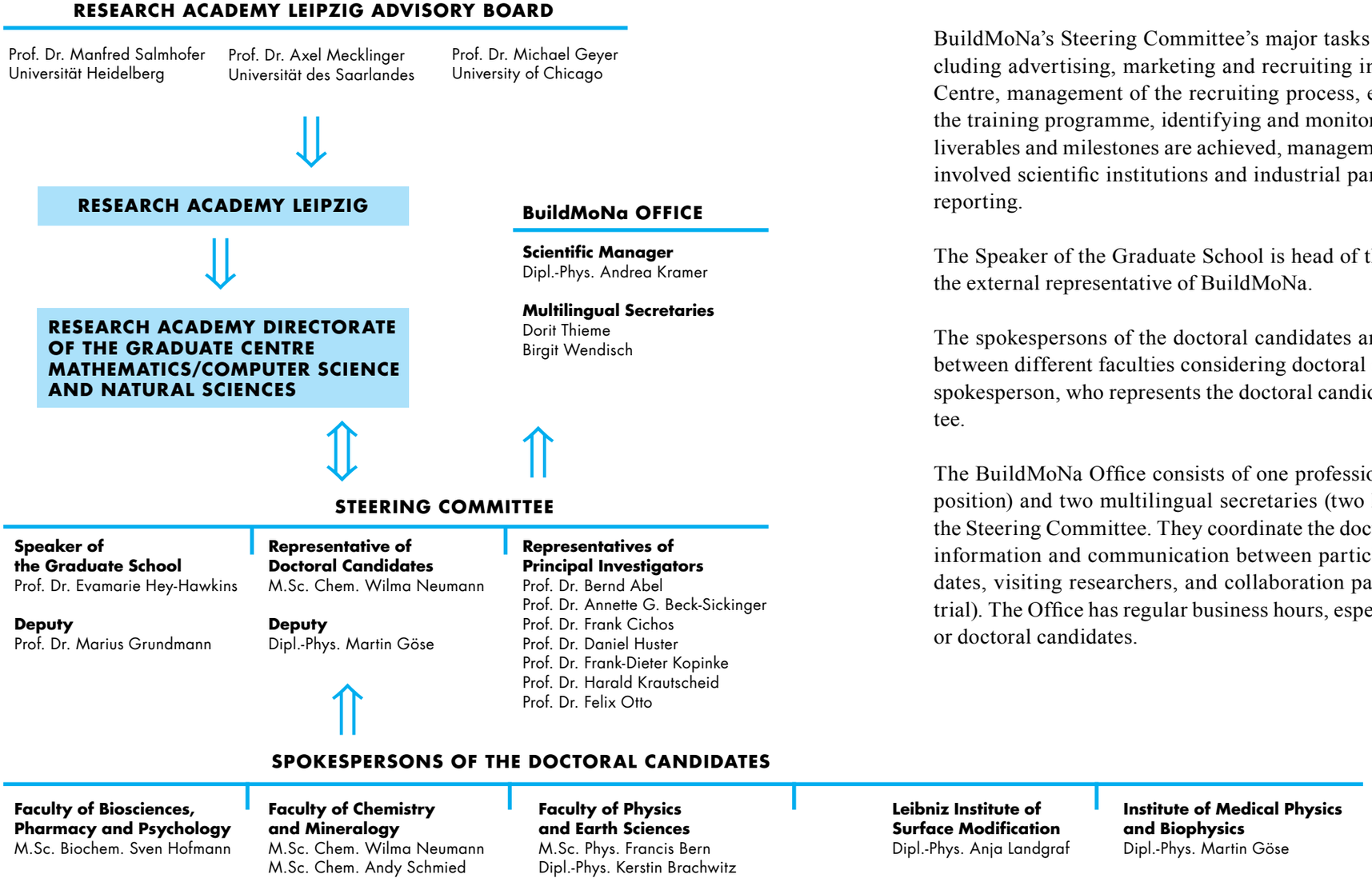
The graduate school provides a well-structured training programme including multi-disciplinary scientific training and a transferable skills programme in cooperation with the Research Academy Leipzig. The scientific training programme consists of introductory modules to bridge interdisciplinary gaps, 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 2013, the minisymposium "Smart and Active Assemblies" was organised by Prof. Evamarie Hey-Hawkins, Prof. Roger Gläser and Prof. Frank-Dieter Kopinke. At the minisymposium, 16 internationally renowned invited speakers presented latest trends in homogeneous catalysis, heterogeneous catalysis and environmental and biocatalysis

Science-related events included the Annual BuildMoNa Conference, which resulted from a combination of the BuildMoNa Symposium and the BuildMoNa Workshop for doctoral candidates. This event especially provides a platform for interdisciplinary exchange and discussion within the graduate school.

Although BuildMoNa will no longer be funded by the DFG within the German Excellence Initiative from November 2014 on, the graduate school will for now be continued with financial support from other sources as a class at the Research Academy Leipzig until October 2017.

Prof. Dr. Evamarie Hey-Hawkins

Organisation and management



The Graduate School BuildMoNa is a class of the *Research Academy Leipzig* within the Graduate Centre for Mathematics, Computer Science and Natural Sciences, its director being Prof. Dr. R. Gläser. BuildMoNa is represented within the Research Academy by Prof. Dr. 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. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phosphaindazole: A promising building block for novel materials*
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. Phys. Ana Isabel Ballestar Balbas	Prof. Dr. P. Esquinazi / Prof. Dr. T. Butz	*Intrinsic anisotropy of multigraphene and transport properties of graphite interfaces*
M.Sc. Chem. Salma Begum	Prof. Dr. H. Krautscheid / Prof. Dr. 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. Chem. Eng. Paul Cosmin Boar	Prof. Dr. 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. 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. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaborane derivatives in tumour therapy and diagnosis*
M.Sc. Phys. Michael Bonholzer	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Magneto-tunnel junctions with oxidic contacts*
Dipl.-Phys. Tammo Böntgen	Prof. Dr. M. Grundmann / Prof. Dr. F.-D. Kopinke	*Optical investigation of $BaTiO_3$-heterostructures with ellipsometry and Raman-scattering*
Dipl.-Phys. Kerstin Brachwitz	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Materials of ferroic order and their interaction*
Dipl.-Phys. Marco Braun	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Gold nanoparticle based thermophoretic nanofluids*
M.Sc. Chem. Martin Brehm	Prof. Dr. B. Kirchner / Prof. Dr. R. Gläser	*Development of a program package for efficient simulation of complex chemical systems*
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*
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. 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*
Dipl.-Phys. Anatol Fritsch	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Growth of soft breast tumour cells in micro- and nanostructured hard 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. 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. Phys. Tom Golde	Prof. Dr. J. Käs / Prof. Dr. E. Hey-Hawkins	*Actin related contractile structures*
Dipl.-Phys. Martin-Patrick Göse	Prof. Dr. D. Huster / Prof. Dr. T. Pompe	*Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake*
M.Sc. Chem. Sina Gruschinski	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Transition metal complexes with spin-crossover properties*
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*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Marcel Handke	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	*Networks based on 4d and 5d-metal ions as possible catalysts*
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. E. Hey-Hawkins	*Chemical modification of peptides*
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. E. Hey-Hawkins	*Design and development of peptides for therapeutic application*
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. Tobias Kießling	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Molecular marker free isolation of pluripotent haematopoetic stem cells and metastatic cancer cells from blood*
Dipl.-Phys. Fabian Klüpfel	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	*Transparent active multi-electrode arrays for the measurement of nerve cell signals*
Dipl.-Math. Melanie Knorr	Prof. Dr. J. Käs	*Role of stochasticity in a moving thin polymer film*
Dipl.-Phys. Jonas Kohlrautz	Prof. Dr. J. Haase / Prof. Dr. P. Esquinazi	*Magnetic resonance under extreme condidtions*
Dipl.-Phys. Wilhelm Kossack	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	*IR-spectroscopy for the analysis of structure and dynamic of polymers*
Dipl.-Phys. Andrea Kramer	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	*How temperature affects cell mechanics*
Dipl.-Phys. Christian Kranert	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	*Electron-photon-interaction in micro- and nanowires*
M.Sc. Appl. Chem. Anusree Viswanath Kuttatheyil	Prof. Dr. J. Haase / Prof. Dr. H. Krautscheid	*Structure determination and host-guest interactions in porous metal-organic frameworks studied by solid-state NMR*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
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. E. Hey-Hawkins	*Stochastic analysis of plasma membrane fluctuations of neuonal growth cones*
M.Sc. Chem. Veronika Mäde	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Modified pancreatic polypeptide for treatment of obesity*
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. 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. Chem. Tobias Möller	Prof. Dr. E. Hey-Hawkins / Prof. Dr. S. Berger	*Synthesis of P-chiral phosphorus compounds derived from low-valent phosphorus species*
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. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Metal-organic frameworks with chiral binaphthalene-based linkers*
Dipl.-Phys. Nils Neubauer	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Photothermal fluctuation spectroscopy on gold nanoparticle dimers*
M.Sc. Chem. Paul Neumann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Switchable dendritic ferrocenyl phosphines*
M.Sc. Chem. Wilma Neumann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Overcoming cisplatin resistance of tumour cells with cytotoxic cyclooxygenase inhibitor conjugates*
M.Sc. Chem. Mareen Pagel	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. 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. Chem. Eva Perlt	Prof. Dr. B. Kirchner / Prof. Dr. B. Abel	*Development of methods and application to complex systems from first principles*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
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. E. Hey-Hawkins	*Heterogeneous photocatalysis: water splitting with visible-light irradiation*
Dipl.-Chem. Stefan Richter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*New selective cytostatics*
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	*Spin polarisation investigations on exciton-polaritons and their condensates*
M.Sc. Phys. Susanne Rönicke	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The development of a novel technique to measure the proteomic content of biological cells by combining microfluidics, laser-based nano-manipulation and optical high-resolution tomography*
Dipl.-Phys. Martin Rothermel	Prof. Dr. T. Butz / Prof. Dr. M. Grundmann	*Spatially resolved characterisation of the composition, structural disorders and electronic properties of inorganic nanostructures*
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*
Dipl.-Phys. Florian Schmidt	Prof. Dr. M. Grundmann / Prof. Dr. R. Gläser	*Characterisation of defects in hetero- and nanostructures*
M.Sc. Chem. Andy Schmied	Prof. Dr. 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. E. Hey-Hawkins	*Chemical modification of peptide analogues*
Dipl.-Phys. Carsten Schuldt	Prof. Dr. J. Käs / Prof. Dr. B. Abel	*Cellular force generation on the single molecule level*
M.Sc. Phys. Ilya Semenov	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Dynamics of DNA under tension and in confinement*
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*
Dipl.-Phys. Marko Stölzel	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Time-resolved spectroscopy on ZnO based micro- and nanowire heterostructures and -cavities*
Dipl.-Phys. Dan Strehle	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Mechanical and dynamic properties of actin bundles*
Dipl.-Phys. Sebastian Sturm	Prof. Dr. K. Kroy / Prof. Dr. F. Kremer	*Nonequilibrium dynamics of forced and confined semiflexible 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*
Dipl.-Phys. Martin Treß	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	*Molecular dynamics in nanometre-thick polymer layers studied by means of broadband dielectric spectroscopy*
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*
Dipl.-Phys. Franziska Wetzel	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Direct staging of primary mammacarcinomas by determining their cellular composition including metastatically competent cells, dormant cancer cells and cancer stem cells*
Dipl.-Phys. Micha Wiedenmann	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Cluster aggregation and condensation of nano-objects*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
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. Chem. Patrick With	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	*Preparation, physico-chemical characterisation and testing of supported metal (oxide) catalysts*
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*

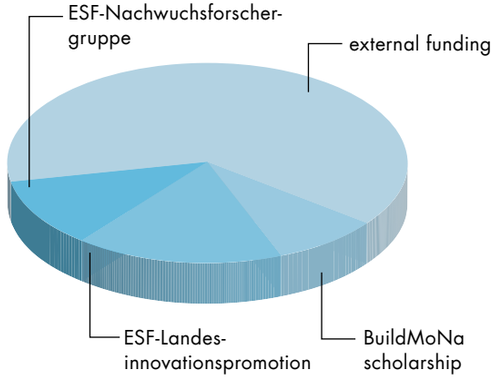
Alumni 2013

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Verena Ahrens	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Tumour targeting peptides – neuropeptide Y based shuttle systems*
Dr. rer. nat. Tobias Andrea	Prof. Dr. T. Butz / Prof. Dr. J. Käs	*3D-visualisation of intracellular drug delivery systems by ion micro-tomography and 3D-inverse tomography sculpting*
Dr. rer. nat. Jorge Luis Cholula Díaz	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmann	*Properties of novel precursor based materials*
Dr. rer. nat. Murali Dama	Prof. Dr. S. Berger / Prof. Dr. J. Haase	*Organo gels as an alignment media for RDC measurements*
Dr. rer. nat. Sylvia Els-Heindl	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Novel ghrelin receptor agonists and inverse agonists to alter energy homeostasis*
Dr. rer. nat. Dirk Friedrich	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmannn	*Synthesis, characterisation and deposition of CIGS precursors*
Dr. rer. nat. Matthias Golecki	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Encapsulation of catalytically active metal complexes*
Dr. rer. nat. Anne Grundmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis and reactivity of transition metal phosphinidene complexes*
Dr. rer. nat. Markus Gyger	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Active and passive biomechanical measurements for characterisation and stimulation of biological cells*
Dr. rer. nat. Anika Kreienbrink	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis and reactions of carba-borane-substituted 1,2-diphosphetanes and other phosphorus-rich heterocycles*
Dr. rer. nat. Jochen Lach	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Thin films of redox-active high-spin molecules*
Dr. rer. nat. Michael Lorenz	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Investigations on the stability of zinc oxide based metal-semi-conductor field-effect-transistors*
Dr. rer. nat. Yanhong Ma	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Magnetic shape memory alloys for miniaturised actuators*
Dr. rer. nat. Lena Neumann	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Hyperthermal ion assisted atomic assembly*
Dr. rer. nat. K. David Nnetu	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The use of biomechanics to reduce metastatic aggressiveness*
Dr. rer. nat. Julian Rodger Frederic Pritzwald-Stegmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	*Phosphorus-based organometallic/ inorganic hybrid materials*

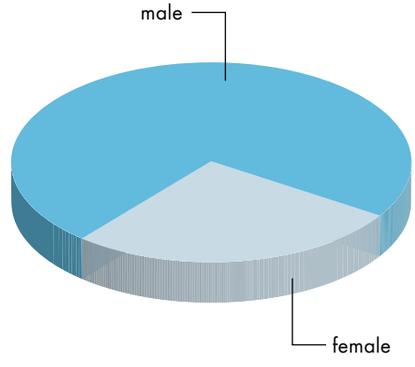
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Anastacia Romanova	Prof. Dr. W. Hackbusch / Prof. Dr. M. Grundmann	*Molecular simulations of ion effects on structural and thermodynamical properties of biopolymers*
Dr. rer. nat. Sebastian Schöbl	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	*Modelling and computer simulations of molecular pattern recognition*
Dr. rer. nat. Max Steinhagen	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Site-specific protein immobilisation for the design of biologically active surfaces*
Dr. rer. nat. Anja Steude	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	*Development and fabrication of novel peptide based biosensors for neuronal diagnostic tools*
Dr. rer. nat. Markus Streitberger	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Building catalytically active bi-metallic nano-frames with flexible bisphosphine ligands*
Dr. rer. nat. Olaf Ueberschär	Prof. Dr. F. Kremer / Prof. Dr. W. Janke	*Investigating stochastic thermody-namics by means of optical tweezers*
Dr. rer. nat. Carolin Wagner	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Investigation of the interaction of receptors and ligands by optical tweezers*

Statistics

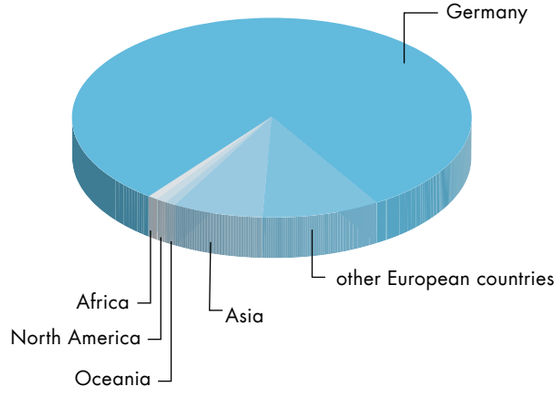
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:

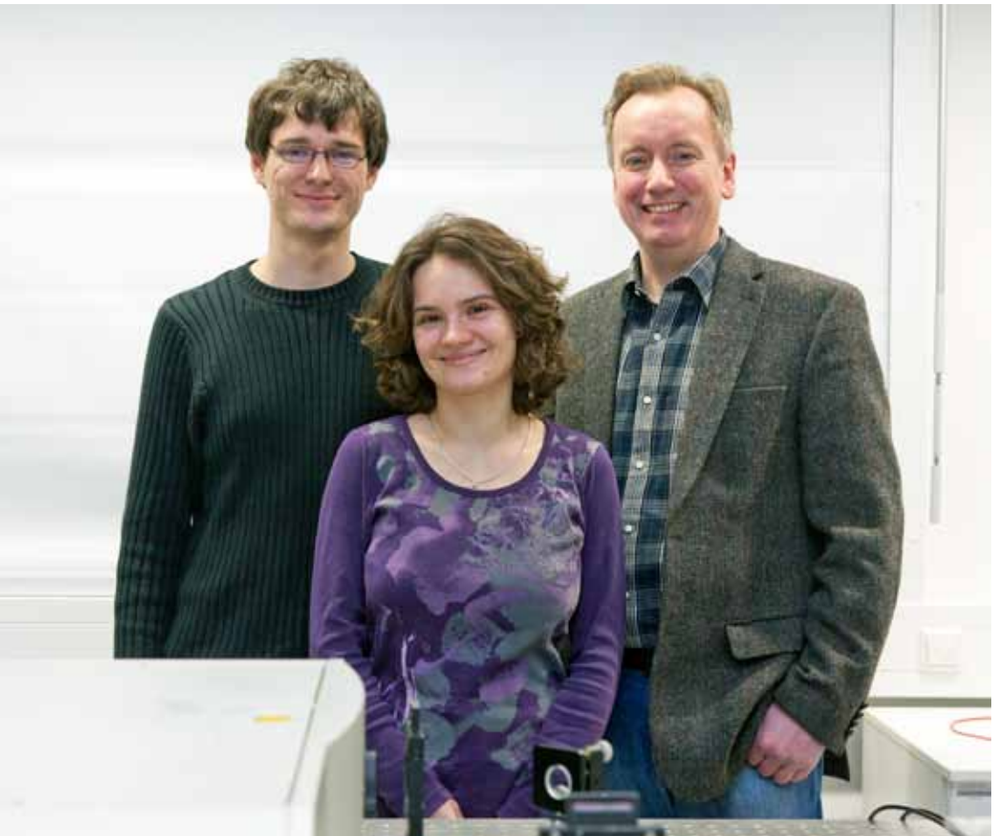


Biophysical and macromolecular chemistry

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

The Abel group works in the fields of biophysical chemistry and macromolecular chemistry as well as smart functional materials. 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.

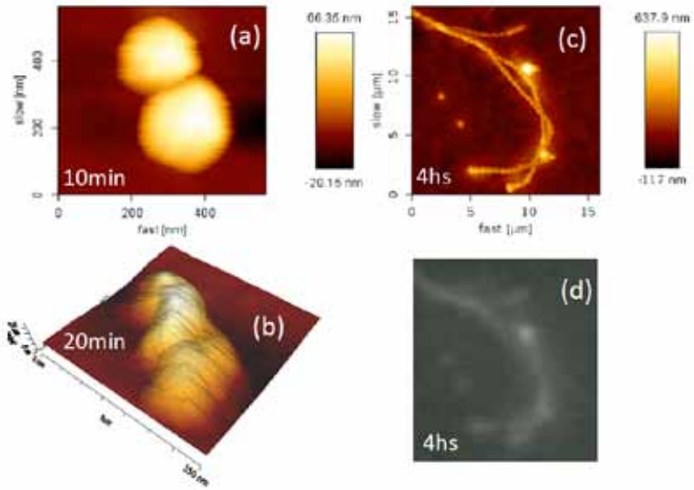
Within BuildMoNa we continued to investigate amyloid aggregation and fibrillation with nanoscale imaging techniques and we aimed at monitoring structures of aggregated proteins near interfaces of nanoparticles to resolve the question whether nanoparticles induce Alzeimer's disease (A. Gladytz).



Together with the Beck-Sickinger group we have successfully investigated biocompatibility at interfaces – being important in the long run for implants and electronic devices. We employed peptide based multifunctional molecules as anchors for cells near inorganic or metal interfaces (A. Gladytz).

The second area of research is amyloid protein/peptide aggregation near interfaces. The process, as well as its mechanisms 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 lasers. Together with theory the investigations have the long-time goal to determine detailed "molecular movies" on ultimate time and space scales.



⇑ AFM measurements of the aggregation of NNFGAIL in aqueous solution. Shown is a series of measurements (10 minutes (a), 20 minutes (b), and after 4 hours (c)). While the initial phase of aggregation is characterised by spheroids and spherical structures (a), which appear to assemble like 'pearls on a string', nice fibrillar structures appear at 3-4 hours, only. They still look like fibrils assembled with a large number of spherical building blocks (c). Epifluorescence of thioflavin-T intercalated into fibrils monitored with a fluorescence microscope verified that the fibrils at 4hrs aggregation time contain amyloid cross-ß-structure (d).

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Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger
Dr. Verena Ahrens, M.Sc. Chem. David Boehme, Dr. Sylvia Els-Heindl, M.Sc. Biochem. Sven Hofmann, Dipl.-Pharm. Cathleen Jendrny, M.Sc. Chem. Veronika Mäde, M.Sc. Chem. Mareen Pagel, Dipl.-Biol. Ria Anne-Rose Schönauer, Dr. Max Steinhagen

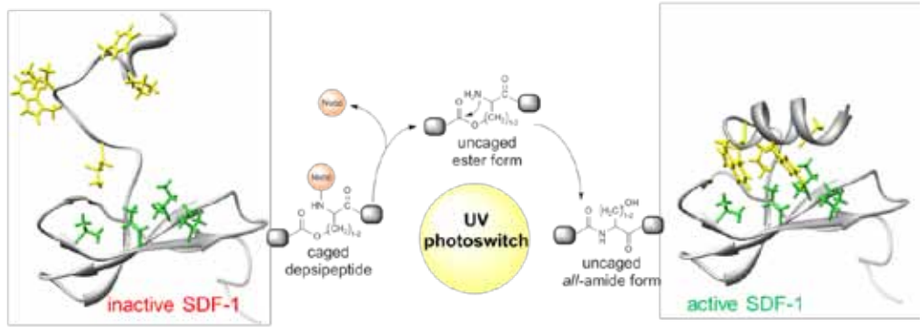
The common aim of the projects includes the synthesis and characterisation of chemically modified peptides and proteins to modulate their function. This includes proteins involved in tumour targeting, proteins for nanomedicine or biomaterial development. Peptides are synthesised by solid phase peptide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

In 2013 Sylvia Els-Heindl (M. Sc. Chem.) successfully finished her PhD in the field of chemically modified peptide hormones. Sylvia Els-Heindl developed the most powerful inverse agonist of the ghrelin receptor, which turned out to be promising candidates to treat metabolic diseases. By chemical modification e. g. palmitoylation she could significantly enhance the half-life from minutes to days. Mass spectrometry revealed the increased half-life in rat. The most powerful molecules have been submitted to patent application. 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.

Sven Hofmann (M. Sc. Biochem.), David Boehme (M. Sc. Chem.) and Verena Ahrens (M. Sc. Biochem.) 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. Verena Ahrens finished her PhD in December. Sven Hofmann could publish as first author novel compounds in which selectivity can be modulated by the incorporation of carboboranes.

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 2013. Mareen Pagel (Dipl. Chem.), and Max Steinhagen (Dipl. Biochem.) work on chemically modified peptides and proteins to improve the properties of biomaterials. Max Steinhagen developed a one pot method to directly immobilise proteins on surfaces. Mareen Pagel has developed a novel biocompatible ligation method, the inverse Diels-Alder reaction, and successfully applied this to the derivatisation of inorganic surfaces. They could impressively show that cells prefer coated surfaces. Four manuscripts have been published by this subgroup, including the paper of L. Baumann and R. Hassert who graduated in 2012. Max Steinhagen finished his PhD in 2013, he could add sortase mediated ligation of proteins as a novel method.



⇑ Photoactivatable stromal derived factor 1 (SDF-1) is the first protein published with a depsipeptide bond. This inactive version of SDF-1 is protected with a photolabile Nvoc-group. After illumination and release of the free N-terminus, this attacks the depsipeptide bond, which leads to a rearrangement and the all-amide form of active SDF-1 (L. Baumann et al. / Angew. Chem. Int. Ed. Engl. (2013) **52** 9550).

⇒ *Photoactivatable Chemokines – Controlling Protein Activity by Light*
L. Baumann, A.G. Beck-Sickinger / Angewandte Chemie International Edition English (2013) **52** 9550

⇒ *In Vitro Modification of Substituted Cysteines as Tool to Study Receptor Functionality and Structure-activity Relationships*
D. Rathmann, X. Pedragosa-Badia, A.G. Beck-Sickinger / Analytical Biochemistry (2013) **439** 173

⇒ *Large Scale Modification of Biomolecules Using Immobilized Sortase A from Staphylococcus Aureus*
M. Steinhagen, K. Zunker, K. Nordsieck, A.G. Beck-Sickinger / Bioorganic Medicinal Chemistry (2013) **21** 3504

⇒ *Manipulating Y Receptor Subtype Activation of Short Neuropeptide Y Analogs by Introducing Carbaborane*
S. Hofmann, R. Frank, E. Hey-Hawkins, A.G. Beck-Sickinger, P. Schmidt / Neuropeptides (2013) **47** 59

⇒ *The Activity of Prolactin Releasing Peptide Correlates with its Helicity*
S.H. DeLuca, D. Rathmann, A.G. Beck-Sickinger, J. Meiler / Biopolymers (2013) **99** 314

⇒ *Preparation of C-terminally Modified Chemokines by Expressed Protein Ligation*
L. Baumann, M. Steinhagen, A.G. Beck-Sickinger / Methods in Molecular Biology (2013) **1047** 103

⇒ *Tuning Peptide Affinity for Biofunctionalized Surfaces*
R. Hassert, A.G. Beck-Sickinger / European Journal of Pharmaceutics and Biopharmaceutics (2013) **85** 69

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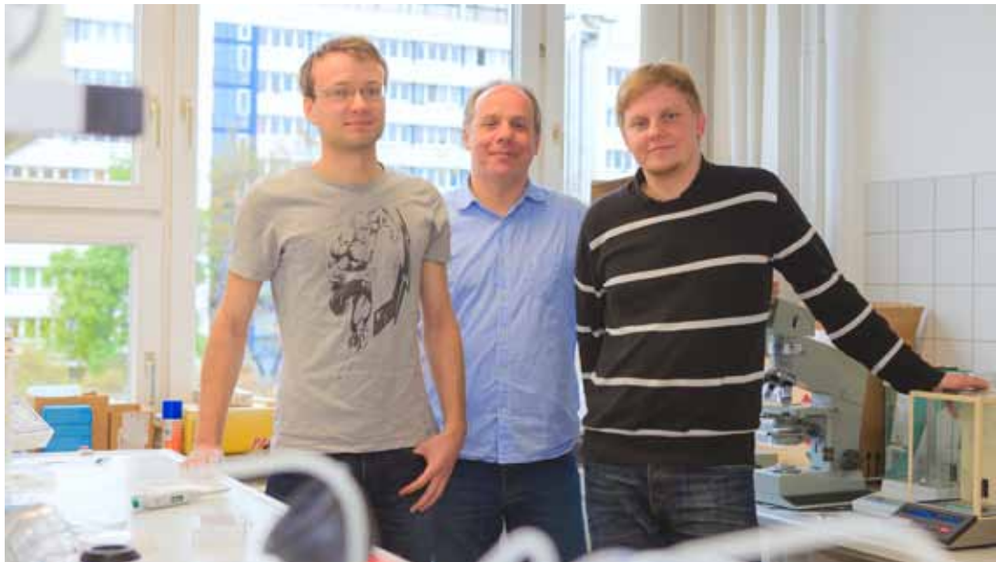
Experiments with optically controlled heat sources

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

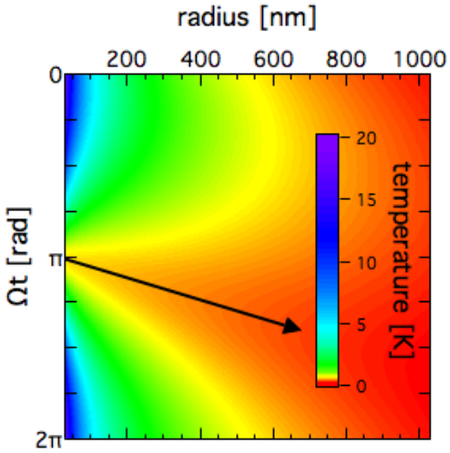
Temperature is one of the important parameters to control the properties of materials in soft as well as in hard matter physics. In hard matter physics, the field of phononics is emerging where the propagation of phonons or heat is controlled by nanostructured materials and circuitry. In soft matter physics, thermal non-equilibrium processes become important as small temperature differences for example readily induce transport processes due to the weak intermolecular interactions.

The research of the "Molecular Nanophotonics Group" within the graduate school BuildMoNa during the last year was devoted to both fields, local temperature fields in soft and hard matter. On one side, the group has developed experimental tools to access heat transfer at the nanoscale with the help of a single metal nanoparticle. The optical microscopy scheme developed by the group captures the propagation of a thermal wave from a single metal nanoparticle by scattering light on the refractive index perturbation. The method allows millisecond time resolution and can be applied to soft and hard materials as well. This method is the foundation for current experiments on ballistic heat coupled plasmonic systems.

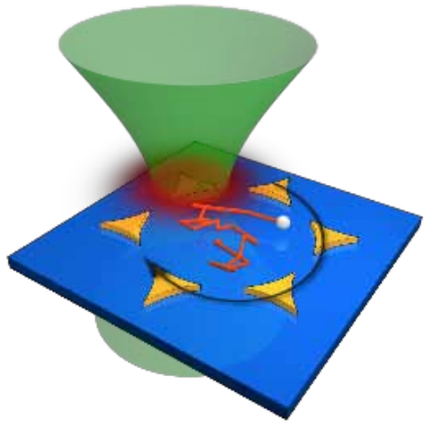
In the field of soft matter physics, the group has established a unique manipulation technique for single nano-objects in solution. The method is based on the



generation of dynamic temperature fields by optically heated metal nanostructures. The resulting temperature gradient creates thermophoretic forces on individual nano-objects or even single molecules and allows for a trapping and steering of these objects. This new scheme, which is able to control the number of interacting nano-objects in a well defined trapping volume, provides a huge perspective on a large variety of studies including enzyme activity or protein interactions on long timescales.



⇑ Time and spatial dependence of the temperature field of a thermal wave injected by a single gold nanoparticle



⇑ Scheme of a thermophoretic trap using dynamic temperature fields generated by optically heated gold nanostructures

⇒ *Optically Controlled Thermophoretic Trapping of Single Nano-Objects*
M. Braun, F. Cichos / ACS Nano (2013) **6** 2741

⇒ *Photothermal Signal Distribution Analysis (PhoSDA)*
M. Selmke, M. Braun, R. Schachoff, F. Cichos / Physical Chemistry Chemical Physics (2013) **15** 4250

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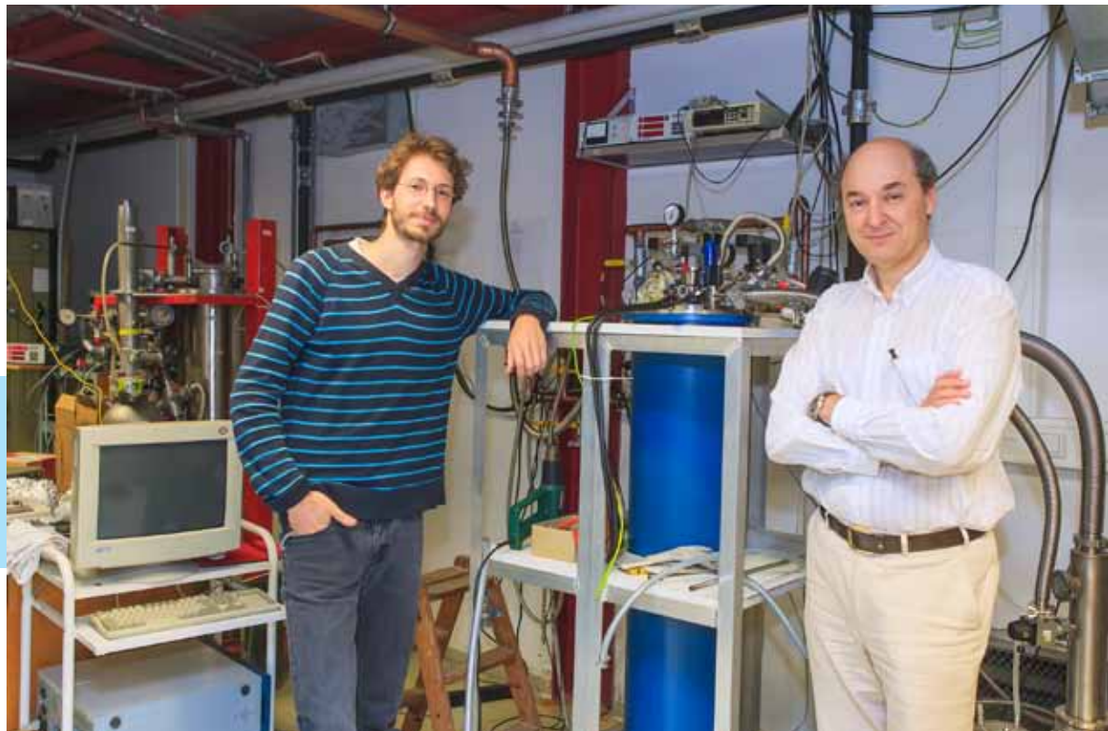
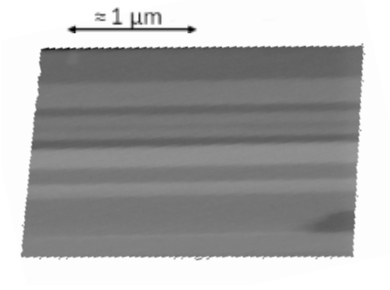
Superconductivity at graphite interfaces

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

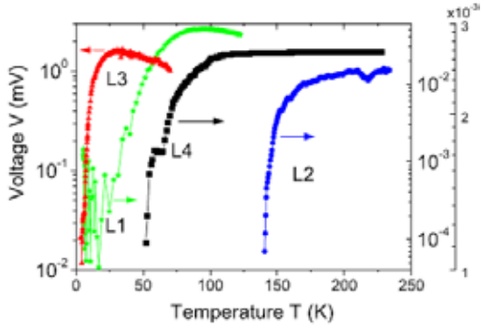
To understand the properties of the embedded interfaces in graphite, we have performed transport measurements contacting the edges of the embedded interfaces in different graphite samples. The TEM lamellae showed non-linear current-voltage characteristic curves, a drop of the voltage decreasing temperature, 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)

⇒ *Large Local Hall Effect in Pin-hole Dominated Multigraphene Spin-valves*
P.K. Muduli, J. Barzola-Quiquia, S. Dusari, A. Ballestar, F. Bern, W. Böhlmann, P. Esquinazi / Nanotechnology (2013) **24** 015703

⇒ *Josephson Coupled Superconducting Regions Embedded at the Interfaces of Highly Oriented Pyrolytic Graphite*
A. Ballestar, J. Barzola-Quiquia, T. Scheike, P. Esquinazi / New Journal of Physics (2013) **15** 023024

⇒ *Hall Effect of Tetragonal and Orthorhombic $SrRuO_3$ Films*
F. Bern, M. Ziese, K. Dörr, A. Herklotz, I. Vrejoiu / physica status solidi - Rapid Research Letters (2013) **7** 204

⇒ *Structural, Magnetic and Electrical Properties of $SrRuO_3$ Films and $SrRuO_3/SrTiO_3$ Superlattices*
F. Bern, M. Ziese, A. Setzer, E. Pippel, D. Hesse, I. Vrejoiu / Journal of Physics: Condensed Matter (2013) **25** 496003

⇒ *Magnetotransport and Hall Effect Studies of $SrRuO_3/SrTiO_3$ Superlattices*
F. Bern, M. Ziese / European Physical Journal: Web of Conferences (2013) **40** 15013

⇒ *Existence of a Magnetically Ordered Hole Gas at the $La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$ Interface*
M. Ziese, F. Bern, A. Setzer, E. Pippel, D. Hesse, I. Vrejoiu / The European Physical Journal B (2013) **86** 42

⇒ *Exchange Bias in Manganite/$SrRuO_3$ Superlattices*
M. Ziese, F. Bern, I. Vrejoiu / Journal of Applied Physics (2013) **113** 063911

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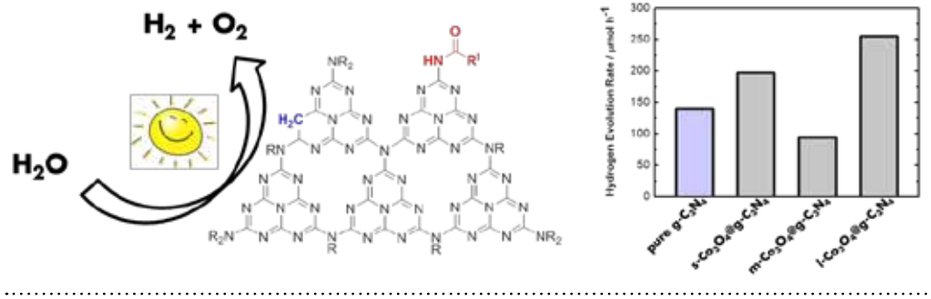
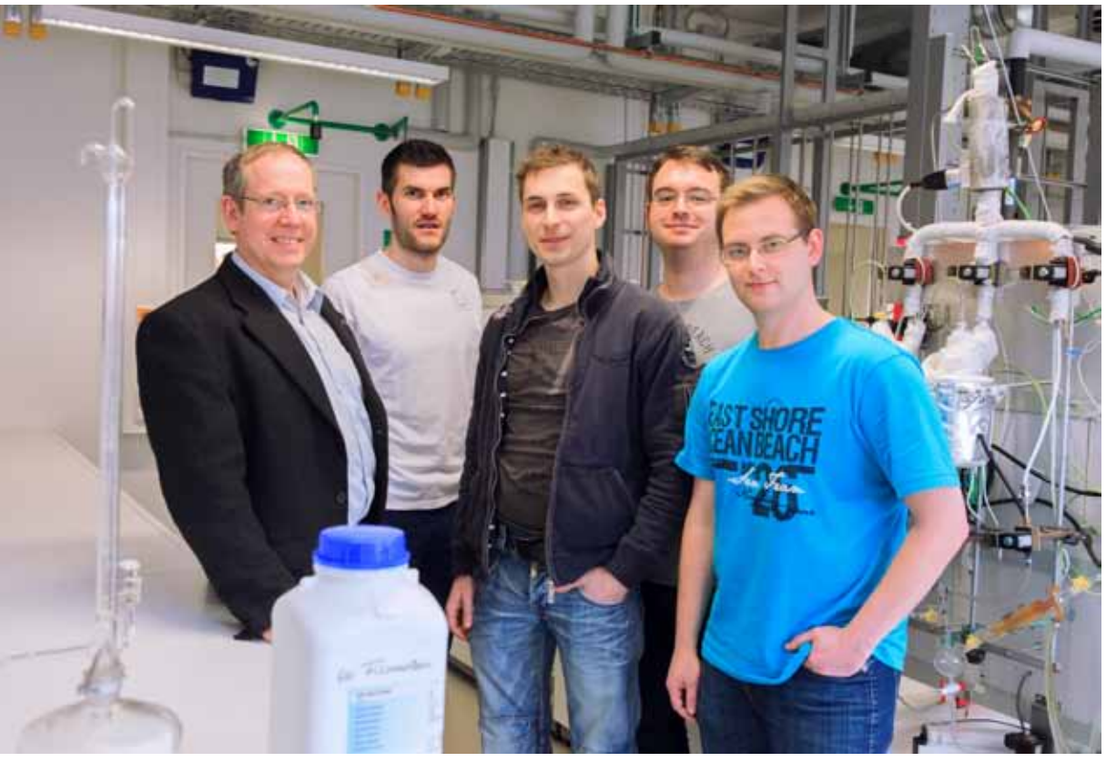
Complex nanomaterials for sustainable catalysis

Prof. Dr. Roger Gläser
M.Sc. Chem. Thomas Heinze, M.Sc. Chem. Michael Marx, M.Sc. Chem. Dennis Richter, M.Sc. Chem. Patrick With

Heterogeneous catalysis continues to play a key role for sustainable technologies. Besides environmental applications, solid catalysts are designed for mastering the raw materials change and energy conversion. The research in our group makes use of tailor-made nanoporous materials with defined porosity and functions for applied catalysis. According to two major foundations of the graduate school, we utilise templating and scaffolding approaches to synthesise novel materials for the use as catalysts and catalyst supports. For instance, we focus on applications in environmental catalysis in the selective catalytic reduction of nitrogen oxides by catalysts with transport-optimised pore systems. Also, we covalently bond Ionic Liquid-functionalities to SiO_2-based nanoporous supports surfaces to obtain highly selective oxidation catalysts by exchanging the anion of the ionic liquid with ruthenium- or manganese-containing species. Another prominent research area deals with energy-related catalysis with the aim of photocatalytic water splitting for hydrogen production. Towards that goal, we modify porous carbon nitrides (g-C_3N_4) with different sensitsers such as dyes, noble metals or transition metal oxides. Thus, the catalytic activity for the hydrogen formation in the overall water splitting with visible light is enhanced and enables efficient harvesting of solar energy.



⇑ Structure of g-C_3N_4 showing two surface modifications (blue and red) for solar water splitting (left) and hydrogen evolution rate over pure g-C_3N_4 and over g-C_3N_4 containing small (s), medium (m), and large (l) Co_3O_4 nanoparticles (right)



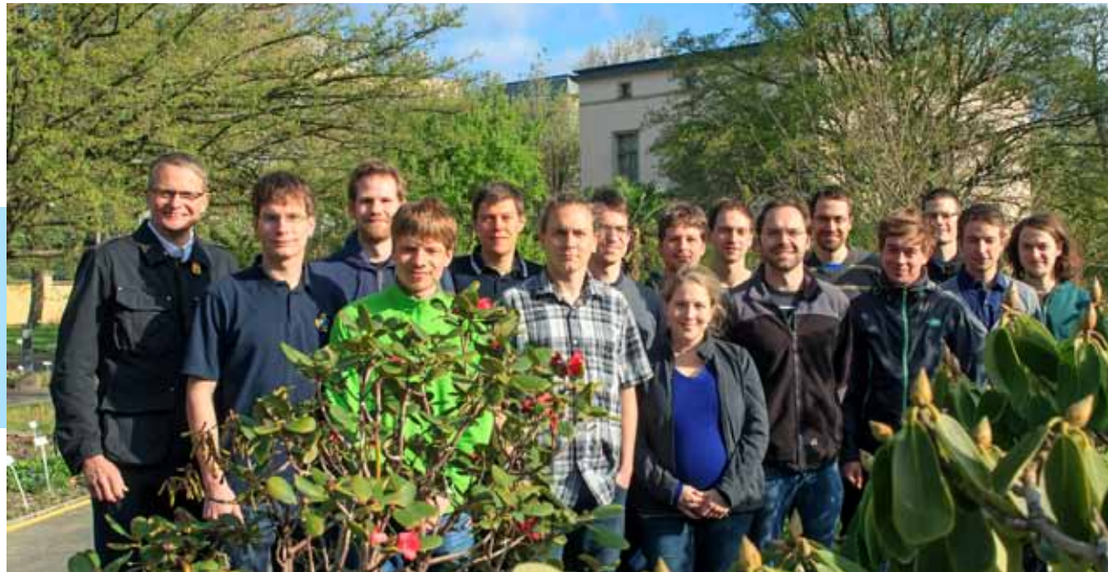
Transparent semiconductors – from materials growth to devices

Prof. Dr. Marius Grundmann

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

Transparent electrodes were initially discovered in Leipzig (K. Bädeker / Ann. Physik (1907) **327** 749) by K. Bädeker and are now ubiquitous in touch screens, flat panel displays, heat insulating glass and as front contact in thin film solar cells. For such "ohmic" applications, the materials are optimised to have as large conductivity as possible, preserving optical transparency.

We take on the huge challenge to develop transparent *semiconducting* materials with controlled conductivity suitable for making diodes and transistors in order to enable completely transparent displays, invisible electronics and solar cells on windows. For n-type conductors several materials have been developed such as zinc oxide, zinc tin oxide or indium-gallium zinc oxide. High performance unipolar devices such as Schottky diodes and MESFETs using such materials have been reported by our BuildMoNa doctoral candidates in the past. p-type conducting trans-



⇒ *Carbon Template Removal by Dielectric-Barrier Discharge Plasma for the Preparation of Zirconia*
Q. Guo, P. With, Y. Liu, R. Gläser, C.-J. Liu / Catalysis Today (2013) **211** 156

⇒ *Hydrierung von p-Nitrophenol zu p-Aminophenol als Testreaktion für die katalytische Aktivität von Pt-Trägerkatalysatoren*
M. Goepel, M. Al-Naji, P. With, G. Wagner, O. Oeckler, D. Enke, R. Gläser / Chemie Ingenieur Technik (2013) **85** 1774

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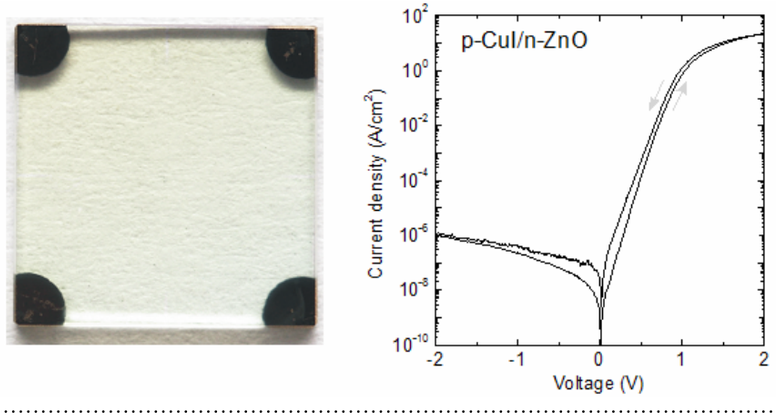
parent materials remain a huge challenge.
The more stringent requirements regarding doping and defect content are supplemented with our desire to develop a *green technology*, i.e. use only non-toxic, abundant, easily available and cheap materials and employ fabrication processes that require a minimum of energy. BuildMoNa doctoral candidate Friedrich Schein has achieved 2013 breakthroughs in this direction by fabricating highly rectifying bipolar oxide diodes using room temperature deposition of the p-conducting materials.

Before our successful research, oxide-based bipolar diodes exhibited rather low rectification (forward current divided by reverse current) with values equal to or often (much) less than 10^3. Using cuprous iodide (CuI), fully transparent diodes with rectification of 10^6 could be realised. Using amorphous zinc cobalt oxide ($ZnCo_2O_4$) as p-type material, the record rectification of more than 10^{10} was achieved. Both CuI and $ZnCo_2O_4$ were deposited at room temperature. Clearly the excellent device properties represent a huge progress in the field. Current further work, conducted by BuildMoNa candidates Peter Schlupp and Robert Karsthof, is targeted towards fully amorphous diodes and using such diodes for solar power harvesting.

A quite interesting group of functional transparent materials are the sesquioxides in the $(In,Ga,Al)_2O_3$ system, covering the band gap range from below 3 to above 7 eV. Possible applications are – besides transparent electronics – high power electronics, UV detectors and infrared optics. Using the recently developed facile method for depositing material libraries (continuous composition spread pulsed laser deposition, CCS-PLD), we can efficiently examine the entire composition range. For Ga_2O_3 thin films, best Schottky diodes have been reported by BuildMoNa doctoral candidate Daniel Splith. For In_2O_3 thin films, almost all theoretically expected Raman lines were reported by Christian Kranert using resonant Raman scattering, a technique set up in Leipzig through funds from the Centre of Excellence (DFG Sonderforschungsbereich) 762. In the meantime, Daniel Splith has also fabricated the first Schottky diodes on In_2O_3, a veritable challenge due to the strong surface electron accumulation layer, previously thought to inhibit Schottky barrier formation altogether.

Thus, BuildMoNa young researchers are at the forefront of the fields of transparent and oxide electronics – fields that are challenging with respect to materials fabrication and semiconductor physics and at the same time rewarding due to the large application potential.



⇑ left: CuI/ZnO diode (on sapphire, with gold corner contacts for Hall effect measurements), right: IV characteristics with high rectification. Adapted from F.-L. Schein et al. / Appl. Phys. Lett. (2013) **102** 092109

⇒ *One Decade of Fully Transparent Oxide Thin Film Transistors: Fabrication, Performance and Stability*
H. Frenzel, A. Lajn, M. Grundmann / physica status solidi RRL (2013) **7** 605

⇒ *Transparent p-CuI/n-ZnO Heterojunction Diodes*
F.-L. Schein, H. von Wenckstern, M. Grundmann / Applied Physical Letters (2013) **102** 092109

⇒ *Continuous Composition Spread Using Pulsed-Laser Deposition with a Single, Segmented Target*
H. von Wenckstern, Z. Zhang, F. Schmidt, J. Lenzner, H. Hochmuth, M. Grundmann / CrystEngComm (2013) **15** 10020

⇒ *Cuprous Iodide – a p-type Transparent Semiconductor: History and Novel Applications*
M. Grundmann, F.-L. Schein, M. Lorenz, T. Böntgen, J. Lenzner, H. von Wenckstern / physica status solidi (a) (2013) **210** 1671

⇒ *Tunneling Dynamics of Excitons in Random Semiconductor Alloys*
A. Müller, M. Grundmann / Physical Review B (2013) **87** 035134

⇒ *Comparative Study of Deep Defects in ZnO Microwires, Thin Films and Bulk Single Crystals*
F. Schmidt, S. Müller, H. von Wenckstern, C.P. Dietrich, R. Heinhold, M.W. Allen, M. Grundmann / Applied Physical Letters (2013) **103** 062102

⇒ *On the Transition Point of Thermally Activated Conduction of Spinel-type MFe_2O_4 Ferrite Thin Films (M=Zn,Co,Ni)*
K. Brachwitz, T. Böntgen, M. Lorenz, M. Grundmann / Applied Physical Letters (2013) **102** 172104

⇒ *Comparison of ZnO-based JFET, MESFET, and MISFET*
F.J. Klüpfel, F.L. Schein, M. Lorenz, H. Frenzel, H. von Wenckstern, M. Grundmann / IEEE Transact. Electr. Dev. (2013) **60** 1828

⇒ *Vacuum Ultraviolett Dielectric Function of $ZnFe_2O_4$ Thin Films*
T. Böntgen, K. Brachwitz, R. Schmidt-Grund, M. Lorenz, M. Grundmann / Journal of Applied Physics (2013) **113** 073503

⇒ *Comparative Study of Transparent Rectifying Contacts on Semiconducting Oxide Single Crystals and Amorphous Thin Films*
A. Lajn, H. von Wenckstern, M. Grundmann, G. Wagner, P. Barquinha, E. Fortunato, R. Martins / Journal of Applied Physics (2013) **113** 044511

⇒ *Temperature Dependent Dielectric Function in the NIR-VUV Spectral Range of Alumina and yttria Stabilized Zirconia Thin Films*
R. Schmidt-Grund, T. Lühmann, T. Böntgen, H. Franke, D. Opper, M. Lorenz, M. Grundmann / Journal of Applied Physics (2013) **114** 223509

⇒ *Growth Control of Nonpolar and Polar ZnO/$Mg_xZn_{1-x}O$ Quantum Wells by Pulsed-Laser Deposition*
J. Zippel, M. Lorenz, M. Lange, M. Stölzel, G. Benndorf, M. Grundmann / Journal of Crystal Growth (2013) **364** 81

⇒ *Excitonic and Optical Confinement in Microwire Heterostructures with Non-Polar (Zn,Cd)O/(Mg,Zn)O Multiple Quantum Wells*
M. Lange, C. Dietrich, M. Lorenz, M. Grundmann / Journal of Physical Chemistry C (2013) **117** 9020

⇒ *Defect-induced Magnetism in Homoepitaxial Manganese Stabilized Zirconia Thin Films*
J. Zippel, M. Lorenz, A. Setzer, M. Rothermel, D. Spemann, P. Esquinazi, M. Grundmann, G. Wagner, R. Denecke, A.A. Timopheev / Journal of Physics D: Applied Physics (2013) **46** 275002

⇒ *Effect of Rare-earth Ion Doping on Multiferroic Properties of $BiFeO_3$ Thin Films Grown Epitaxially on $SrTiO_3(100)$*
V.V. Lazenka, M. Lorenz, H. Modarresi, K. Brachwitz, P. Schwinkendorf, T. Böntgen, J. Vanacken, M. Ziese, M. Grundmann, V.V. Moshchalkov / Journal of Physics D: Applied Physics (2013) **46** 175006

⇒ *Degenerate Interface Layers in Epitaxial Scandium-doped ZnO Thin Films*
M. Lorenz, C. Schmidt, G. Benndorf, T. Böntgen, H. Hochmuth, R. Böttcher, A. Pöppl, D. Spemann, M. Grundmann / Journal of Physics D: Applied Physics (2013) **46** 065311

⇒ *Damp Heat Treatment of $Cu(In,Ga)Se_2$ Solar Cells with Different Sodium Content*
F. Daume, S. Puttnins, C. Scheit, H. Zachmann, A. Rahm, A. Braun, M. Grundmann / Materials (2013) **6** 5478

⇒ *Oxidation State of Tungsten Oxide Thin Films Used as Gate Dielectric for Zinc Oxide Based Transistors*
M. Lorenz, M. Grundmann, S. Wickert, R. Denecke / Proceedings Materials Research Society (2013) **1494** 1649

⇒ *Surface- and Point-defect-related Raman Scattering in Wurtzite Semiconductors Excited above the Band Gap*
C. Kranert, R. Schmidt-Grund, M. Grundmann / New Journal of Physics (2013) **15** 113048

⇒ *Martensitic Phase Transition and Subsequent Surface Corrugation in Manganese Stabilized Zirconia Thin Films*
J. Zippel, M. Lorenz, G. Wagner, J. Lenzner, M. Grundmann / Philosophical Magazine (2013) **93** 2329

⇒ *Determination of Unscreened Exciton States in Polar ZnO/(Mg,Zn)O Quantum Wells with Strong Quantum-confined Stark Effect*
M. Stölzel, A. Müller, G. Benndorf, M. Brandt, M. Lorenz, M. Grundmann / Physical Review B (2013) **88** 045315

⇒ *Effect of Sodium on Material and Device Quality in Low Temperature Deposited $Cu(In,Ga)Se_2$*
S. Puttnins, S. Levcenco, K. Schwarzburg, G. Benndorf, F. Daume, A. Rahm, A. Braun, M. Grundmann, T. Unold / Solar Energy Materials & Solar Cells (2013) **119** 281

⇒ *Magnetic Anisotropy of Epitaxial Zinc Ferrite Thin Films Grown by Pulsed Laser Deposition*
A.A. Timopheev, A.M. Azevedo, N.A. Sobolev, K. Brachwitz, M. Lorenz, M. Ziese, P. Esquinazi, M. Grundmann / Thin Solid Films (2013) **527** 273

⇒ *Transparent Rectifying Metal/Metal Oxide/Semiconductor Contact Structure and Method for the Production Thereof and Use*
M. Grundmann, H. Frenzel, A. Lajn, H. von Wenckstern / CA 2765981 C (Canadian Intellectual Property Office, 2013)

⇒ *Transparente gleichrichtende Metall-Metalloxid-Halbleiterkontaktstruktur und Verfahren zu ihrer Herstellung und Verwendung*
M. Grundmann, H. Frenzel, A. Lajn, H. von Wenckstern / EP 2 446 484 B1 (European Patent Office, Munich, 2013)

⇒ *Transparent Rectifying Metal/Metal Oxide/Semiconductor Contact Structure and Method for the Production Thereof and Use*
M. Grundmann, H. Frenzel, A. Lajn, H. von Wenckstern / US 8,445,904 B2 (United States Patent, 2013)

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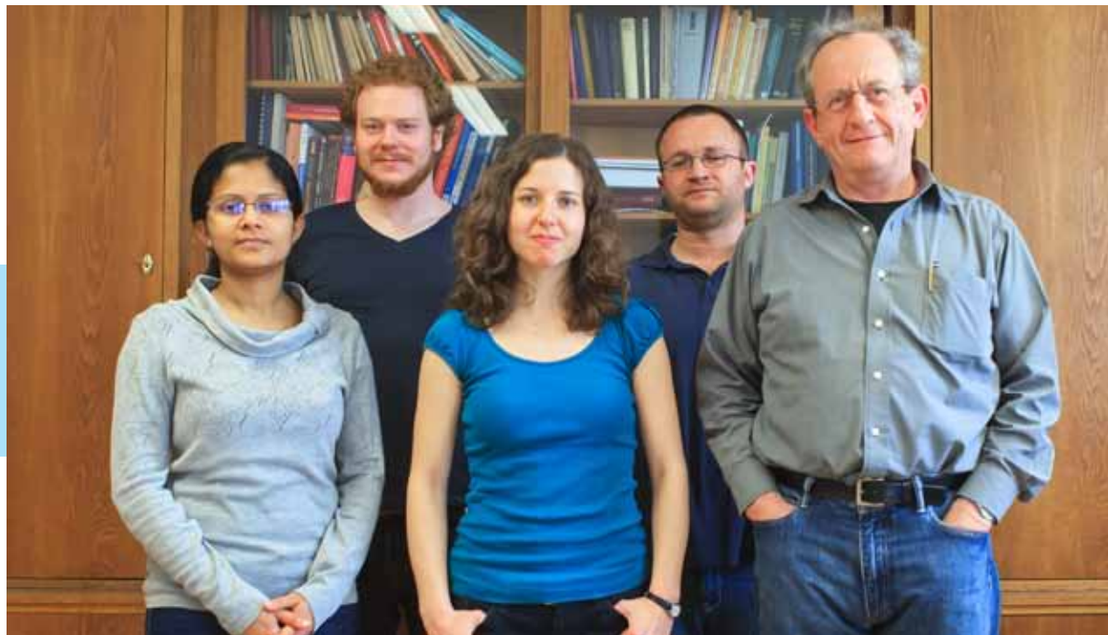
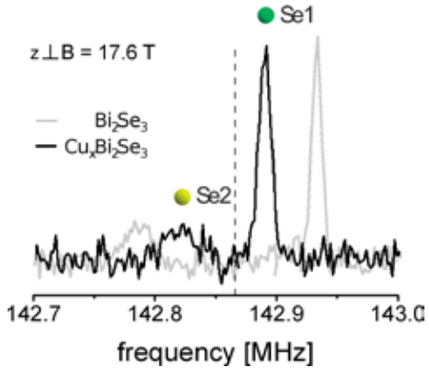
Magnetic resonance technique to investigate the properties of modern materials

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

We are interested in the investigation of the properties of materials with the methods of Nuclear Magnetic Resonance (NMR), and Electron Paramagnetic Resonance (EPR). The materials under research range from high-temperature superconductors, and topological insulators to porous materials like metal-organic frameworks (MOFs).

The highest magnetic fields can only be obtained through pulsed magnetic fields. Here, the availability of NMR is highly desirable since the field strength is an important parameter for many solid-state systems. In case of the high-temperature superconductors, the physical state can be changed and new results contribute to a better understanding. Recently, we obtained first ^{17}O signals on the cuprate parent compound Nd_2CuO_4. Furthermore, we developed a method to obtain the longitudinal relaxation time T_1 in a single field pulse.





⇐ ^{77}Se NMR spectra of Bi_2Se_3 and $Cu_{0.15}Bi_2Se_3$ measured at an external magnetic field strength B = 17.6 T with the crystal z-axis perpendicular to the magnetic field. The two signals correspond to the two distinct crystal sites that Se occupies.

Using ^{77}Se NMR in single crystals, we investigated the topological insulator Bi_2Se_3 and the change of its properties under Cu intercalation. We find two Se signals with intensities in agreement with to the two anticipated non-equivalent lattice sites. NMR frequencies, relaxation times, and linewidths were measured in dependence on magnetic field strength and crystal orientation in the external field. The results, however, are very unusual and not yet fully understood (so far there are no publications on ^{77}Se NMR in Bi_2Se_3 and $Cu_xBi_2Se_3$ single crystals). They must be caused by the topological nature of the material.

Unprecedented ^{63}Cu and in particular ^{17}O NMR experiments on single crystals of the electron-doped high-temperature superconducting cuprate $Ln_{2-x}Ce_xCuO_4$ (with Ln = Pr, Nd) gave new insights into the compound- and doping-dependent charge distribution within electron- as well as hole-doped samples, which promise to further increase the understanding of the still enigmatic mechanism of high-Tc superconductivity.

We also investigate cadmium based coordination polymers (MOFs) using ^{113}Cd NMR. The isotropic chemical shifts as well as chemical shift anisotropies are sensitive on the coordination geometry, especially useful when no X-ray data exists.

⇒ *Charge Inhomogeneity in Electron-Doped $Pr_{1.85}Ce_{0.15}CuO_4$ Determined with ^{63}Cu NMR*
M. Jurkutat, J. Haase, A. Erb / Journal of Superconductivity and Novel Magnetism (2013) **26** 2685

⇒ *Synthesis, Crystal Structure, and Solid-State NMR Investigations of Heteronuclear Zn/Co Coordination Networks – A Comparative Study*
A.V. Kuttatheyil, D. Lässig, J. Lincke, M. Kobalz, M. Baias, K. König, J. Hofmann, H. Krautscheid, C.J. Pickard, J. Haase, M. Bertmer / Inorganic Chemistry (2013) **52** 4431

⇒ *A Solid-Solution Approach to Mixed-Metal Metal-Organic Frameworks – Detailed Characterization of Local Structures, Defects and Breathing Behaviour of Al/V Frameworks*
O. Kozachuk, M. Meilikhov, K. Yusenko, A. Schneemann, B. Jee, A.V. Kuttatheyil, M. Bertmer, C. Sternemann, A. Pöppl, R.A. Fischer / European Journal of Inorganic Chemistry (2013) **2013** 4546

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

Prof. Dr. Evamarie Hey-Hawkins
M.Sc. Chem. Anup Kumar Adhikari, M.Sc. Chem. Eng. Paul Cosmin Boar, M.Sc. Chem. Solveig Boehnke, Dr. Anne Grundmann, Dr. Anika Kreienbrink, M.Sc. Chem. Tobias Möller, M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon, M.Sc. Chem. Paul Neumann, M.Sc. Chem. Wilma Neumann, Dr. Julian Pritzwald-Stegmann, Dipl.-Chem. Stefan Richter, M.Sc. Chem. Andy Schmied, Dr. Markus Streitberger

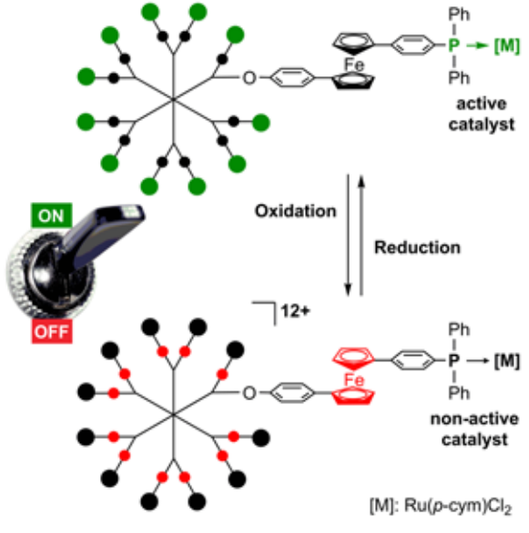
The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carbaborane clusters and antitumour drugs).

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, A. Schmied, M. Streitberger), 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 nano-sized 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.

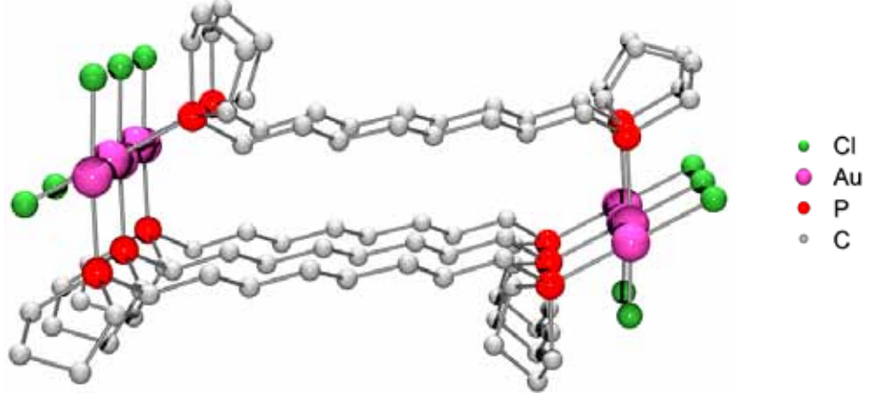
From Molecules to Novel Materials:
Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear 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: terminal phosphinidene complexes [L_nM=PR] (A. Grundmann), strained inorganic (A. Kreienbrink) or organic (T. Möller) phosphorus-based rings, alkylene-bridged bis(phospholanes) (P.C. Boar, A. Schmied, M. Streitberger) or (planar-chiral) ferrocene derivatives (J. Pritzwald-Stegmann).



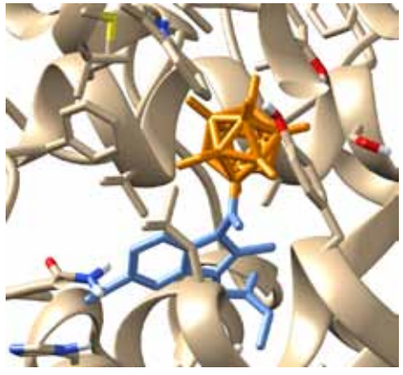
⇐ Redox-switchable ferrocenylphosphine-based dendrimer

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) as molecular precursors.

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) inhibitors (W. Neumann) 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).
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)).



⇑ Section of a gold(I)-based "nano-tube" formed via aurophilic interactions



⇐ Docking studies of carbaborane-based COX inhibitor (indoborin) with COX-2

⇒ *Manipulating Y Receptor Subtype Activation of Short Neuropeptide Y Analogs by Introducing Carbaboranes*
S. Hofmann, R. Frank, E. Hey-Hawkins, A.G. Beck-Sickinger, P. Schmidt / Neuropeptides (2013) **47** 59

⇒ *2-Carbaborane-3-phenyl-1H-indoles – Synthesis via McMurry Reaction and COX Inhibition Activity*
M. Laube, W. Neumann, M. Scholz, P. Lönnecke, B. Crews, L.J. Marnett, J. Pietzsch, T. Kniess, E. Hey-Hawkins / ChemMedChem (2013) **8** 329

⇒ *Microwave-assisted Catalytic Amination of Phenothiazines; Reliable Access to Phenothiazine Analogues of Tröger's Base*
L.I. Găină, L.N. Mătărângă-Popa, E. Gal, P. Boar, P. Lönnecke, E. Hey-Hawkins, C. Bischin, R. Silaghi-Dumitrescu, I. Lupan, C. Cristea, L. Silaghi-Dumitrescu / European Journal of Organic Chemistry (2013) 5500

⇒ *1,2-Disubstituted Aryl-Based Ferrocenyl Phosphines*
M. Madalska, P. Lönnecke, E. Hey-Hawkins / Organometallics (2013) **32** 2019

⇒ *Functionalisation of the nido-Dicarbaborate Anion nido-7,8-$C_2B_9H_{12}^-$ by Hydride Abstraction*
R. Frank, H. Auer, E. Hey-Hawkins / Journal of Organometallic Chemistry (2013) **747** 217

⇒ *Vibrational Spectra of a Ferrocenyl Phosphine Derivative Chemisorbed on 3-aminopropylsilyl Modified Silica Gel*
V. Ivanovski, M. Bukleski, M. Madalska, E. Hey-Hawkins / Vibrational Spectroscopy (2013) **69** 57

⇒ *Terminal Alkylphosphinidene Organotantalum(V) Complexes*
A. Grundmann, M.B. Sárosi, P. Lönnecke, R. Frank, E. Hey-Hawkins / European Journal of Inorganic Chemistry (2013) 3137

⇒ *Synthesis of 1,1',2-Trisubstituted Aryl-Based Ferrocenyl Phosphines as Precursors for Immobilized Ligands*
M. Madalska, P. Lönnecke, V. Ivanovski, E. Hey-Hawkins / Special Issue: Ferrocene – Beauty and Function, Organometallics (2013) **32** 5852

⇒ *Facile Synthesis of the Versatile Trifunctionalized Building Block 1,2-bis(hydroxymethyl)-9-mercapto-1,2-dicarba-closo-dodecaborane(12)*
S. Boehnke, S. Saretz, M. Kellert, E. Hey-Hawkins / Inaugural Issue of Biochemical and Biophysical Journal of Neutron Therapy & Cancer Treatments (2013) **1** 22

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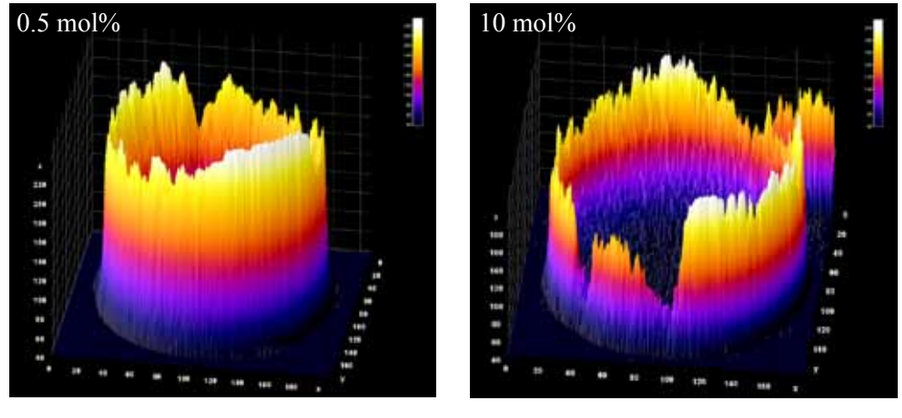
Surface functionalisation of Layer-by-Layer coated colloidal microcarriers for specific cell uptake

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

In recent years the Layer-by-Layer (LbL) technology, based on the alternative coating of oppositely charged polyelectrolytes, attracts more and more interest in the field of biotechnology and biomedicine due to the modular principle of construction which provides the opportunity to create novel drug delivery systems (microcarriers) with unique features. The structure of these microcarriers allows to integrate multiple active agents into one delivery system which can be gradually and independently released. Nevertheless, the underlying principle of the LbL technology presents a charged microcarrier surface, which may lead to unspecific cell and serum protein interaction and therefore to a non-targeted delivery of the active agents.

The work of Dipl.-Phys. Martin Göse focuses on a procedure to overcome this restriction while preserving the advantages of the LbL microcarriers. An artificial lipid membrane is assembled onto the microcarrier surface to inhibit unspecific interaction and to serve as a platform for the integration of functionalised lipids,



⇑ 3D Surface Plot of the fluorescence intensity of lipid layer coated SiO_2-microparticles obtained by STED-Microscopy. (left): POPS/POPC 1:1 + 0.5 mol% PE-PEG-Biotin (right): POPS/POPC 1:1 + 10 mol% PE-PEG-Biotin, revealing inhomogeneous lipid layer distribution at high PE-PEG-Biotin concentrations

which are acting as surface anchors for antibodies providing targeted delivery. The amount of such functionalised lipids but also the assembly parameters of the lipid layer itself show a strong influence on the surface characteristics necessitating the investigation of optimal parameters for obtaining a homogeneous lipid distribution.

Multiple techniques like Atomic Force Microscopy, Confocal Laser Scanning Microscopy, Stimulated Emission Depletion Microscopy and Flow Cytometry have been used to investigate lipid layer formation strategies in a comprehensive way.

⇒ *Development of LbL Biopolymer Capsules as a Delivery System for the Multilayer-assembled Anti-inflammatory Substance α1-antitrypsin*
V. Strehlow, J. Lessig, M. Göse, U. Reibetanz / Journal of Materials Chemistry B (2013) **1** 3633

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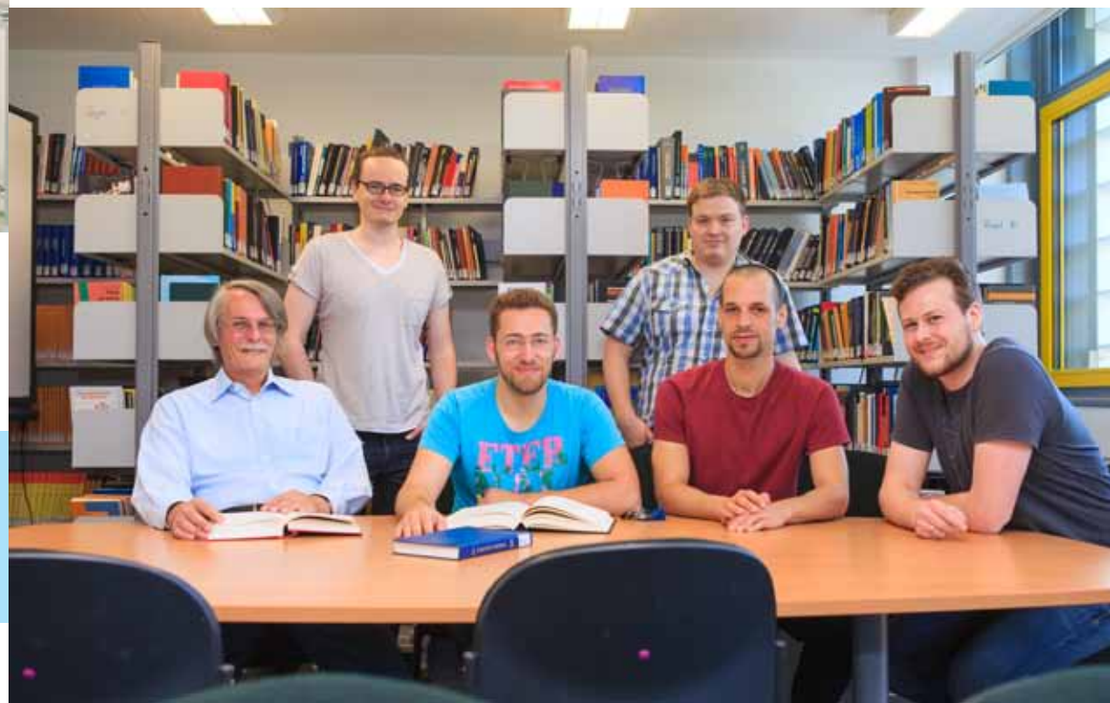
Monte Carlo and molecular dynamics simulations of structure formation processes

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

The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on several interrelated subprojects. In all projects, the employed methodology relies mainly on sophisticated Monte Carlo computer simulations based on multicanonical ensembles, parallel tempering techniques and chain-growth algorithms with population control, quantum Monte Carlo simulations based on stochastic series expansions, and thermostated Molecular Dynamics methods, which 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) Sebastian Schöbl employs a special type of chain-growth algorithms for investigations of polymers in disordered environments. Some of the results have been validated by additional multicanonical simulations performed in collaboration with Johannes Zierenberg. His findings are an important basic building block for a better understanding of, e.g., the universal properties of the cycloskeleton investigated by several other BuildMoNa groups. In February 2013 he has successfully defended his PhD Thesis on this topic.

(ii) Micha Wiedenmann investigates condensation phenomena at the liquid-gas or solid-gas coexistence described by a simplified lattice gas model, which are of relevance for aggregation processes in general and for polymer and peptide aggregation in particular.

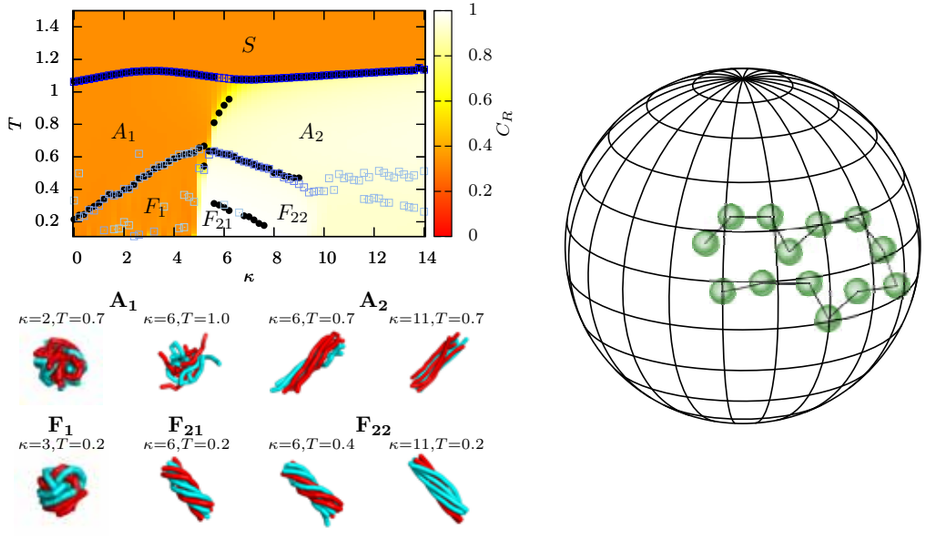
(iii) Johannes Zierenberg builds on Micha Wiedenmann's work and studies the aggregation properties of a number of polymers, both in lattice and off-lattice models, with emphasis on the distinguishing differences between flexible and semiflexible macromolecules. In the latter case he recently found very interesting twisted bundle-like structures for large bending stiffness and low temperatures.

(iv) 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 interacting 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 and structure formation processes under confinement are in the focus of interest.

(v) Niklas Fricke extended our recently proposed novel renormalisation group inspired exact enumeration method for self-avoiding random walks on a percolation cluster, modeling polymers in disordered environments with fractal properties, to up to seven space dimensions. This novel method allows us to enumerate walks of more than 1000 steps in a couple of minutes for which standard techniques would have needed over 10^{170} years.

(vi) Johannes Bock focuses 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 extends the work of Sebastian Schöbl to the three-dimensional case subject to additional confinement constraints.

(vii) Philipp Schierz aims 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.



⇑ left: Phase diagram for 8 polymers consisting of $N=13$ monomers each, combining the surface plot of the end-to-end correlation parameter C_R, the maxima of the heat capacity (black dots) and the temperature derivative of the phase separation parameter I^2 (blue squares). We identify several structural phases, namely S (separated), A (aggregated) and F (frozen), and present typical conformations for the low-temperature phases.
right: Sketch of a confined polymer fluctuating inside a spherical cage

⇒ *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*
J. Zierenberg, M. Marenz, W. Janke / Computer Physics Communications (2013) **184** 1155

⇒ *Self-Avoiding Walks on Strongly Diluted Lattices: Chain-Growth Simulations vs Exact Enumeration*
N. Fricke, W. Janke / European Physical Journal – Special Topics (2013) **216** 175
(Fig. 1 selected for the cover page of this volume)

⇒ *Diffusion and Polymers in Fractal, Disordered Environments*
N. Fricke, J. Bock, W. Janke / diffusion-fundamentals.org (2013) **20** 111

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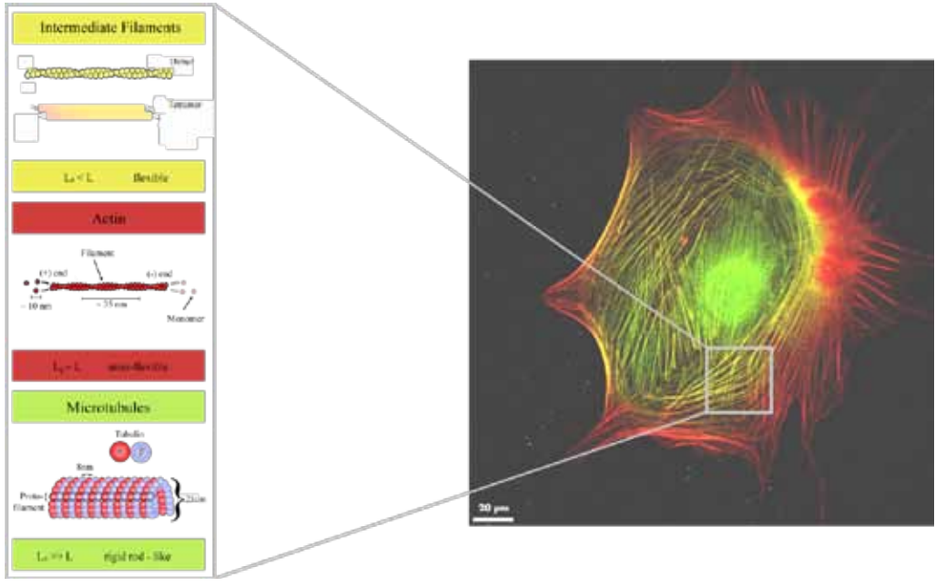
Emergent complexity of the cytoskeleton

Prof. Dr. Josef Alfons Käs
Dipl.-Phys. Anatol Fritsch, M.Sc. Phys. Tom Golde, M.Sc. Phys. Martin Glaser, Dr. Markus Gyger, Dipl.-Phys. Chris Händel, Dipl.-Phys. Tina Händler, Dipl.-Phys. Tobias Kießling, Dipl.-Math. Melanie Knorr, M.Sc. Phys. Jürgen Lippoldt, Dr. David K. Nnetu, Dipl.-Phys. Steve Pawlizak, M.Sc. Phys. Susanne Rönicke, Dipl.-Phys. Jörg Schnauß, Dipl.-Phys. Carsten Schuldt, Dipl.-Phys. Dan Strehle, Dipl.-Phys. Franziska Wetzel

In January 2013 we published the article "Emergent complexity of the cytoskeleton: from single filaments to tissue" in Advances in Physics. This journal is ranked as the number one in the discipline of condensed matter physics. Mainly written by BuildMoNa members this article reviews physics of different scales (levels of complexity) in biological systems.
Biophysical investigations and theoretical approaches were presented aiming to introduce the physics of the cytoskeleton. To explain this intra-cellular biopolymer scaffold appropriately, effects ranging from single biopolymer filaments to cells and multicellular organisms are summarised. In that course a wide range of phenomena is presented and the intertwined nature of different levels of complexity is emphasised. Numerous emergent properties are explained by the means of self-organisation or self-assembly.



⇑ The cellular cytoskeleton consists of three main components. Due to the cytoskeleton cell can remain organised and various higher ordered structures can emerge.

⇒ *Fluorescent Beads Disintegrate Actin Networks*
T. Golde, C. Schuldt, J. Schnauß, D. Strehle, M. Glaser, J.A. Käs / Physical Review E (2013) **88** 044601

⇒ *Keratins Significantly Contribute to Cell Stiffness and Impact Invasive Behavior*
K. Seltmann, A.W. Fritsch, J.A. Käs, T.M. Magin / Proceedings of the National Academy of Science USA (2013) **110** 18507

⇒ *Slow and Anomalous Dynamics of an MCF-10A Epithelial Cell Monolayer*
K.D. Nnetu, M. Knorr, S. Pawlizak, T. Fuhs, J.A. Käs / Soft Matter (2013) **9** 9335

⇒ *Thermorheology of Living Cells—Impact of Temperature Variations on Cell Mechanics*
T.R. Kießling, R. Stange, J.A. Käs, A.W. Fritsch / New Journal of Physics (2013) **15** 045026

⇒ *Analysis of Multiple Physical Parameters for Mechanical Phenotyping of Living Cells*
T.R. Kießling, M. Herrera, K.D. Nnetu, E.M. Balzer, M. Girvan, A.W. Fritsch, S.S. Martin, J.A. Käs, W. Losert / European Biophysics Journal (2013) **42** 383

⇒ *Emergent Complexity of the Cytoskeleton: From Single Filaments to Tissue*
F. Huber, J. Schnauß, S. Rönicke, P. Rauch, K. Müller, C. Fütterer, J. Käs / Advances in Physics (2013) **62** 1

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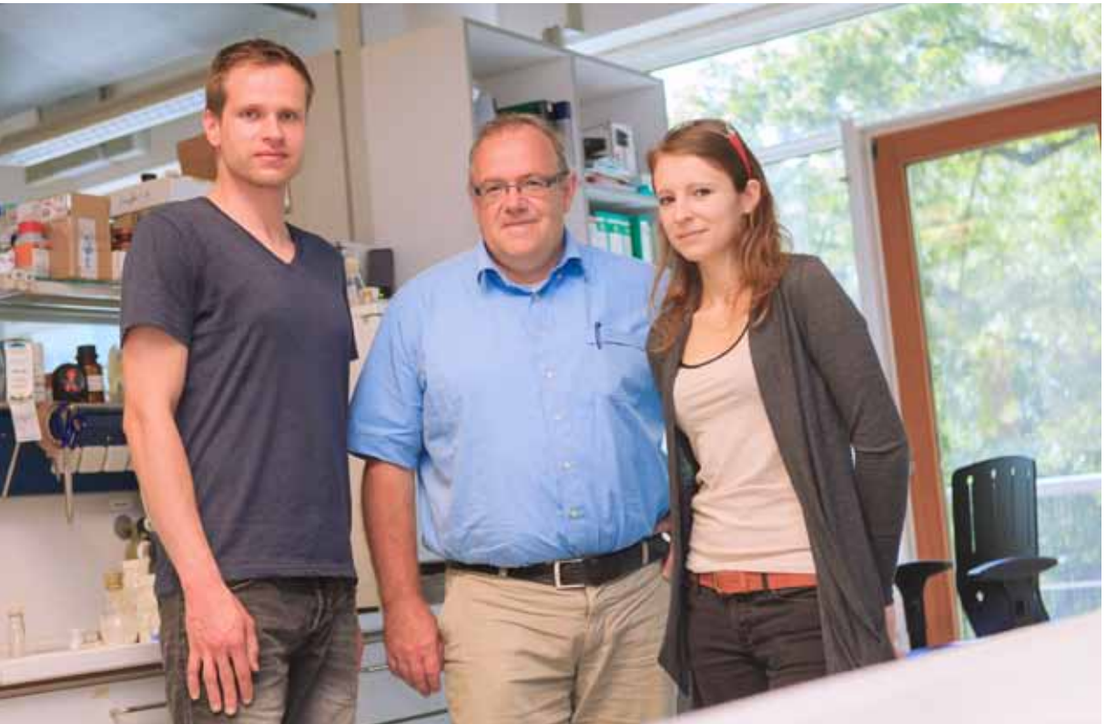
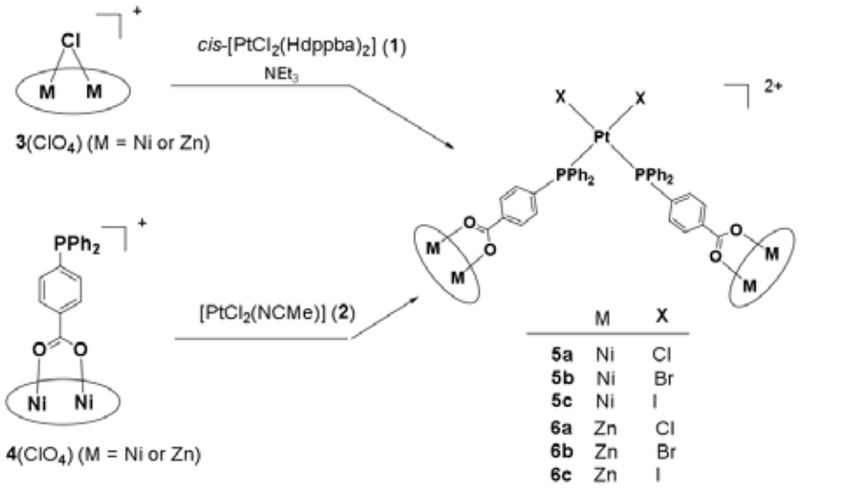
Coordination compounds in supramolecular chemistry and materials chemistry

Prof. Dr. Berthold Kersting
Dr. Matthias Golecki, M.Sc. Chem. Sina Gruschinski, Dr. Jochen Lach, M.Sc. Chem. Steve Ullmann

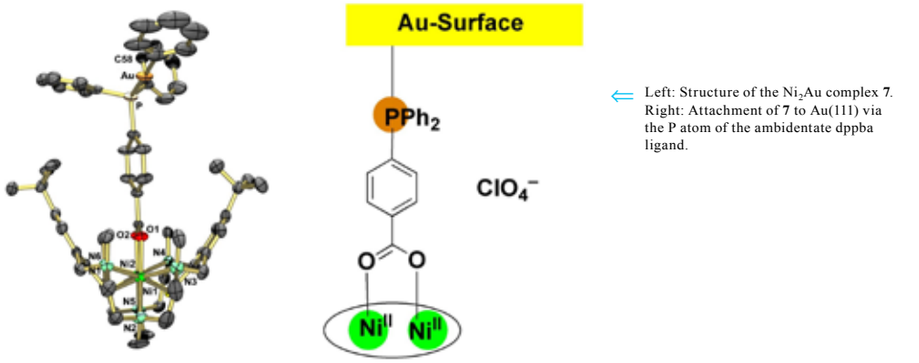
The studies focusing on the encapsulation of catalytically active transition metal complexes were continued. The ability of square-planar complexes such as *cis*-$[PtCl_2(Hdppba)_2]$ (**1**) (or $[PtCl_2(NCMe)_2]$ (**2**)) to act as bridging metalloligand for dinuclear macrocyclic $[Ni_2L]^{2+}$ and $[Zn_2L]^{2+}$ complexes was demonstrated (L^{2-} represents a 24-membered macrocyclic hexaaza-dithiophenolate ligand). Pentanuclear Ni_4Pt and Zn_4Pt complexes of composition $[(M_2L)_2(\mu\text{-dppba})_2PtCl_2]^{2+}$ (M = Ni or Zn) were synthesised either from substitution reactions between **1** and the corresponding $[M_2L(\mu\text{-Cl})]^+$ compounds (M = Ni, Zn) or by treatment of $[PtCl_2(NCMe)_2]$ with the $[M_2L(\mu\text{-dppba})]^+$ complexes (M = Ni, Zn). The Pt and Rh dppba complexes act in all cases as quadridentate bridging ligands linking two bioctahedral LNi_2 (or LZn_2) units via $\mu_{1,3}$-bridging carboxylate functions. The ^{31}P chemical shifts and the $^1J(P, Pt)$ and $^1J(P, Rh)$ coupling constants further show that the *cis*- and *trans*-stereochemistry of the mononuclear educts is maintained in the pentanuclear products. It is also demonstrated that the terminal Cl^- ligands can be substituted by Br^- and I^- without affecting the pentanuclear nature of the complexes.



The studies focusing on the synthesis of novel molecular-based magnetic materials were also continued. A novel strategy for the fixation of redox-active dinickel(II) complexes with high-spin ground states to gold surfaces was developed. The dinickel(II) complex $[Ni_2L(dppba)]ClO_4$ (**4**ClO_4) reacts with AuCl to a monoaurated $Ni^{II}_2Au^I$ complex $[Ni^{II}_2L(dppba)Au^ICl]ClO_4$ (**7**ClO_4). Temperature dependent magnetic susceptibility measurements reveal a ferromagnetic coupling J = +15.9 cm^{-1} between the two Ni(II) ions in **7**ClO_4 ($H = -2JS_1S_2$). HF-ESR measurements yield a negative axial magnetic anisotropy ($D < 0$) which implies a bistable (easy axis) magnetic ground state. The binding of the $[Ni_2L(dppba)]ClO_4$ complex to gold was ascertained by four complementary surface analytical methods: contact angle measurements, atomic force microscopy, X-ray photoelectron spectroscopy and spectroscopic ellipsometry. The results indicate that the complexes are attached to the Au surface via coordinative Au–P bonds in a monolayer.



⇑ Synthesis of pentanuclear Ni_4Pt and Zn_4Pt complexes **5**-**6**



⇐ Left: Structure of the Ni_2Au complex **7**. Right: Attachment of **7** to Au(111) via the P atom of the ambidentate dppba ligand.

⇒ *Synthesis and Characterization of Pentanuclear Complexes Composed of Pairs of Macrocyclic Ni_2L and Zn_2L Complexes Linked by cis-[$PtCl_2$(dppba)$_2$] and trans-[RhCl(CO)(dppba)$_2$] (dppba = (4-diphenylphosphino) benzoate, L=macrocyclic ligand)*
M. Golecki, B. Kersting / Z. Anorg. Allg. Chem. (2013) **639** 2473

⇒ *Chemisorption of Exchange-Coupled [Ni_2L(dppba)]$^+$ Complexes on Gold via Ambidentate 4-(Diphenyl) phosphinobenzoate Coligands*
M. Golecki, J. Lach, A. Jeremies, F. Lungwitz, M. Fronk, G. Salvan, D.R.T. Zahn, J. Park, Y. Krupskaya, V. Kataev, R. Klingeler, B. Büchner, B. Mahns, M. Knupfer, P.F. Siles, O.G. Schmidt, A. Reis, W.R. Thiel, D. Breite, B. Abel, B. Kersting / Chem. Eur. J (2013) **19** 7787

⇒ *Dinuclear Zinc Complexes Supported by Macrobinucleating Hexaaza-dithiophenolate Macrocycles: Synthesis of Zinc Thiolate Complexes with Biologically Relevant N_3S and N_2SCl Donor Sets*
U. Lehmann, B. Kersting / Z. Anorg. Allg. Chem. (2013) **639** 1543

⇒ *Preparation and Characterization of Dinuclear Nickel(II) Complexes Containing $N_3Ni(\mu_{1,3}\text{-}SO_3R)_2(\mu\text{-}RCN_4)NiN_3$ Cores: Crystal Structures and Magnetic Properties*
J. Lach, E. Perlt, B. Kersting, B. Kirchner / Z. Anorg. Allg. Chem. (2013) **639** 524

⇒ *2- tert -Butyl-5-(2-pyridyl)-2 H -tetrazole as Chelating Ligand in Direct Synthesis of Novel Cu(II) and Heterobimetallic Cu(II)/Mn(II) Complexes*
A.P. Mosalkova, S.V. Voitekhovich, A.S. Lyakhov, L.S. Ivashkevich, J. Lach, B. Kersting, P.N. Gaponik, O.A. Ivashkevich / Dalton Trans. (2013) **42** 2985

⇒ *The Effects of Ring Expansion and N-Methylation on the Complexation Behaviour of Macrobinucleating Hexaaza-Dithiophenolate Macrocycles: Destabilization of the CoIII Oxidation Level and Lowering of Coordination Number*
U. Lehmann, J. Lach, F. Schleife, A. Jeremies, B. Kersting / Eur. J. Inorg. Chem. (2013) 1336

⇒ *Tetranuclear Complexes Composed of Dinickel(II) Macrocyclic Fragments Bridged by 5,5'-(1,3-phenylene) bis-1 H -tetrazolato and N,N-bis(tetrazol-5-ato)amine Coligands: Synthesis, Structures and Magnetic Properties*
J. Lach, A.P. Mosalkova, S.V. Voitekhovich, P.N. Gaponik, B. Kersting / Polyhedron (2013) **49** 183

⇒ *Binuclear Nickel Complexes with an Edge Sharing Bis(Square-pyramidal) $N_3Ni(u\text{-}S_2)NiN_3$ Core: Synthesis, Characterization, Crystal Structure and Magnetic Properties*
U. Lehmann, J. Lach, C. Loose, T. Hahn, B. Kersting, J. Kortus / Dalton Trans. (2013) **42** 987

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Complex systems from theoretical methods – development and applications

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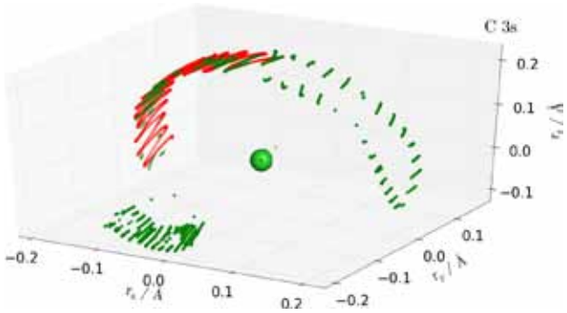
M.Sc. Chem. Martin Brehm, M.Sc. Chem. Eva Perlt

Nowadays, molecular dynamics is one of the most important tools for the investigation of complex systems. Thereby the whole range between small systems that can be investigated to extremely high accuracy from first principles applying ab initio molecular dynamics, to huge systems and biological processes, which are studied by classical molecular dynamics with the appropriate force fields and coarse grained methods, is covered. All of these methods have in common that they result in a multi-dimensional trajectory where the results have to be extracted from. The program Travis developed by Martin Brehm is able to extract a multitude of data out of these trajectories. It is still being improved and extended and in the meanwhile, it is frequently used by external groups.

A new kind of ab initio molecular dynamics has been developed by Eva Perlt. In that approach the orbitals are no longer fixed on the atomic cores but are optimised in order to lower the total energy. Many new implementations have been made including the possibility to simulate open-shell systems, the evaluation of the dipole moment, partial charges and bond orders.



⇐ Optimised positions of the 3s basis function of carbon in the methane molecule along the trajectory

⇒ *Liquid Structure and Cluster Formation in Ionic Liquid/Water Mixtures – An Extensive ab initio Molecular Dynamics Study on 1-Ethyl-3-Methylimidazolium Acetate/Water Mixtures – Part 2*
M. Brehm, H. Weber, A.S. Pensado, A. Stark, B. Kirchner / Z. Phys. Chem. (2013) **227** 177

⇒ *Carbene Formation in Ionic Liquids: Spontaneous, Induced, or Prohibited?*
O. Holloczki, D.S. Firaha, J. Friedrich, M. Brehm, R. Cybik, M. Wild, A. Stark, B. Kirchner / J. Phys. Chem. B (2013) **117** 5898

⇒ *Computing Vibrational Spectra from ab initio Molecular Dynamics*
M. Thomas, M. Brehm, R. Fligg, P. Vöhringer, B. Kirchner / Phys. Chem. Chem. Phys. (2013) **15** 6608

⇒ *Preparation and Characterization of Dinuclear Nickel(II) Complexes Containing $N_3Ni(\mu_{1,3}\text{-}SO_3R)_2(\mu\text{-}RCN_4)NiN_3$ Cores: Crystal Structures and Magnetic Properties*
J. Lach, E. Perlt, B. Kirchner, B. Kersting / ZAAC (2013) **639** 524

⇒ *Understanding the Evaporation of Ionic Liquids using the Example of 1-Ethyl-3-Methylimidazolium Ethylsulfate*
F. Malberg, M. Brehm, O. Hollóczki, A.S. Pensado, B. Kirchner / Phys. Chem. Chem. Phys. Chem. Chem. Phys. (2013) **15** 18424

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Structural flexibility and gate opening behaviour in porous coordination polymers

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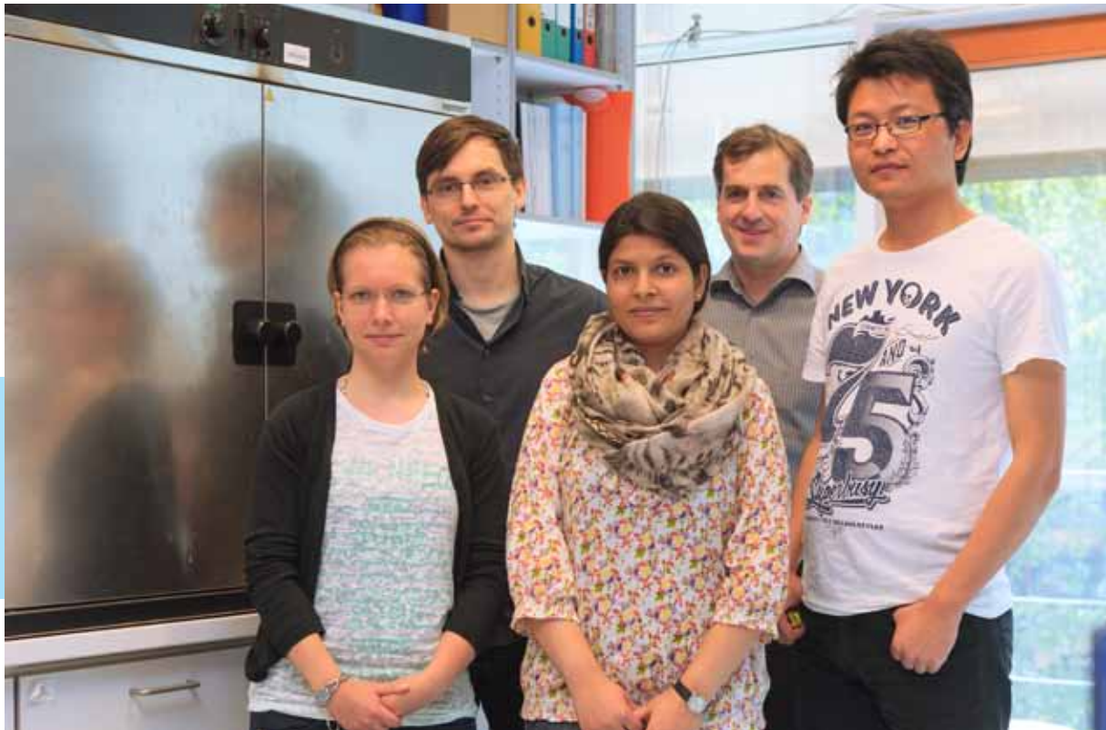
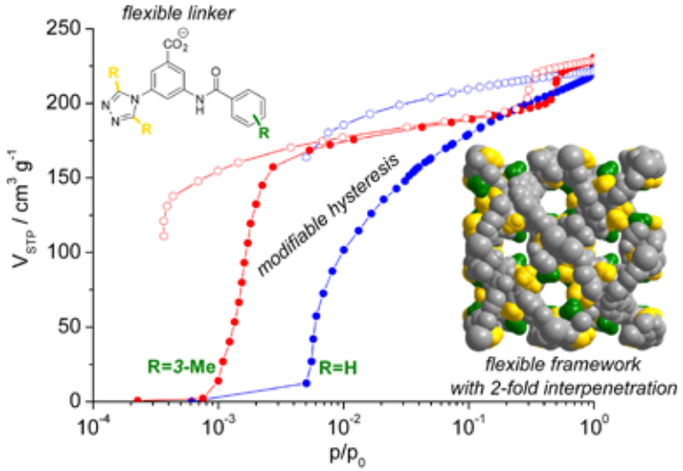
M.Sc. Chem. Salma Begum, Dr. Jorge Luis Cholula Díaz, Dr. Dirk Friedrich, M.Sc. Chem. Marcel Handke, M.Sc. Chem. Karolin Stein, M.Sc. Chem. Zhaoyang Wang

Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) are a new class of porous materials with distinct adsorption properties and high diversity of possible framework structures. They possess great potential for applications in gas separation and storage, as sensors, in heterogeneous catalysis and in thermal energy storage. Some MOFs are structurally flexible resulting in adsorption-desorption isotherms with hysteresis loops. Such flexible materials reveal a so-called *gate opening* process in which the framework undergoes a structural transformation along with a sudden increase in adsorption capacity – a response to external stimuli such as pressure or temperature.



A series of 15 isostructural Ag^+ based MOFs consisting of interpenetrated 3D networks and a thermal stability up to 250 °C could be obtained under solvothermal conditions. Their pore diameters and pore volumes can be adjusted by substituents of the 3-(1,2,4-triazol-4-yl)-5-benzamidobenzoate linker. Sorption studies with N_2 and CO_2 demonstrate the high flexibility of the new materials, the sorption experiments result in isotherms with one or two hysteresis loops and pore volumes of up to 0.38 $cm^3\ g^{-1}$ (49%). The variation of the sterical demand of the substituents of the triazole and the benzoyl group adjust the pore shape. Thus, this series of isostructural MOFs was employed for systematic studies of the influence of linker substitution on network porosity and *gate opening* behaviour in order to study origin and consequences of structural flexibility.



⇑ Influence of linker substitution on N_2 sorption isotherms (77 K, p_0 = 0.0972 MPa, closed symbols adsorption, open symbols desorption) in $[Ag_2(L)_2]$.

⇒ *Synthesis and Crystal Structures of $[(^iPr_3P)_2Cu(\mu\text{-}ESiMe_3)(InMe_3)]$ (E = S. Se) – Lewis Acid-Base Adducts with Chalcogen Atoms in Planar Coordination*
R. Biedermann, O. Kluge, H. Krautscheid / European Journal of Inorganic Chemistry (2013) 4727

⇒ *Unprecedented Trapping of Difluorooctamolybdate Anions within an α-Polonium Type Coordination Network*
O.V. Sharga, A.B. Lysenko, M. Handke, H. Krautscheid, E.B. Rusanov, A.N. Chernega, K.W. Krämer, S.-X. Liu, S. Decurtins, A. Bridgeman, K.V. Domasevitch / Inorganic Chemistry (2013) **52** 8784

⇒ *Tetranuclear Organometallic Complexes based on 1,2-ethanedithiolate Ligands as Potential Precursors for $CuMS_2$ (M = Ga, In)*
D. Friedrich, O. Kluge, M. Kischel, H. Krautscheid / Dalton Transactions (2013) **42** 9613

⇒ *Synthesis, Crystal Structure and Solid State NMR Investigations of Heteronuclear Zn/Co MOFs – A Comparative Study*
A. Viswanath Kuttatheyil, D. Lässig, J. Lincke, M. Kobalz, M. Baias, K. König, J. Hofmann, H. Krautscheid, C. J. Pickard, J. Haase, M. Bertmer / Inorganic Chemistry (2013) **52** 4431

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From glassy dynamics of condensed isolated polymer coils to molecular biophysics in basic research and application

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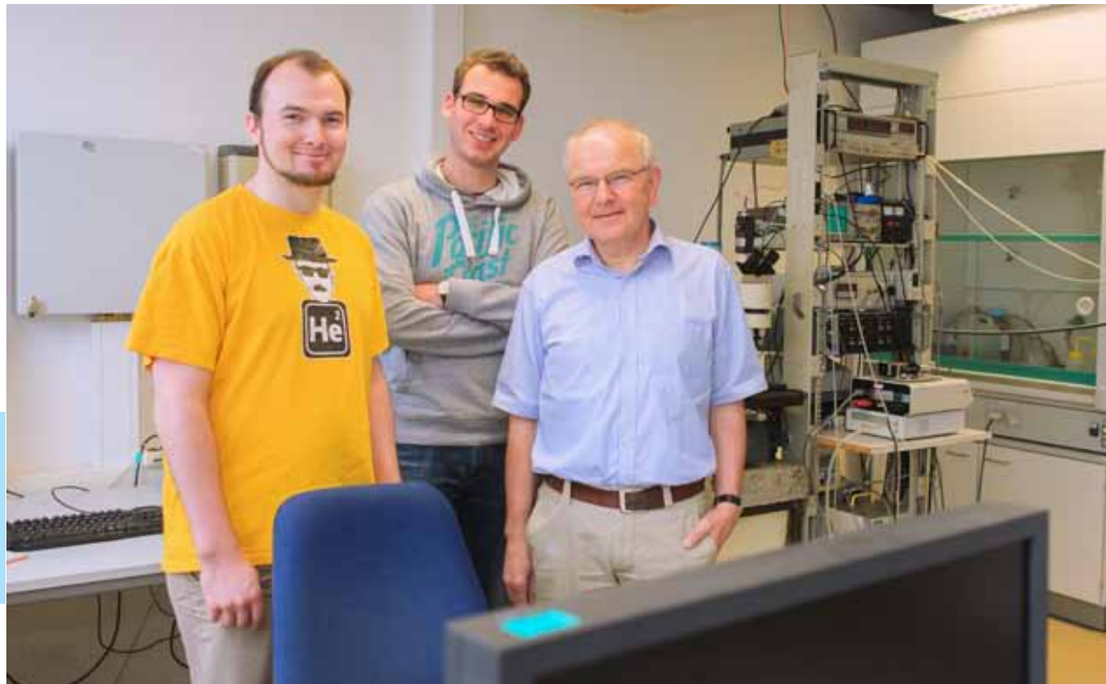
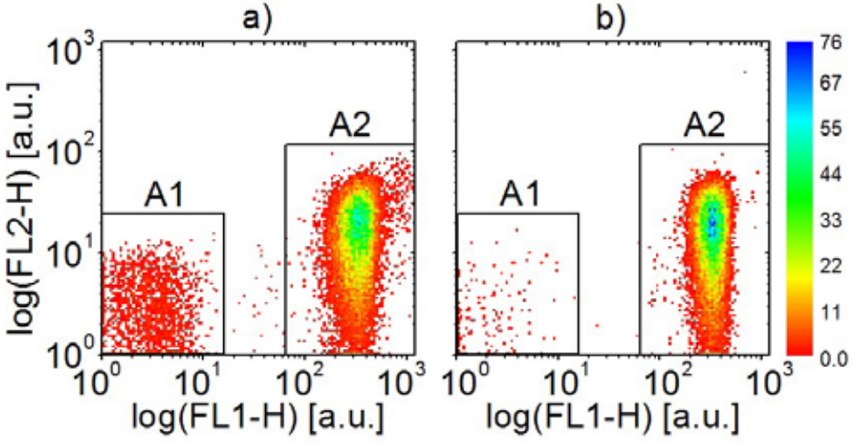
FACS-sorted particles reduce the data variance in optical tweezers assisted Dynamic Force Spectroscopy measurements: By combining optical tweezers assisted dynamic force spectroscopy experiments with fluorescence activated cell sorting (FACS), we demonstrate a new approach to reduce the data variance in measuring receptor-ligand-interactions on a single molecule level by ensuring similar coating densities. Therefore, the carboxyfluorescein-labeled monophosphorylated peptide tau226-240[pThr231] is anchored on melamine resin beads and these beads are sorted by FACS to achieve a homogeneous surface coverage. To quantify the impact

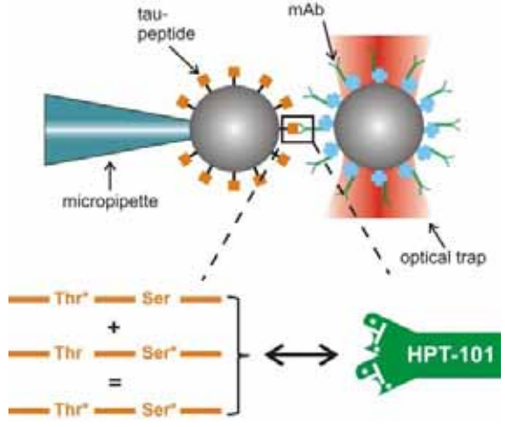


of the fluorescence dye on the bond parameters between the phosphorylated peptide and the corresponding phosphorylation specific anti-human tau monoclonal antibody HPT-104, we perform dynamic force spectroscopy and compare the results to data using unsorted beads covered with the non-fluorescence peptide analogue. Finally, we demonstrate that the data variance of the relative binding frequency is significantly decreased by a factor of 3.4 using pre-sorted colloids with a homogeneous ligand coating compared to unsorted ones.



⇑ 2D-density plot of tau-peptide labeled MF-particles (diameter: 2.3 µm) in dependence on intensity signal of channel FL2-H vs. FL1-H. a) FACS data before the selection process. Two populations are visible: A1 contains uncoated colloids and A2 contains the fluorescence tagged tau-particles. It is apparent that both populations can be distinguished. b) Same batch of colloids as in a), but after sorting. Population A1 is sorted out, only the target population A2 remains with a significant reduction in width and a pronounced increase in density (blue color).

Determining the specificity of monoclonal antibody HPT-101 to tau-peptides with optical tweezers: Optical tweezers-assisted dynamic force spectroscopy is employed to investigate specific receptor-ligand-interactions on the level of single binding events. In particular, we analyse binding of the phosphorylation-specific monoclonal antibody (mAb) HPT-101 to synthetic tau-peptides with two potential phosphorylation sites (Thr231 and Ser235), being the most probable markers for Alzheimer's disease. Whereas the typical interpretation of enzyme-linked immunosorbent assay (ELISA) suggests that this monoclonal antibody binds exclusively to the double-phosphorylated tau-peptide, we show here by DFS that the specificity of mAb HPT-101 is only apparent. In fact, binding occurs also to each sort of the monophosphorylated peptides. Therefore, we characterise the unbinding process by analysing the measured rupture force distributions, from which the lifetime of the bond without force τ_0, its characteristic length x_{ts} and the free energy of activation ΔG are extracted for the three mAb/peptide combinations. This information is used to build a simple theoretical model to predict features of the unbinding process for the double-phosphorylated peptide purely based on data on the monophosphorylated ones. Finally, we introduce a method to combine binding and unbinding measurements to estimate the relative affinity of the bonds. The values obtained for this quantity are in accordance with ELISA, showing how DFS can offer important insights about the dynamic binding process which are not accessible to this common and widespread assay.



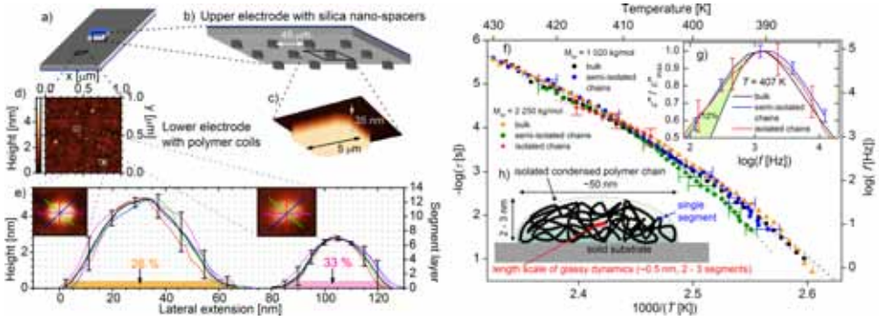
⇑ Experimental setup. One peptide-coated colloid is immobilised at the tip of a custom-made micropipette by capillary force and a second colloid, bearing the mAb HPT-101 on its surface, is trapped with the optical tweezers. (Inset) It is shown by our measurements and a simple theoretical model that the binding of mAb HPT-101 to the doubled phosphorylated peptide can be describe as the sum of the two monophosphorylated cases.

Amino acid-sequence dependent interactions between receptors and ligands studied with optical tweezers: For diagnostic procedures that rely on monoclonal antibodies (mAbs), it is imperative to know whether the antibody (e.g. mAb HPT-101) recognises the epitope of its target peptide/protein (e.g. tau-protein) specific or whether possible cross-reactions to other forms of the protein may occur. In a previous study, non-specific interactions of the phosphorylation-specific mAb HPT-101 to tau-peptides with similar epitopes, differing only by a single isolated phosphorylation site, were detected. Based on this result, it is obvious that the specificity of mAb HPT-101 refers not exclusively to the phosphorylation pattern but depends also on the surrounding amino acid sequence in the tau peptide. Here, we investigate with the help of optical tweezers assisted dynamic force spectroscopy the influence of single amino acids on the binding of mAb HPT-101 to the doubled phosphorylated peptide tau[pThr231/Ser235]. For this purpose, we characterise the unbinding process by analysing the measured rupture force distributions, from which the lifetime of the bond without force τ_0, its characteristic length x_{ts}, and the free energy of activation ΔG are extracted for the all mAb/peptide combinations. Furthermore, the binding process is specified by means of the relative binding frequency. Using these parameter, it is possible to identify essential as well as secondary amino acids for the interaction between mAb HPT-101 and tau[pThr231/pSer235].

Sequence	V	A	V	V	R	pT	P	P	K	pS	P	S	S	A	K
HPT-101 (pT & pS)	V	A	V	V	R	pT	P	P	K	pS	P	S	S	A	K

⇑ Epitop mapping of monoclonal antibody HPT-101. The antibody specific phosphorylation sites are underlined (abbreviation: p = phosphorylation) and essential amino acids are shown in red. Secondary amino acids, which contribute to the binding, are highlighted in orange. White fields are not significant for the specific interaction between antigen and antibody.

Glassy dynamics of condensed (semi)-isolated polymer coils: The glassy dynamics of *condensed isolated* poly(2-vinylpyridine) (P2VP) polymer chains is studied by means of Broadband Dielectric Spectroscopy (BDS). For this purpose, a recently developed nano-structured electrode arrangement is refined to achieve an electrode-to-electrode distance of only 35 nm. The polymer coils are deposited on highly conductive silicon electrodes, a subsequent annealing removed the solvent. Atomic Force Microscopy (AFM) scans of the identical samples reveal that the mean volume of the coils resembles that calculated for a single chain. ~30 % of the segments directly contact the substrate which are hence expected to exhibit traces of interfacial interaction. The BDS measurements show, that even isolated condensed polymer chains exhibit glassy dynamics. Further, the mean relaxation time corresponds to the bulk. This demonstrates that glassy dynamics relies on fluctuations of 2–3 segments, a unit much smaller than the coil which is in accord with results from thin layers. An extensive analysis of the relaxation time distribution



⇑ a) Sketch of the sample arrangement with upper and lower electrode of an area of 1 x 1 mm² and 4 x 10 mm², respectively. b) Scheme of the upper electrode with its regular matrix of insulating silica nano-structures serving as spacers. c) 3D display of an AFM image of an individual nano-structure. d) AFM image of the lower electrode with isolated condensed P2VP chains on the silica surface; e) height profiles taken along the coloured lines as indicated in the respective insets. f) Mean relaxation time of segmental motion vs. inverse temperature for P2VP bulk, semi-isolated and isolated condensed polymer chains of different molecular weight as indicated. g) Loss spectra corrected for artificial contributions (conductivity and wafer resistance) and normalised with respect to the peak maximum. h) Schematic drawing for comparison of the dimensions of a single polymer chain and the intrinsic length scale of glassy dynamics.

reveals a broadening at lower frequencies: ~12 % of the mobile segments are slower than in bulk. The mismatch by a factor of ~2 with the fraction of segments directly contacting the interface is due to the fact that only half of the latter establish bonds with the substrate surface which is revealed by complementary measurements by means of infrared spectroscopy.

⇒ *Intra- and Inter-molecular Dynamics in Glass-forming Liquids*
P. Papadopoulos, W. Kossack, F. Kremer / Soft Matter (2013) **9** 1600

⇒ *Comparative Study on the Molecular Dynamics of a Series of Polypropylene Glycols*
K. Kaminski, W. Kipnusu, K. Adrjanowicz, E. Mapesa, C. Iacob, M. Jasiurkowska, P. Wlodarczyk, K. Grzybowska, M. Paluch, F. Kremer / Macromolecules (2013) **46** 1973

⇒ *The Interplay Between Inter- and Intramolecular Dynamics in a Series of Alkylcitrates*
W. Kipnusu, W. Kossack, C. Iacob, P. Zeigermann, M. Jasiurkowska, J.R. Sangoro, R. Valiullin, F. Kremer / Soft Matter (2013) 9 4681

⇒ *FACS-sorted Particles Reduce the Data Variance in Optical Tweezers Assisted Dynamic Force Spectroscopy Measurements*
T. Stangner, D. Singer, C. Wagner, C. Gutsche, O. Ueberschär, R. Hoffmann, F. Kremer / Physical Biology (2013) **10** 046004

⇒ *Segmental and Chain Dynamics in Nanometric Layers of Poly (cis-1,4-isoprene) as Studied by Broadband Dielectric Spectroscopy and Temperature-modulated Calorimetry*
E. Mapesa, M. Tress, G. Schulz, H. Huth, C. Schick, M. Reiche, F. Kremer / Soft Matter (2013) **9** 10592

⇒ *Glassy Dynamics in Condensed Isolated Polymer Chains*
M. Tress, E. Mapesa, W. Kossack, W. Kipnusu, M. Reiche, F. Kremer / Science (2013) **341** 1371

⇒ *Determining the Specificity of Monoclonal Antibody HPT-101 to Tau-Peptides with Optical Tweezers*
T. Stangner, C. Wagner, D. Singer, S. Angioletti-Uberti, C. Gutsche, J. Dzubiella, R. Hoffmann, F. Kremer / ACS Nano (2013) **7** 12

⇒ *Molecular Order and Dynamics of Nanometric Thin Layers of Poly(styrene-b-1,4-isoprene) Diblock Copolymers*
W.K. Kipnusu, M.M. Elmahdy, M. Tress, M. Fuchs, E.U. Mapesa, D.-M. Smilgies, J. Zhang, C. Papadakis, F. Kremer / Macromolecules (2013) **46** 9729

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Slow biopolymer dynamics

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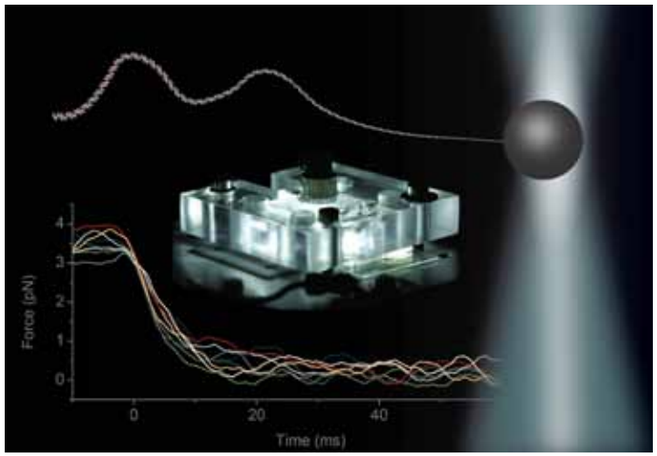
Dipl.-Phys. Jakob Tómas Bullerjahn, M.Sc. Phys. Gianmaria Falasco, Dipl.-Phys. Andrea Kramer, Dipl.-Phys. Marc Lämmel, Dipl.-Phys. Sebastian Sturm, M.Sc. Phys. Guillermo Zecua

Reversible chemical bonds are a recurrent theme in biophysics, determining the effectivity of enzymes as well as the elastic and plastic behaviour of biopolymers, reconstituted polymer solutions or the cytoskeleton. Building on our minimal "Glassy Wormlike Chain" model of polymer network dynamics, we were successful in quantitatively describing the slow dynamics and linear and nonlinear viscoelasticity as a function of temperature for pectin gels.

In collaboration with the Keyser group at the University of Cambridge, UK, we also investigated the hydrodynamic friction forces generated by a rapidly recoiling molecular linker (specifically a dsDNA molecule), an effect that may become relevant to the practical implementation of rapid force spectroscopy protocols. We were able to show, both experimentally and theoretically, that the friction "actively generated" through the conformational dynamics of the DNA may evoke a severalfold increase in the effective friction coefficient. We derived a semi-analytical, generic formula for this effective friction coefficient in dependence on linker properties, pulling force and transducer stiffness.



⇑ The decay of the tension in a recoiling DNA molecule is inferred, using a precise theory (developed in Leipzig), from the relaxation of an attached tracer bead in an optical trap. The measurements (performed in Cambridge) reveal a drastically increased friction "actively generated" by the recoiling dynamics.

⇒ *Micro-rheological Behaviour and Nonlinear Rheology of Networks Assembled from Polysaccharides from the Plant Cell Wall*
R.R.R. Vincent, B.W. Mansel, A. Kramer, K. Kroy, M.A.K. Williams / New J. Phys. (2013) **15** 035002

⇒ *Rapid Internal Contraction Boosts DNA Friction*
O. Otto, S. Sturm, N. Laohakunakorn, U. Keyser, K. Kroy / Nature Communications (2013) **4** 1780

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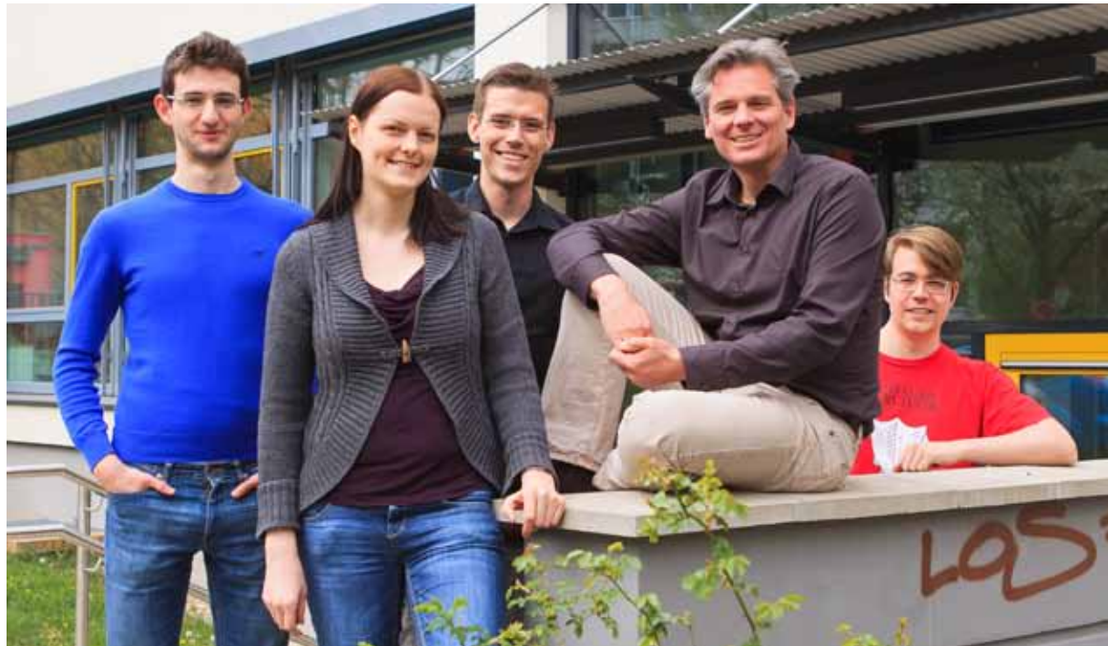


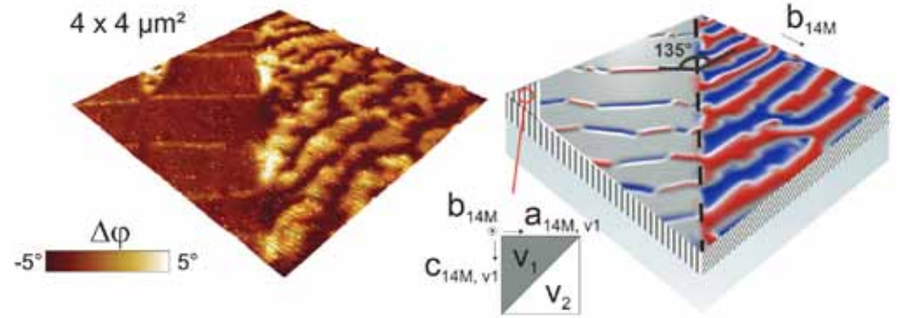
Functional materials, materials physics at the nanoscale, interfaces between hard matter and living cells and tissue

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

Our group employs state-of-the-art synthesis and characterisation techniques, as well as computer modeling to develop and study new functional materials with emphasis on possible applications in biomedical sciences. Within BuildMoNa, the following topics are currently addressed: bimetallic magnetic nanoparticles, mechanical properties at the nanoscale and, as a special focus of ongoing research, ferromagnetic shape memory alloys (FSMA). Recent results and achievements within this field shall be presented in the following.

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 focused specifically on Fe_7Pd_3 and Ni_2MnGa. While Ni_2MnGa can yield strains as high as 10% and exhibits high ductility, Fe_7Pd_3 leads to smaller strains but has the advantage of being biocompatible. Two key aspects of FSMAs have recently been put under scrutiny by our group: i) the connection between structural and magnetic properties of FSMA thin films and ii) the interaction mechanisms of biocompatible Fe_7Pd_3 with living cells.

i) Magnetic Force Microscopy studies on FSMA thin films: The correct orientation of the martensitic cell constitutes an essential prerequisite for magnetic actuation. Therefore, it is necessary to systematically examine the relationship between the magnetic domain pattern and underlying structure. During our studies we found experimental evidence showing that magnetic domain appearance is strongly connected to the presence and absence of nanotwinning. While the martensite–austenite transformation of as-deposited films upon temperature variation is clearly reflected in topography, the magnetic domain pattern is hardly affected. These observations are strongly influenced by significant thermal stresses arising in the austenite phase due to the Invar properties of Fe_7Pd_3. Meanwhile, freestanding martensitic films exhibit a hierarchical structure of micro- and nanotwinning with a more complex associated domain configuration, since the dominance of magnetic energy contributors is altered within this length scale regime. We also observed clear correlations between magnetic and crystalline structures at various temperatures for as-deposited Ni_2MnGa thin films. With the micromagnetic simulations the development of magnetic domains in these films was successfully simulated.



⇑ Experimental (left) and theoretical (right) results of local magnetic structure of a martensitic Ni_2MnGa sample. Simulations consider local magneto crystalline features, twinning periodicity as well as film thickness and MFM conditions such as tip dimensions and lift height. Schematics illustrate the presence of twin variants v_1 and v_2 as well as local orientation of the 14M modulated lattice.

ii) Biocompatibility and biological functionalisation of smart materials: Foregoing research proposed that Fe_7Pd_3 films could be used for applications in biomedicine. Therefore, we tested their interaction with living cells and coatings, such as the RGD amino acid sequence, which is crucial to cellular adhesion. Through delamination tests and cell culture assays, we proved decent adhesion of RGD to the substrate and cells to the RGD, respectively. Theoretical *ab initio* calculations via density functional theory confirmed the experimental results and explained the strong connection between RGD and Fe_7Pd_3 in a fundamental physical way; it is mainly mediated by coordinate bonds between iron atoms of the films and nitrogen/oxygen atoms of the RGD. Thus surface functionalisation with biological coatings is possible and desirable.

⇒ *Nanoindentation Response of Substrate-attached and Freestanding Single-crystalline Fe_7Pd_3 Ferromagnetic Shape Memory Thin Films around the Martensite Transition - Impact of Constraints and Beyond*
Y. Ma, S.G. Mayr / Acta Materialia (2013) **61** 6756

⇒ *Nanoscale Magneto-structural Coupling in as-deposited and Freestanding Single Crystalline Fe_7Pd_3 Ferromagnetic Shape Memory Alloy Thin Films*
A. Landgraf, A.M. Jakob, Y. Ma, S.G. Mayr / Sci. Technol. Adv. Mater. (2013) **14** 045003

⇒ *Interaction of Ferromagnetic Shape Memory Alloys and RGD Peptides for Mechanical Coupling to Cells: from Ab Initio Calculations to Cell Studies*
M. Zink, F. Szillat, U. Allenstein, S.G. Mayr / Adv. Func. Mat. (2013) **23** 1383

⇒ *Coupling of Micromagnetic and Structural Properties across the Martensite and Curie Temperatures in Miniaturized Ni-Mn-Ga Ferromagnetic Shape Memory Alloys*
A.M. Jakob, M. Hennes, M. Müller, D. Spemann, S.G. Mayr / Adv. Func. Mat. (2013) **23** 4694

⇒ *Fe-Pd Based Ferromagnetic Shape Memory Actuators for Medical Applications: Biocompatibility, Effect of Surface Roughness and Protein Coatings*
U. Allenstein, Y. Ma, A. Arabi-Hashemi, M. Zink, S.G. Mayr / Acta Biomaterialia (2013) **9** 5845

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Engineering biomimetic microenvironments for *in vitro* cell studies

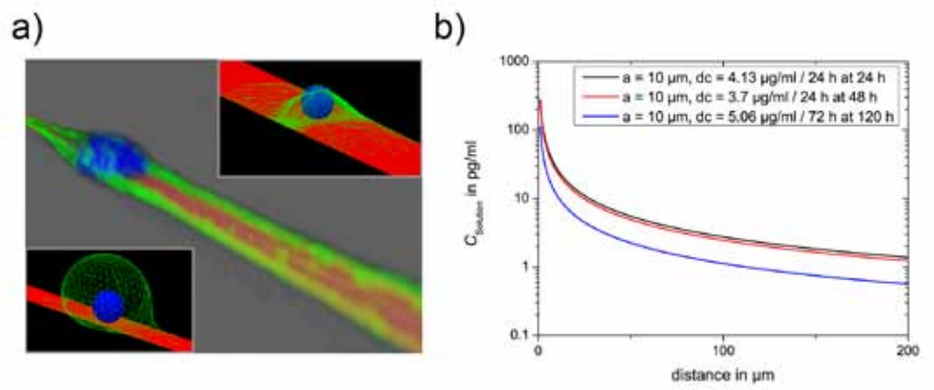
Prof. Dr. Tilo Pompe
M.Sc. Chem. Michael Ansorge, Dipl.-Phys. Andreas Müller

The extracellular microenvironment controls many cellular processes including cell growth, differentiation and apoptosis. In order to better understand 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 gradients of soluble mediators of hematopoietic stem cell fate in the bone marrow niche. He constructs polymeric microparticles with glycosaminoglycan functionalisation exhibiting a controlled and slow release of signalling molecules like SDF-1, GM-CSF and others, which allow to establish microscale gradients in 2D and 3D cell culture scaffolds.

In recent work directed migration of different populations of hematopietic stem and progenitor cells was shown.

A. Müller uses synthetic hydrogel layers to model the impact of materials stiffness, ligand affinity and spatial constraints on cell adhesion. Spatial constraints are modelled by introducing micropatterns on top of the polymer-coated hydrogels as they were recently shown to impact the intracellular structure of the actin cytoskeleton.



⇑ An illustration of experimental and modelled cell shapes on micropatterned substrates

⇑ Modelled gradients of the signalling molecule GM-CSF established by the release from protein-laden microparticles demonstrate sustained gradients at physiological relevant levels

⇒ *Dissipative Interactions in Cell–Matrix Adhesion*
C. Müller, A. Müller, T. Pompe / Soft Matter (2013) **9** 6207

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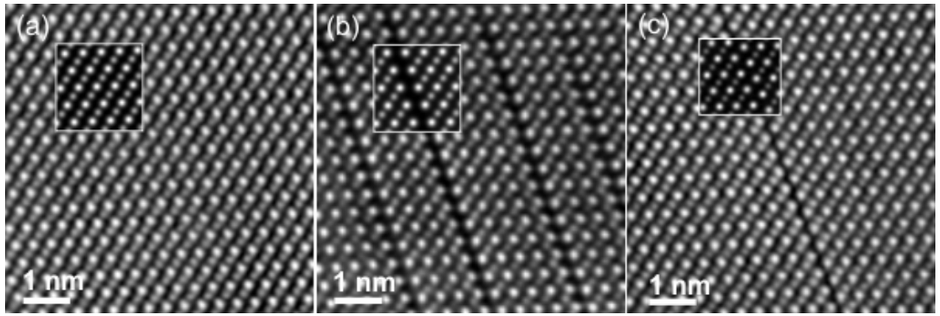
Ion and laser beam induced thin films and nanostructures

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

The research was focused on the formation of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium. Preferentially ion and laser beam techniques are used. These methods influence the nucleation and growth as well as the structural, optical and electrical properties of growing films as a consequence of atomic rearrangement. A main emphasis of this research was the preparation (i) of high-quality GaN films on SiC by ion beam assisted molecular beam epitaxy, (ii) the formation of Ge and Si sculptured thin films by ion beam assisted glancing angle deposition and (iii) the deposition of phase change material thin films by pulsed laser deposition. Especially, phase-change composites are of

interest as active components in next generation electronics phase-change random access memory (PCRAM). They display a rapid, reversible transition in resistance and reflectivity states due to their unique crystallisation behaviour from amorphous to metastable crystalline phase, as well as a low threshold to re-amorphisation. The atomic structure transition is therefore closely linked to those electronic and optical properties making the material class useful for data retention.

We have applied the analytical capabilities of a state-of-the-art probe Cs-corrected FEI Titan³ G2 60–300 TEM were used to the investigation of the atomic structure and phase transition in various thin film samples deposited by pulsed laser deposition. The chosen material systems of ternary compounds along the $(GeTe)_x$ -$(Sb_2Te_3)_{1-x}$ pseudo-binary line are widely used as test cases for phase change behaviour.



⇑ High resolution STEM images of metastable lattice in a textured $Ge_2Sb_2Te_5$ layer and corresponding image simulations (insets). (a) Defect-free lattice with randomly distributed vacancies, (b) vacancy layered structure, (c) antisite boundary.

⇒ *Single Pulse Laser-Induced Phase Transitions of PLD-Deposited $Ge_2Sb_2Te_5$ Films*
H. Lu, E. Thelander, J.W. Gerlach, U. Decker, B. Rauschenbach / Adv. Func. Mater. (2013) **23** 3621

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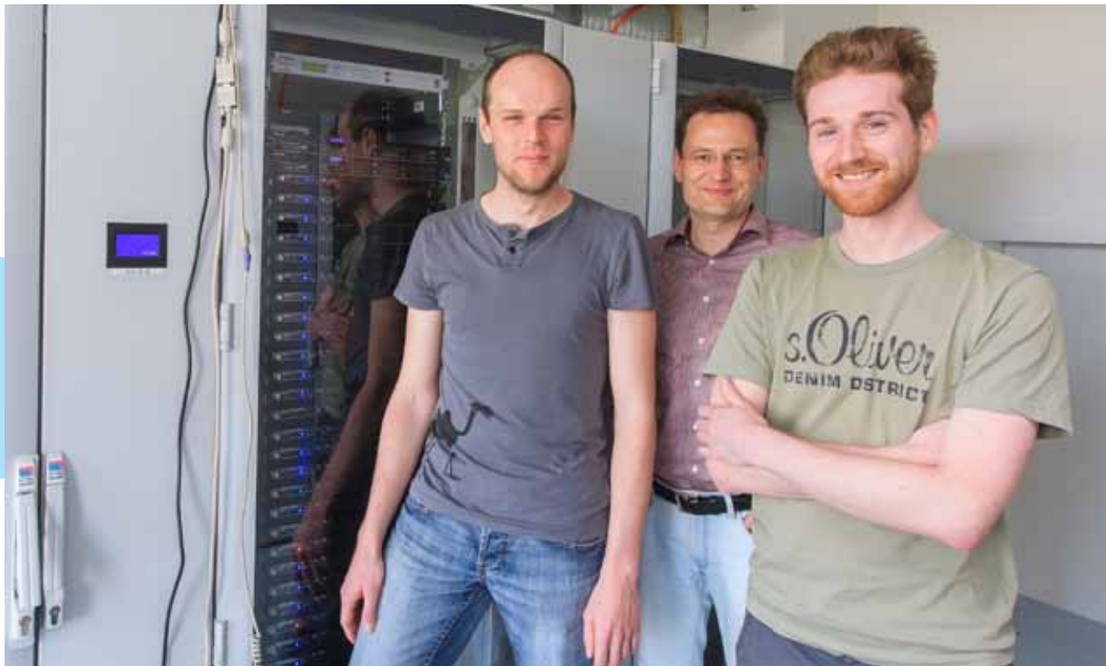
Coherent transport in quantum condensates: from quantum Hall nano-structures to exciton-polariton condensates

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

Research in the group is focused on the analysis of quantum condensates and topological quantum systems. Examples for quantum condensates are superconductors and exciton-polariton condensates. The common characteristic of these states of matter is the existence of a macroscopic wave function, which describes the collective quantum dynamics of the system. An exciton-polariton condensate, in contrast to a common condensate, is a non-equilibrium macroscopic state. This allows for a variety of novel fascinating phenomena, like condensation at finite momenta, disorder induced phase fluctuations or the discovery of new dynamical critical exponents. Quantum Hall fluids are a prime example for topological quantum systems exhibiting a novel phase of matter which cannot be characterised by standard order



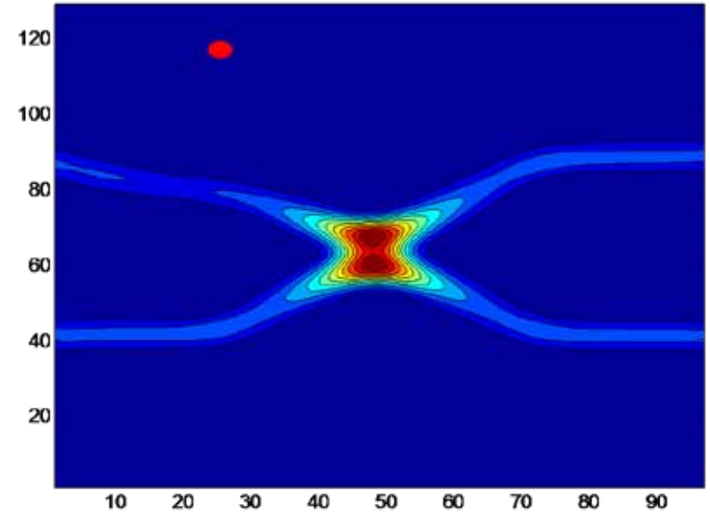
parameters. As a hallmark, for example, they exhibit perfectly conducting, topologically protected edge states.

We investigated both correlation functions and superfluid stiffness for a dissipative, driven quantum condensate (e.g. polariton condensate) in a disordered environment. We found that the disorder induced phase fluctuations destroy the quasi-longe-range order, which would survive in a disordered equilibrium condensate. For the disordered, driven system the response to external perturbation remains rigid only over a finite length scale. Thus, a non-equilibrium condensate is not a superfluid in the thermodynamic limit, although superfluid behaviour would persist at sufficiently small length scales. Our theoretical findings allow to understand experimental findings for an exciton-polariton condensate in a ZnO microcavity.

The active research on topological quantum systems has stimulated our search for a topologically non-trivial order in polariton systems. Specifically, we focus on cavity photons coupled to electrons of a quantum spin Hall insulator. For a chiral cavity and topologically trivial electrons restricted to one spin sector only, a topologically non-trivial phase arises. Taking the full cavity and electron space into account shows topological hallmarks if the electron system has an inverted band structure.

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. In recent experiments, quantum Hall edge states were imaged by means of scanning gate microscopy, allowing a detailed analysis of the edge state structure.

With the transport algorithm that we developed, we attempt to numerically implement a scanning gate experiment. In a first approach, the quantum point contact was modeled by a harmonic saddle point potential, using parameters that were found experimentally. In addition to this saddle point, a Lorentzian tip potential, which is moved around the system, implement the description of the scanning tip. In this way, a qualitative understanding of the results of scanning gate microscopy is achieved. To improve the quantitative agreement with experiment, 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 changes the results dramatically. 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.



⇑ The local density of states inside a quantum point contact tuned to have one Landau level completely filled shows a single edge state on either side of the system. Inside the constriction the channels are bent towards one another. The electron density can be manipulated with a scanning tip. The position of the tip is indicated with a red dot. Electron channels close to the tip are bent such that the electrons continue to follow equipotential lines.

⇒ *Superfluid Stiffness of a Driven Dissipative Condensate with Disorder*
A. Janot, T. Hyart, P.R. Eastham, B. Rosenow / PRL (2013) **111** 230403

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Experiences

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

Prof. Dr. Daniel Huster

In its 6th year, BuildMoNa continued to be a very successful graduate school with incredibly exciting scientific results and high ranking interdisciplinary teaching.

As a PI, I am very impressed to see how our doctoral candidates perform and develop in this highly interdisciplinary environment. In my view, a big step forward was the new structure of the scientific modules introduced in 2012. I particularly like the three basic modules "Basic Concepts in Physics/Chemistry/Biochemistry", which have been designed for doctoral candidates who did not do their major in the respective field. These modules provide an excellent introduction into the scientific fields of the other researchers in BuildMoNa and set up the stage for truly interdisciplinary collaborations within the graduate school, for which we can proudly present numerous examples. The interdisciplinary character of the modules is also fostered by the fact that the organisers and teachers in the modules come from various scientific backgrounds.

But also organising such a module is a fun experience. Being a physicist working in the field of biophysics and structural biology, I was involved in the "Basic Concepts in Biochemistry" module. Two things made this module a very special experience for me: (i) the fact that the doctoral candidates from various scientific backgrounds and expertise are also highly motivated to learn about new fields of science, and (ii) the PI who has been working in the field for many years also learns quite a lot in these modules, not just from the teachers but also from the doctoral candidates. This I think describes the spirit and the atmosphere that BuildMoNa is all about –mutual learning, rigorous discussions, and interdisciplinary research.

So it is not surprising that our doctoral candidates take on this spirit in their research projects and more and more start collaborating with colleagues from different fields and backgrounds. Suffice to say that our collaborative projects are often initiated and fully driven by our doctoral candidates. As a PI, one is then in the comfortable situation to lean back, watch the next generation researchers do their work and develop in the creative and exciting collaborative research environment of BuildMoNa. With a few guidelines from our side, I strongly believe that BuildMoNa prepares its graduates with the best possible background for a successful career in industry or academia.

Prof. Dr. Daniel Huster

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

Dipl.-Phys. Martin Göse

BuildMoNa is now in its 6th year and has continued its excellent work as an interdisciplinary graduate school for young scientists. Within this time, the graduate school established a well organised structure and arranged scientific programmes and modules, designed to convey fundamental background knowledge as well as highly specialised education for the doctoral candidates. Such an ambitious goal is hard to achieve, considering the different scientific backgrounds of the doctoral candidates due to their original field of study (e.g. physics or chemistry). BuildMoNa has developed a successful approach in overcoming this issue by offering basic scientific modules, summarising the basics of the three main topics: physics, chemistry and biochemistry, as well as research modules to discuss novel investigations and findings. This sensitises doctoral candidates to specific approaches of other disciplines, inspiring their own research as well as facilitating future interdisciplinary collaborations. But yet, the training programme exhibits potential further enhancements. Here the scientific information per module and examinations could be more focused on the key questions to prevent discouraging some candidates from other fields of study.

In addition to the scientific education programme, the graduate school offers a variety of different training modules for transferable skills. As some modules are specific to the every-day work of the doctoral candidates, other modules are intended to communicate specific abilities, which are more and more demanded by today's science and industry (e.g. scientific writing, grant proposal writing or presentation skills). That way, BuildMoNa not only supports the candidates on their way of achieving their doctorate, but prepares them for postgraduate issues and demands. Furthermore, the established connections with other doctoral candidates from different fields of research at, for example, the Annual BuildMoNa Conference lay the basis of fruitful collaborations as well as the development of new ideas.

Altogether, I think that the concept of the Graduate School BuildMoNa is a good example for a comprehensive graduate education for young and excellent scientists, as it promotes the personal as well as the scientific development of the doctoral candidates. However, the development of the graduate school should not stop at this point, but doctoral candidates as well as the Steering Committee should continue to work together to adapt the current concepts to new needs and future expectations improving BuildMoNa even further.

Dipl.-Phys. Martin Göse

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

BuildMoNa training programme: M, 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 (2013-B1)

21 / 22 March 2013,
written exam, 2 credit points, yearly recurrence, 12 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 (2013-B2)

25 / 26 March 2013,
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 Scientists:
Prof. Dr. H. Harms, Prof. Dr. D. Huster

Lecturers:
Dipl.-Biochem. S. Berndt, Universität Leipzig, Germany; Dr. A. Chatzinotas, UFZ, Leipzig, Germany; Prof. Dr. H. Harms, UFZ, Leipzig, Germany; Dr. Falk Harnisch, UFZ, Leipzig, Germany; Prof. Dr. D. Huster, Universität Leipzig, Germany; M.Sc. Biochem. G. Künze, Universität Leipzig, Germany; Dr. P. Schmidt, Universität Leipzig, Germany

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

Basic concepts in physics (2013-B3)

12 / 14 February 2013,
written exam, 2 credit points, yearly recurrence, 7 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. P. Esquinazi, Prof. Dr. J. Haase, Prof. Dr. W. Janke

Contents:
⇒ Solid-state physics (bonding in solids, crystal structures, classical theory of a harmonic crystal, thermal properties of the crystal lattice, electrons in metals, electrons in a periodic potential)
⇒ Spin physics (magnetic resonance, spin currents)
⇒ Optics (ray optics, nonlinear optics)
⇒ Computer simulations (molecular dynamics, Markov chain Monte Carlo methods)
⇒ Polymer physics (entropic forces, viscoelasticity, polymer dynamics)

Multifunctional scaffolds: Modelling and simulating macromolecules (2013-T2)

20 / 21 June 2013,
written exam, 2 credit points, bi-yearly recurrence with modification, 5 participants

The basic background in modelling and simulating macromolecules was taught to enable the students to use highly dynamic polymer scaffolds as an organising matrix for smart nanoelements and active devices. A particular focus was on methods for bridging the many length and time scales which hamper efficient computer simulations of multifunctional polymer scaffolds.

Responsible Scientists:
Prof. Dr. W. Janke, Prof. Dr. F. Kremer

Lecturers:
Dr. S. Förster, Martin-Luther-Universität Halle-Wittenberg, Germany; Dr. H.-P. Hsu, Universität Mainz, Germany; Prof. Dr. K. Kremer, Max Planck Institute for Polymer Research, Mainz, Germany; Prof. Dr. S. Kumar, Banaras Hindu University, Varanasi, India

Contents:
⇒ General concepts of statistical and polymer physics
⇒ Basic ideas and selected applications of multiscale modelling
⇒ Polymer adsorption
⇒ Experimental deposition techniques
⇒ Polymers under external forces
⇒ Force measurements by optical tweezers
⇒ Bending stiffness effects of semiflexible polymers
⇒ Chain-growth computer simulations (PERM)
⇒ Monte Carlo simulations (generalised ensembles)

Methods:
⇒ Theory and modelling concepts (polymers in confinements and under external forces, stiffness effects)
⇒ Computer simulation methodologies for (semi)flexible polymers (chain-growth algorithms, Monte Carlo methods, scaling theories, etc.)
⇒ Polymer deposition techniques
⇒ Interaction measurements by optical tweezers

Complex nanostructures: Hot nanoparticles (2013-T3)

28 – 30 May 2013,
written exam, 2 credit points, bi-yearly recurrence with modification, 13 participants

The module aimed to provide participants with some understanding of the chemical and physical properties of nanoparticles and nanostructures, such as their synthesis, experimental control, theoretical description, numerical modelling, specific nanoscale effects and interactions, and emerging complexity. The module gave an interdisciplinary perspective covering chemical, physical, experimental and theoretical aspects.

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

Lecturers:
Prof. Dr. E. Bertin, ENS Lyon, France; Prof. Dr. K. Martens, University of Geneva, Switzerland; Dr. S. Sanchez Ordonez, IFW Dresden, Germany; Prof. Dr. G. Volpe, Bilkent University, Ankara, Turkey; Prof. Dr. A. Würger, Université Bordeaux 1, France

Contents:
⇒ Aspects of driven and self-propelled transport of nanoparticles and nanostructures
⇒ Thermal gradients and thermodynamic forces
⇒ (Self-)thermophoresis
⇒ Effective temperatures in driven systems
⇒ Hydrodynamics
⇒ Wet electrostatics

⇒ Topological and geometric effects
⇒ Energy transfer mechanisms and strong light-matter interactions
⇒ The emergence of complexity
⇒ Collective dynamics
⇒ Networks and swarm properties

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

From biomolecules to cells: The good and the bad – Analysis and manipulation of stem and tumour cells (2013-T5)

10 / 11 October 2013,
written exam, 2 credit points, bi-yearly recurrence with modification, 16 participants

This module provided biochemistry, biophysics and molecular biology to manipulate cells and use them as smallest bioreactors. It provided an understanding how the cellular machinery changes when intracellular proteins are changed or molecules are added from the extracellular side, including internalisation, trafficking and cell-specific targeting.

Responsible Scientists:
Prof. Dr. T. Pompe

Lecturers:
Prof. Dr. U. Anderegg, Universität Leipzig, Germany; Prof. Dr. M. Cross, Universität Leipzig, Germany; Prof. Dr. L. Ferreira, Biocant/University of Coimbra, Portugal; F. Krumpfe, JPK Instruments AG, Berlin, Germany; Prof. Dr. C. Mierke, Universität Leipzig, Germany; Prof. Dr. T. Pompe, Universität Leipzig, Germany

Contents:
⇒ Cell compartments and their functions (cytoskeleton, cell membrane, Golgi, endoplasmic reticulum, mitochondria, role in various cell types)
⇒ Biophysical techniques (characterise cells [AFM, optical tweezers], manipulation of cell growth [modulation of substrate stiffness, mechanotransduction], orientation with physical and chemical tools [durotaxis, printing of chemical gradients], application of cell manipulation in biosensor technology)
⇒ Eukaryotic cell culture (expression of proteins, 2D and 3D tissue culture, comparison of primary versus tumour cells, methods to modulate cells recombinantly, genetic modification, transfection methods)
⇒ Signal transduction
⇒ Synthesis and screening of bioactive molecules (tests for agonist/antagonistic compounds, consequences for development of molecules, theoretical methods for molecular pharmacology)

Methods:
⇒ Techniques to characterise cells (microscopy, staining, optical analysis, transfection to create artificial cells with different activities)
⇒ Assays to study biological activity, binding, signal transduction (fluorescence-based methods, radioactive assays, impedance spectrometry)
⇒ Modification of cell substrates (stiffness, nanocontact printing, electronic devices)
⇒ Cell manipulation (AFM, optical and magnetical traps)
⇒ Cell sorting (FACS, magnetic sorting)
⇒ qPCR

Transport and entropy production in soft matter (2013-T7)

6 May – 24 June 2013,
oral exam, 2 credit points, lecture of the Leibniz-Professor in summer term 2013, 7 participants

The main goal of this module was to relate dissipative and irreversible phenomena in soft matter systems to fundamental principles of nonequilibrium thermodynamics. This should provide understanding of various transport phenomena and the underlying physical mechanisms

Responsible Scientists/Lecturers:
Prof. Dr. A. Würger, Université Bordeaux 1, France

Contents:
⇒ Entropy in equilibrium; ideal gas
⇒ Entropy production and dissipation
⇒ Stationary state and mechanical equilibrium
⇒ Massieu functions and thermodynamic forces
⇒ Examples: Gradient diffusion; sedimentation; electrophoresis
⇒ Thermal forces on molecules
⇒ Thermal forces on micron-size colloids
⇒ The role of enthalpy

Chemical biology and biophysics of cancer: Novel developments of anticancer therapeutics (2013-A2)

17 / 18 September 2013,
written exam, 2 credit points, yearly recurrence with modification, 23 participants

Molecular biology shows the complexity and ambiguity that arises from the variability of tumours. Nevertheless, some biochemical and biophysical changes are universal to solid tumour progression and may provide both, novel diagnostic as well as therapeutic concepts. The state of the art in diagnostics and therapeutics were discussed to identify the current needs.

Responsible Scientists:
Prof. Dr. A.G. Beck-Sickinger

Lecturers:
Prof. Dr. A.G. Beck-Sickinger, Universität Leipzig, Germany; PD Dr. U. Hacker, Universitätsklinikum Leipzig, Germany; Dr. M. Heroult, Bayer AG Berlin, Germany; Dr. D. Kosel, Ontochem Halle, Germany; Dr. H.-G. Lerchen, Bayer AG Wuppertal, Germany; Prof. Dr. T. Pompe, Universität Leipzig, Germany; Dr. B. Riedl, Bayer AG Wuppertal, Germany

Contents:
⇒ Tumour progression (tumour growth and homeostasis, uncontrolled proliferation, invasion and metastasis, tumour induced alterations of the stroma, vascular system and immune system, role of chemical cues as well as active and passive forces in triggering cell division and apoptosis)
⇒ Therapy (surgery, radiation, chemotherapy [antineoplastic drugs, cytostatic molecules, protein kinase inhibitors])
⇒ Targeted tumour therapy (specific and unspecific shuttles, specific expression of cell surface proteins, internalisation of biomolecules into tumour cells, linkers for controlled release, etc.)
⇒ Development of novel tumour therapeutics, from target identification, to chemistry and biology of tumour models

Methods:
⇒ Biochemistry and biology to identify tumour targets
⇒ Medicinal chemistry methods to make drugs out of bioactive molecules
⇒ Conjugation
⇒ Hybrid molecules

Quantum coherent structures: Quantum structures for energy applications (2013-A3)

30 September / 1 October 2013,
poster presentation, 2 credit points, yearly recurrence with modification, 25 participants

This module treated materials, structures and quantum effects that have relevance for energy transport and energy efficiency. Thermoelectrics convert temperature difference into electrical current and rely on management of electronic and heat transport. Here, phonon scattering should be maximised in order to reduce thermal conductivity. Macroscopic condensates of polaritons can form at room temperature; here phonon scattering should be reduced in order to enhance the coherence time. The module combined lectures of introductory/overview nature and presentations on current research topics.

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

Lecturers:
Dr. Helena Franke, Universität Leipzig, Germany; Dr. Heiko Frenzel, Universität Leipzig, Germany; Prof. Dr. Tero Heikkilä, University of Jyväskylä/Aalto University, Finland; Dr. Jan König, Fraunhofer-Institut für Physikalische Messtechnik, Freiburg i. Br., Germany; Prof. Dr. Oliver Oeckler, Universität Leipzig, Germany; Dr. Gabi Schierning, Universität Duisburg-Essen, Germany; Prof. Dr. Sabine Schlecht, Justus-Liebig-Universität Gießen, Germany; Prof. Dr. Luis Vina, Universidad Autonoma de Madrid, Spain; Prof. Dr. Matthias Vojta, TU Dresden, Germany; Dr. Holger von Wenckstern, Universität Leipzig, Germany

Contents:
⇒ Thermoelectrics
⇒ Oxide electronics
⇒ Superconductivity
⇒ Bose-Einstein(-like) condensates

Methods:
⇒ Electronic transport and thermal measurements
⇒ Device characteristics
⇒ Optical properties

Scientific minisymposium

Smart and Active Assemblies for Catalysis (2013-A1)

23 / 24 September 2013

The fourth BuildMoNa Minisymposium was organised by the research groups of Prof. Dr. E. Hey-Hawkins, Prof. Dr. R. Gläser and Prof. Dr. F.-D. Kopinke.

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

Internationally renowned speakers covered three aspects of the minisymposium: Homogeneous catalysis, heterogeneous catalysis and environmental and biocatalysis. The speakers were:

⇒ Prof. Dr. Anne-Marie Caminade, Laboratoire de Chimie de Coordination du CNRS, Toulouse, France: *Smart Nano-objects for Catalysis: Dendrimeric Catalysts*
⇒ Prof. Dr. Joaquim Faria, University of Porto, Portugal: *Carbon-based Materials as Catalysts for Water Treatment*
⇒ Dr. Robert N. Grass, ETH Zurich, Switzerland: *Smart (Nano)materials Interfacing Biochemistry: Moving Molecules and Tracing Polymers*
⇒ Dr. Peter Hausoul, RWTH Aachen, Germany: *Heterogeneous Catalysis and Renewable Feedstocks – A Combination for the Future*
⇒ Prof. Dr. Harald Horn, Karlsruhe Institute of Technology, Germany: *Sorption of Magnetic Nanoparticles on Biofilm Structures and Identification with MRI*
⇒ Prof. Dr. Petra de Jongh, Utrecht University, The Netherlands: *The Impact of Collective Properties on the Stability of Supported Nanoparticles for Catalytic and Sustainable Energy Applications*
⇒ Prof. Dr. Andrey Karasik, Russian Academy of Sciences, Kazan, Russia: *Novel Phosphino Amino Pyridines for Construction of Biomimetic Catalysts for Hydrogen Economy*
⇒ Prof. Dr. Gregory Lowry, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA: *Optimizing Fe^0-based in situ Groundwater Remediation Agents*
⇒ Dr. Katrin Mackenzie, Helmholtz Centre for Environmental Research – UFZ, Germany: *Nanomaterials as Adsorbents, Reagents and Catalysts for Water Treatment*
⇒ Prof. Dr. Vera Meynen, University of Antwerp, Belgium: *Controlled Synthesis of Multimodal Materials, Creating Designed Materials Properties for Catalysis*
⇒ Prof. Dr. Russell Morris, University of St Andrews, UK: *Manipulating Zeolites and MOFs for Application*
⇒ Prof. Dr. Martin Muhler, Ruhr-Universität Bochum, Germany: *Carbon Nanotubes – Synthesis, Functionalisation, and Applications in Heterogeneous Catalysis*
⇒ Prof. Dr. Martin Schröder, University of Nottingham, UK: *Porous Metal-Organic Materials for Gas Storage and Selectivity*
⇒ Dr. Jennifer Strunk, Ruhr-Universität Bochum, Germany: *Transition Metal Oxides in Mesoporous Silica: Structural Characterisation, Adsorption and Photocatalysis*
⇒ Ass. Prof. Jarl Ivar van der Vlugt, University of Amsterdam, The Netherlands: *Design of Reactive Ligands for Cooperative Activation of Small Molecules*
⇒ Prof. Dr. Dieter Vogt, University of Edinburgh, UK: *Building Catalysts with Molecules and Nano-objects – From Molecules to Processes*
⇒ Prof. Dr. Paul Wright, University of St Andrews, UK: *Designed Synthesis, Adsorption and Catalytic Performance of Structurally Flexible MOFs and Zeolites*

Additionally, postdoctoral and doctoral researchers presented their scientific results in a poster session and in short talks. The best short talk and the best poster were honoured with prizes. M.Sc. Chem. Paul Neumann (Institute of Inorganic Chemistry) received the prize for his talk on “Dendritic ferrocenyl phosphanes in redox-switchable catalysis”. The prize for the best poster was awarded to M.Sc. Chem. Nicole Wilde (Institute of Chemical Technology) for her poster “Epoxidation of biodiesel with H_2O_2 over hierarchically structured TS-1 catalysts prepared by desilication and transformation”.

⇐ Paul Neumann and Nicole Wilde, the winners of the award for the best short talk and the best poster, respectively

Transferable skills workshops

Presentation workshop

Dr. Frank Lorenz, Rhetoric Excellence,
26 February / 7 March 2013 in combination with the Annual BuildMoNa Conference,
10 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.

C++ programming

PD Dr. habil Rainer Pickenhain,
14–16 May 2013, 17 participants

Contents:
⇒ Introduction to Visual C++ 2008
⇒ C++: data types, operators, job control, functions, arrays, structures, pointers and references, memory management, classes, inheritance
⇒ .Net Framework: Programming: C++/CLI, managed code, libraries; Introduction to Windows Forms: project templates, user interface of Windows, event handling, dialog boxes, graphics, threads

The doctoral degree as a project: Managing complex research projects

Uni support,
3 / 4 June 2013, in cooperation with the Research Academy Leipzig, 10 participants

This workshop is designed for PhD students who face the task of independently structuring and implementing their research project while often at the same time teaching and managing administrative tasks. This workshop offered learning opportunities on:
⇒ Gaining methodological knowledge about professional processes of project planning and implementation
⇒ Getting to know the basics of project management in the specific context of academic research and in different disciplinary cultures
⇒ Focusing as well on the bottom-up-perspective, i.e. on the organisation and management of day-to-day jobs and tasks
⇒ Identifying under what conditions working best
⇒ Learning effective methods of setting priorities and guidelines for handling tasks
⇒ Taking a look at the framework conditions of academic works in terms of both personal and outside influences

Career planning for PhD students: Application standards – personal strategies

Golin Wissenschaftsmanagement,
25 / 26 November 2013, in cooperation with the Research Academy Leipzig, 11 participants

An occupation in research and teaching, a career in the economic or service sector or in a nonprofitorganisation – after the doctorate there are numerous career paths open. Because of this, strategic career planning is necessary. A series of important questions has to be answered: What are my goals and interests, what are my strengths and weaknesses? Where can I apply? Do I know what is expected of me and how to deal with that?

On the basis of these questions the current application standards were conveyed and individual application strategies were worked out. With the help of selected examples from practice, the participants developed the competencies needed for a successful approach to the application process.

Colloquia

⇒ Prof. Dr. Frank Uhlig, Technische Universität Graz, Austria:
Organosilanes and -stannanes – old building blocks for novel materials?
19 June 2013, Faculty of Chemistry and Mineralogy

Annual BuildMoNa Conference

The first annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held on 4 and 5 March 2013 at the Helmholtz Centre for Environmental Research (UFZ) and at the Faculty of Chemistry and Mineralogy. On the first day, renowned guest speakers from science gave talks on current topics of BuildMoNa.

Invited speakers were:

⇒ Prof. Dr. Katharina Al-Shamery, Carl von Ossietzky Universität Oldenburg, Germany:
Ultrafast processes at nanostructured surfaces
⇒ Prof. Dr. Jörg Matysik, Universität Leipzig, Germany:
Towards mesoscopic organisation in biological systems
⇒ Prof. Dr. Felix Otto, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany:
Domain and wall pattern in thin-film ferromagnets
⇒ Prof. Dr. Jörg Wrachtrup, Universität Stuttgart, Germany:
Hybrid quantum systems from molecules, defects and plasmons

⇐ Participants of the Annual BuildMoNa Conference

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

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

Lars Baumann (Institute of Biochemistry) received the first prize for his publications:

A Novel, Biased-like SDF-1 Derivative Acts Synergistically with starPEG-based Heparin Hydrogels and Improves eEPC Migration in vitro
L. Baumann et al. / J. Control. Release (2012) **162** 68
and
Preparation of C-terminally Modified Chemokines by Expressed Protein Ligation
L. Baumann et al. / Methods Mol. Biol. (2013) **1047** 103

Helena Franke (Institute for Experimental Physics II) received the second prize for the detection of the ballistic propagation of a Bose–Einstein condensate, published in:

Ballistic Propagation of Exciton-Polariton Condensates in a ZnO-based Microcavity
H. Franke et al. / New J. Phys. (2012) **14** 013037

Jörg Lincke (Institute of Inorganic Chemistry) was awarded the third prize for his work on Metal-Organic Frameworks (MOFs), which led to the following publications:

A Novel Zn_4O-based Triazolyl Benzoate MOF: Synthesis, Crystal Structure, Adsorption Properties and Solid State ^{13}C NMR Investigations
J. Lincke et al. / Dalton Trans. (2012) **41** 817
and
An Isomorphous Series of Cubic, Copper Based Triazolyl Isophthalate MOFs: Linker Substitution and Adsorption Properties
J. Lincke et al. / Inorg. Chem. (2012) **51** 7579

⇑ Winners of the BuildMoNa Awards 2013: Lars Baumann, Helena Franke, Jörg Lincke (right)

On the second day, 18 doctoral candidates presented their scientific results with short talks. Presentations covered the whole research profile of the graduate school: Development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. Mechanisms of material formation from building blocks, e.g. self-organisation, were also included.

For the 10 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 Mareen Pagel for her presentation “Orthogonal click chemistry to synthesize a multifunctional peptide that promotes cell adhesion”, the second to Paul Neumann for his presentation “Switchable dendritic ferrocenyl phosphines” and the third to Martin Treffkorn for “Interference in single quantum point contacts”.

⇑ Winners of the presentation awards at the Annual BuildMoNa Conference: Mareen Pagel, Paul Neumann (right) and Martin Treffkorn

Childcare

Flexible childcare services at BuildMoNa

Within the graduate school, childcare is guaranteed at times which are not covered by usual childcare institutions, such as municipal children education institutions or child minders of the Research Academy Leipzig. This service enables parents to take part in the training programme of the graduate school and to avoid an excessive extension of the graduation time. For this flexible childcare service at BuildMoNa, Ms. Christina Kny is employed as child minder and teacher.

Funding of doctoral candidates

DFG

WR WISSENSCHAFTSRAT

Europa fördert Sachsen.
ESF Europäischer Sozialfonds

Bundesministerium für Bildung und Forschung

Freistaat Sachsen

Europa fördert Sachsen.
EFRE Europäischer Fonds für regionale Entwicklung

GIPIO

SFB TR 102

Funktionalität Oxidischer Grenzflächen SFB 762

Marie Curie Fellowships

Studienstiftung des deutschen Volkes

Konrad Adenauer Stiftung

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