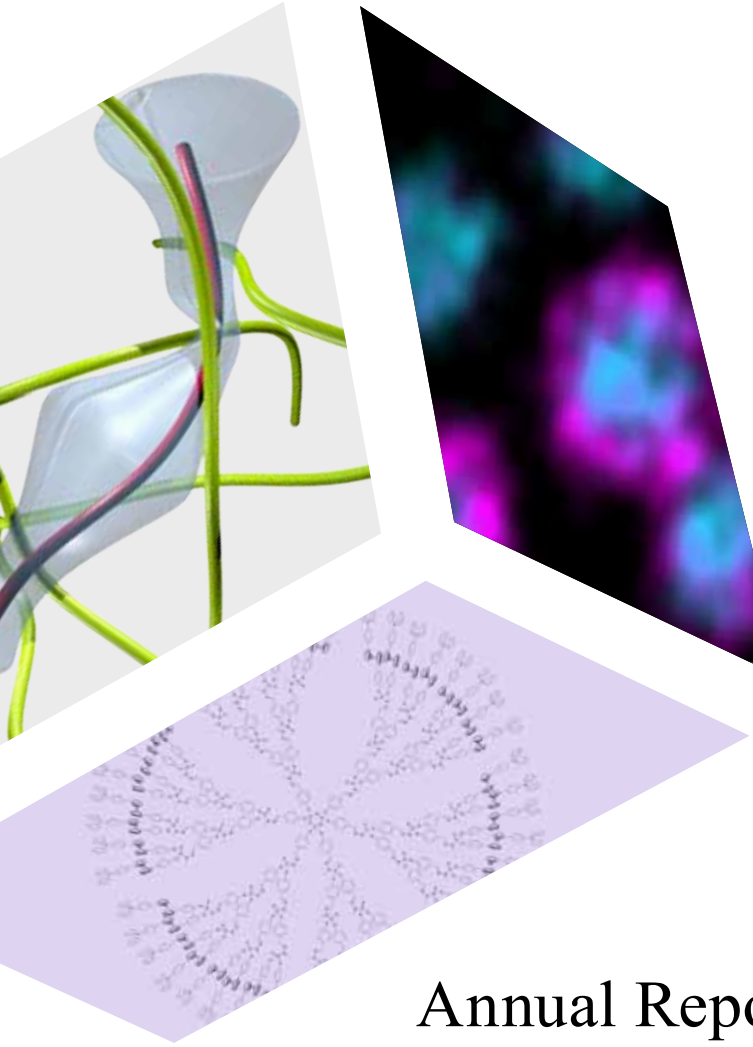
UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2012

Cover image:
⇒ *Left:* Test polymer (red) in a network, sterically confined to a tube-like cage (blue) by its impenetrable neighbour filaments
⇒ *Right:* Cu/Ni core shell nanoparticles
⇒ *Bottom:* Redox-active ferrocenyl-substituted dendrimer

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Leipzig school of natural sciences – the fifth 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 2012, 103 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 54 young scientists have already finished their doctoral studies. In 2012, 15 doctoral candidates were awarded a BuildMoNa scholarship, and 77 doctoral candidates were funded by third-party grants. Additionally, 21 doctoral candidates were funded by ESF (European Social Fund) doctoral positions, and 13 doctoral as well as two postdoctoral researchers were involved in two ESF-funded young researchers groups affiliated with the graduate school.

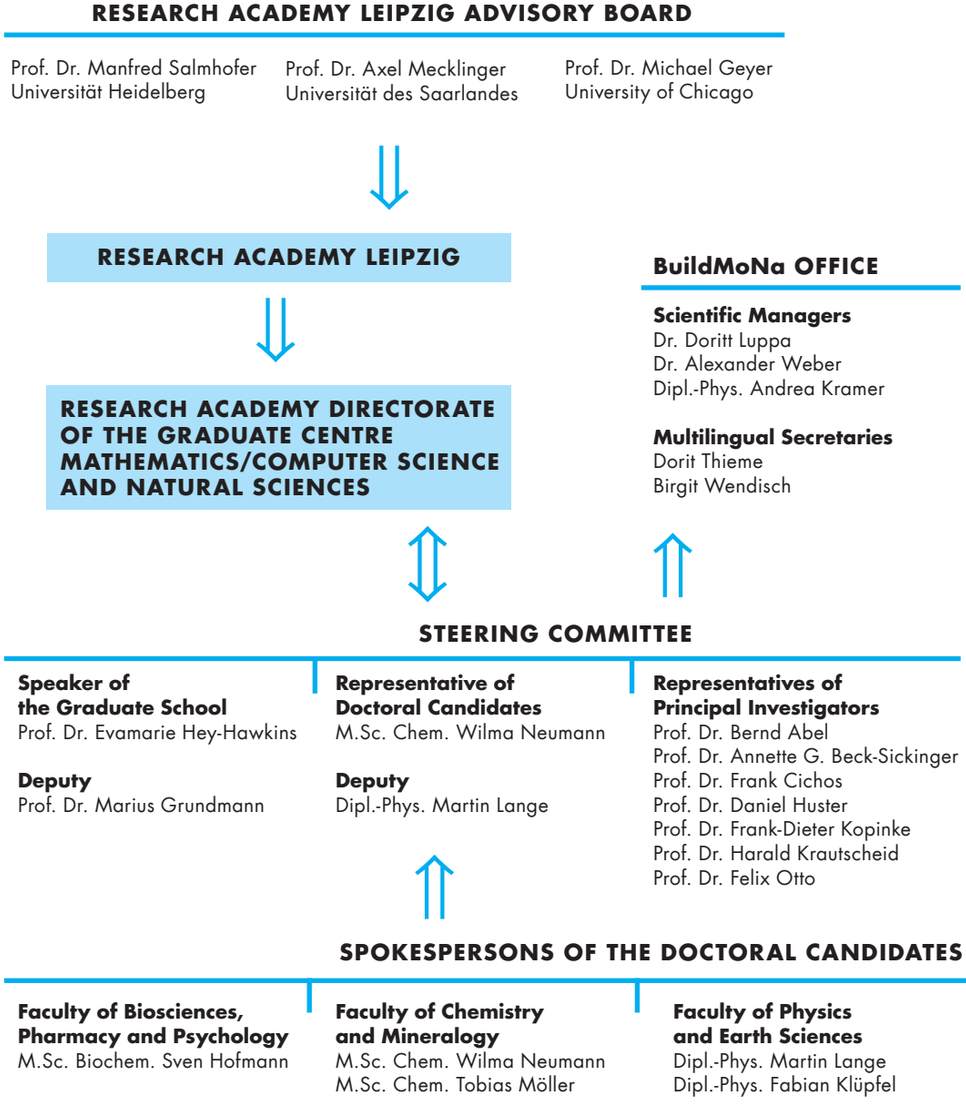
The graduate school provides a well-structured training programme including multi-disciplinary scientific training and a transferable skills programme in cooperation with the Research Academy Leipzig. As part of the further development of the graduate school, the scientific training programme was revised. Besides thematic training modules, introductory modules are now offered to bridge interdisciplinary gaps. Furthermore, three advanced modules linked to ongoing research and technological applications are included, and each year one of them is planned to be the topic of an international minisymposium. In 2012, the minisymposium "Quantum Coherence in Nanostructures" was organised by Prof. Marius Grundmann and Prof. Bernd Rosenow. The minisymposium dealt with macroscopic coherent quantum states such as superfluids, superconductors and Bose–Einstein condensates, which hold great promise for applications such as frictionless, dissipationless transport and ultralow-threshold lasers if brought to room temperature. It also discussed the role of spins and light–matter interactions in nanoscience.

Science-related events organised by BuildMoNa included the 5th BuildMoNa Symposium and the 5th BuildMoNa Workshop for doctoral researchers. These events especially provide a platform for interdisciplinary exchange and discussion within the graduate school.

The renewal proposal of the graduate school played a central role in 2012. Although BuildMoNa will no longer be funded by the DFG within the German Excellence Initiative, the reviewers of the DFG strongly suggested continuing the started developments. BuildMoNa will therefore be continued as a class at the Research Academy Leipzig until 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 Wilma Neumann 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 two professional scientific managers (two half-time positions) 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
Dipl.-Biochem. Verena Ahrens	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Modified peptides for biotechnology*
M.Sc. Phys. Uta Allenstein	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	*Dynamic mechanical cell manipulation and characterisation using magnetostrain*
Dipl.-Phys. 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*
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. 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*
M.Sc. Chem. Murali Dama	Prof. Dr. S. Berger / Prof. Dr. J. Haase	*Organo gels as an alignment media for RDC measurements*
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*
B.Sc. Chem. Jorge Luis Cholula Díaz	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmann	*Properties of novel precursor based materials*
M.Sc. Chem. Sylvia Els-Heindl	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Gastrointestinal peptides related to obesity*
M.Sc. Phys. Gianmaria Falasco	Prof. Dr. K. Kroy / Prof. Dr. F. Cichos	*Non-equilibrium dynamics of heated and self-propelled nanoparticles*
Dipl.-Phys. Niklas Fricke	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	*Polymer conformations in disordered environments*
M.Sc. Chem. Dirk Friedrich	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmannn	*Synthesis, characterisation and deposition of CIGS precursors*
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*
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. Matthias Golecki	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Encapsulation of catalytically active metal complexes*
Dipl.-Phys. Anja Graumann	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*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Anne Grundmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis and reactivity of transition metal phosphinidene complexes*
M.Sc. Chem. Sina Gruschinski	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Transition metal complexes with spin-crossover properties*
M.Sc. Phys. Markus Gyger	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Active and passive biomechanical measurements for characterisation and stimulation of biological cells*
Dipl.-Phys. Chris Händel	Prof. Dr. J. Käs / Prof. Dr. B. Abel	*Chemical oscillations in cell membranes*
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*Principles of mechanosensitivity and durotaxis in mammalian cells*
M.Sc. Chem. Marcel Handke	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	*Networks based on 4d and 5d-metal ions as possible catalysts*
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*
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*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
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. Chem. 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*
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*
Dipl.-Chem. Jochen Lach	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Thin films of redox-active high-spin molecules*
Dipl.-Phys. Marc Lämmel	Prof. Dr. K. Kroy / Prof. Dr. W. Janke	*Stiff biopolymer solutions and networks*
Dipl.-Phys. Michael Lorenz	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	*Investigations on the stability of zinc oxide based metal-semi-conductor field-effect-transistors*
M.Sc. Phys. Chem. Yanhong Ma	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	*Magnetic shape memory alloys for miniaturised actuators*
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. 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*
Dipl.-Phys. Nils Neubauer	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	*Photothermal fluctuation spectroscopy on gold nanoparticle dimers*
Dipl.-Phys. Lena Neumann	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Hyperthermal ion assisted atomic assembly*
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*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. K. David Nnetu	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The use of biomechanics to reduce metastatic aggressiveness*
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*
M.Sc. Chem. Julian Rodger Frederic Pritzwald-Stegmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	*Phosphorus-based organometallic/ inorganic hybrid materials*
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. 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*
M.Sc. Chem. Anastacia Romanova	Prof. Dr. W. Hackbusch / Prof. Dr. M. Grundmann	*Molecular simulations of ion effects on structural and thermodynamical properties of biopolymers*
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*
Dipl.-Phys. Florian Schmidt	Prof. Dr. M. Grundmann / Prof. Dr. R. Gläser	*Characterisation of defects in hetero- and nanostructures*
Dipl.-Phys. Jörg Schnauß	Prof. Dr. J. Käs / Prof. Dr. A.G. Beck-Sickinger	*Biomimetic actin networks*
Dipl.-Phys. Sebastian Schöbl	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	*Modelling and computer simulations of molecular pattern recognition*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Biolog. 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*
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*
Dipl.-Biochem. Max Steinhagen	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	*Enzyme analytics*
Dipl.-Biochem. Anja Steude	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	*Development and fabrication of novel peptide based biosensors for neuronal diagnostic tools*
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*
M.Sc. Chem. Markus Streitberger	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Building catalytically active bimetallic nano-frames with flexible bisphosphine ligands*
Dipl.-Phys. Sebastian Sturm	Prof. Dr. K. Kroy / Prof. Dr. F. Kremer	*Nonequilibrium dynamics of forced and confined semiflexible polymers*
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*
Dipl.-Phys. Olaf Ueberschär	Prof. Dr. F. Kremer / Prof. Dr. W. Janke	*Investigating stochastic thermodynamics by means of optical tweezers*
M.Sc. Chem. Steve Ullmann	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Extration of rare earths by means of preorganised calixarene*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Carolin Wagner	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Investigation of the interaction of receptors and ligands by optical tweezers*
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 mamma-carcinomas 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*
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. Johannes Zierenberg	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	*Aggregation of polymers in crowded confinement with correlated disorder*

Alumni 2012

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Lars Baumann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	*Structure-activity relation of chemokines*
Dr. rer. nat. Christof Peter Dietrich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Growth and charactisation of ZnO-based microstructures*
Dr. rer. nat. Srujana Dusari	Prof. Dr. P. Esquinazi / Prof. Dr. H. Morgner	*Measurements of the mean free path and spin diffusion length in multigraphene*
Dr. rer. nat. René Frank	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranyl amino acids for applications in BNCT*
Dr. rer. nat. Helena Franke	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Growth and characterisation of UV-microcavities*
Dr. rer. nat. Sina Haas	Prof. Dr. A. Robitzki / Prof. Dr. J. Käs	*Development of a bioforce microarray sensor for measuring cellular biomechanical forces of ischemic cell layers*
Dr. rer. nat. Rayk Hassert	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. M. Grundmann	*Peptides for specific adhesion to hard matters*
Dr. rer. nat. Julia Haushälter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phosphine-baskets – ligands for selective catalysis*
Dr. rer. nat. Florian Huber	Prof. Dr. J. Käs / Prof. Dr. M. Grundmann	*Artificial cell motility*
Dr. rer. nat. Ciprian-Ghiorghita Iacob	Prof. Dr. F. Kremer / Prof. Dr. R. Gläser	*Molecular dynamics of organic materials confined in nano-pores*
Dr. rer. nat. Chinmay Khare	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Glancing angle deposition*
Dr. rer. nat. Alexander Lajn	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	*Fabrication and characterisation of transparent field-effect transistors*
Dr. rer. nat. Martin Lange	Prof. Dr. M. Grundmann / Prof. Dr. W. Cichos	*Growth and characterisation of quantum wire heterostructures*
Dr. rer. nat. Jörg Lincke	Prof. Dr. K. Krautscheid / Prof. Dr. R. Gläser	*Coordination polymers with nitrogen-rich ligands*
Dr. rer. nat. Martyna Madalska	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Immobilised switchable phosphine-based catalysts*
Dr. rer. nat. Benno Meier	Prof. Dr. J. Haase / Prof. Dr. S. Berger	*Ultra-high field magnetic resonance of modern materials*
Dr. rer. nat. Monika Möddel	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	*Modelling and computer simulations of adsorption specifity of synthetic peptides*

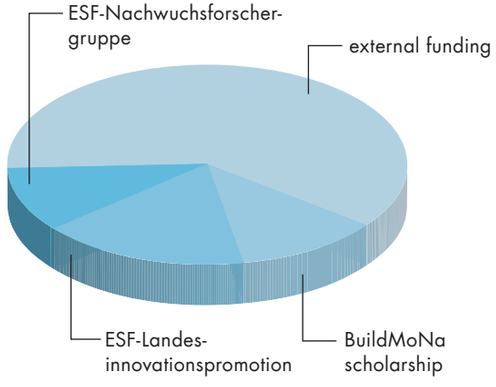
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Alexander Müller	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	*Investigation of carrier dynamics in ZnO films and microcavities*
Dr. rer. nat. Souvik Pandey	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*P-based polymers: synthesis and applications in materials science*
Dr. rer. nat. Daniel Rathmann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	*Structure activity relationships of RF-amide peptide receptors with chemical modified peptides*
Dr. rer. nat. Klara Rusevova	Prof. Dr. F.-D. Kopinke / Prof. Dr. R. Gläser	*Iron-based nanoparticles catalysts for oxidation of pollutants in water*
Dr. rer. nat. Jens Schneider	Prof. Dr. F.-D. Kopinke / Prof. Dr. M. Grundmann	*Studies of dissociation processes of water exposed to high-frequency electromagnetic fields*
Dr. rer. nat. Ksenia Jolanta Surudo	Prof. Dr. F.-D. Kopinke / Prof. Dr. R. Gläser	*Thermodynamic activity versus total concentration of xenobiotics as predictors of bioavailability*
Dr. rer. nat. Jan Zippel	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Magnetic tunnel junctions*

Mini-projects

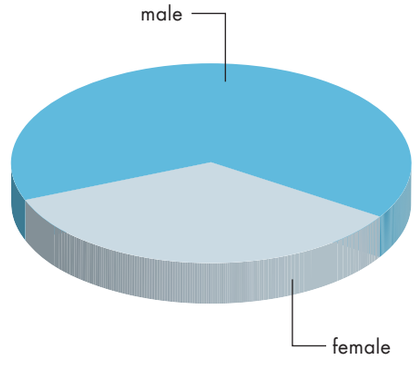
Student name	Doctoral candidate (supervisor)	Topic of mini-project
Rodger John	Dipl.-Phys. Tammo Böntgen	*Calculation of the complex optical response of nanostructured interfaces*

Statistics

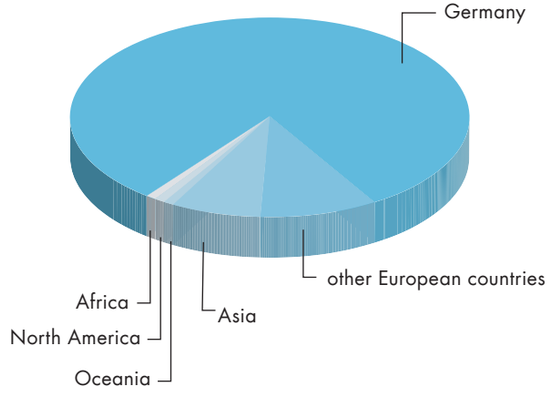
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:



Molecular physical and biophysical chemistry

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

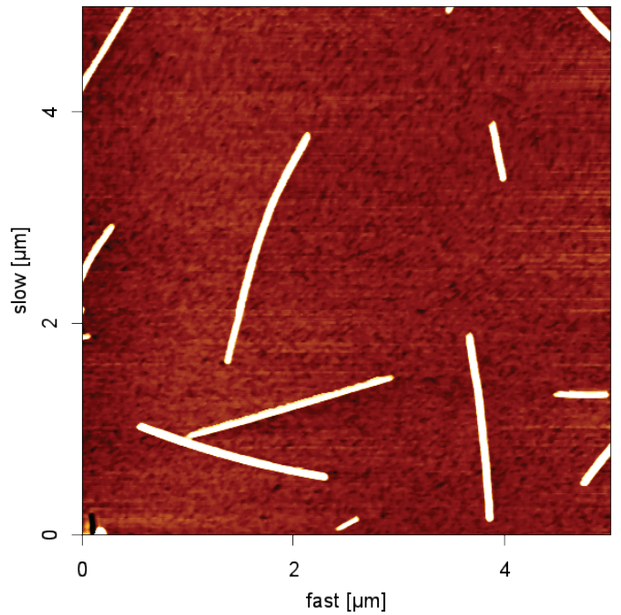
The Abel group works in the fields of molecular physical chemistry and macromolecular chemistry, structure and dynamics with the long term goal of obtaining fundamental knowledge of matter from smaller molecules up to large polymeric systems. Another goal is also to develop new molecular and analytical probes for fundamental research and to develop advanced analytical devices for industry and industrial applications.

Within BuildMoNa we mainly employ nanoscale imaging techniques of molecules and molecular aggregates to monitor nanostructures of aggregated proteins near interfaces of surfaces and nanoparticles.

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.



⇐ Amyloid fibrils of GNNQQNY (fibril forming sequence from Yeast prion protein SUP35)

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Chemical modification of peptides and proteins

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

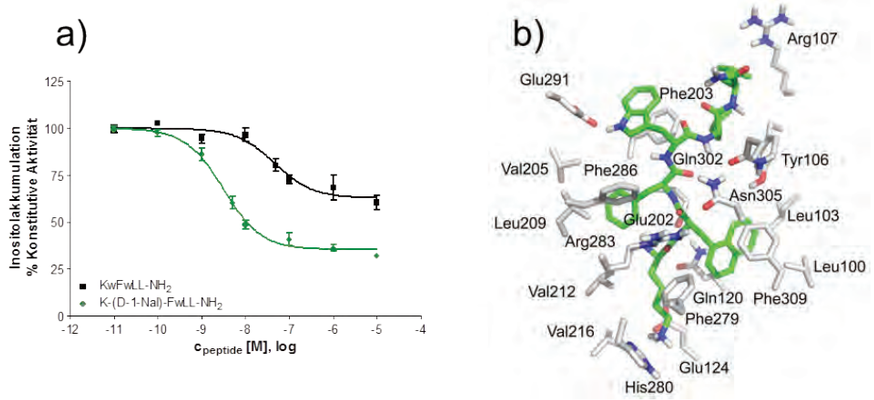
The common aim of the projects includes chemically modified peptides and proteins that are developed to modulate their function. This includes proteins involved in tumour targeting, proteins for nanomedicine or biomaterial development. Peptides are synthesised by solid phase peptide synthesis. Proteins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

Sylvia Els-Heindl (M.Sc. Chem.), Veronika Mäde (M.Sc. Chem.) and Daniel Rathmann (Dipl.-Chem.) synthesise chemically modified peptide hormones that are modified by non-natural amino acids, lipid or polyethylene glycol moieties to improve stability in biological system. They address ghrelin, pancreatic polypeptide, prolactin-releasing peptide and neuropeptide FF, respectively. Significant contributions have been achieved in the field of prolactin-releasing peptide as the molecular mechanism of ligand binding was elucidated. The difference between agonist and antagonist binding was identified by synthetic analogs, mutagenesis and molecular modelling in the field of NPFF-ligand/receptor interactions. Furthermore, Sylvia Els-Heindl developed the most powerful inverse agonist of the ghrelin receptor, which turned out to be a promising candidate to treat metabolic diseaeses. Daniel Rathmann finished his Ph.D. in August 2012.

Sven Hofmann (M.Sc. Biochem.), David Böhme (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.

In the field of chemical modification of proteins Ria Schönauer (Dipl.-Biol.), Cathleen Jendrny (Dipl.-Pharm.) and Lars Baumann (Dipl.-Biochem.) were very successful. They work on adrenomedullin, vaspin and stromal derived factor 1 alpha, cytokines and inhibitors that play a role in the regulation of regeneration diseases and metabolism. Lars Baumann finished his Ph.D. in May 2012.

Mareen Pagel (M.Sc. Chem.), Rayk Hassert (Dipl.-Biochem.) and Max Steinhagen (Dipl.-Biochem.) work on chemically modified peptides and proteins to improve the properties of biomaterials. Rayk Hassert developed high affinity peptides for different surfaces, whereas 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. Rayk Hassert finished his Ph.D. in December 2012.



⇑ a) Inverse activity of one of the most potent inverse agonist K-(D-1-Nal)-FwLL-NH_2 at the human ghrelin receptor b) Molecular modelling yielded the hypothetical conformation of the inverse agonist at the receptor (Els et al. / J. Med. Chem. (2012) **55** 7437)

⇒ *On-resin Synthesis of an Acylated and Fluorescence-labeled Cyclic Integrin Ligand for Modification of Poly(lactic-co-glycolic Acid)*
R. Hassert, P.G. Hoffmeister, M. Pagel, M. Hacker, M. Schulz-Siegmund, A.G. Beck-Sickinger / Chem Biodivers. (2012) **9** 2648

⇒ *Molecular Tools to Characterize Adiponectin Activity*
C. Juhl, A.G. Beck-Sickinger / Vitam. Horm. (2012) **90** 31

⇒ *Biocompatible Silicon Surfaces Through Orthogonal Click Chemistries and a High Affinity Silicon Oxide Binding Peptide*
R. Hassert, M. Pagel, Z. Ming, T. Häupl, B. Abel, K. Braun, M. Wiessler, A.G. Beck-Sickinger / Bioconjug. Chem. (2012) **23** 2129

⇒ *An Aromatic Region to Induce a Switch between Agonism and Inverse Agonism at the Ghrelin Receptor*
S. Els, E. Schild, P.S. Petersen, T.M. Kilian, J. Mokrosinski, T.M. Frimurer, C. Chollet, T.W. Schwartz, B. Holst, A.G. Beck-Sickinger / J. Med. Chem. (2012) **55** 7437

⇒ *Peptides and Peptide Conjugates: Therapeutics on the Upward Path*
V.M. Ahrens, K. Bellmann-Sickert, A.G. Beck-Sickinger / Future Med. Chem. (2012) **4** 1567

⇒ *Ligand-mimicking Receptor Variant Discloses Binding and Activation Mode of Prolactin-releasing Peptide*
D. Rathmann, D. Lindner, S.H. DeLuca, K.W. Kaufmann, J. Meiler, A.G. Beck-Sickinger / J. Biol. Chem. (2012) **287** 32181

⇒ *Selective Mode of Action of Guanidine-containing Non-peptides at Human NPFF Receptors*
M. Findeisen, C. Würker, D. Rathmann, R. Meier, J. Meiler, R. Olsson, A.G. Beck-Sickinger / J. Med. Chem. (2012) **55** 6124

⇒ *A Novel, Biased-like SDF-1 Derivative Acts Synergistically with starPEG-based Heparin Hydrogels and Improves eEPC Migration in vitro*
L. Baumann, S. Prokoph, C. Gabriel, U. Freudenberg, C. Werner, A.G. Beck-Sickinger / J. Control. Release (2012) **162** 68

⇒ *Two Motifs with Different Function Regulate the Anterograde Transport of the Adiponectin Receptor 1*
C. Juhl, D. Kosel, A.G. Beck-Sickinger / Cell. Signal. (2012) **24** 1762

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Polyisocyanides as reagent to observe residual dipolar couplings in NMR

Prof. Dr. Stefan Berger
M.Sc. Chem. Murali Dama

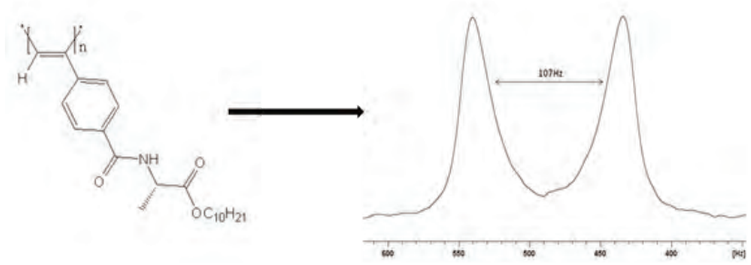
Murali Dama has investigated the alignment possibilities of organic molecules in the strong magnetic field of an NMR spectrometer. If molecules adept to a very small degree a certain orientation with respect to the magnetic field, residual dipolar couplings can be measured. Residual dipolar couplings (RDC's) are an important parameter in organic structure determination. These RDC's are useful in configuration, conformation and constitutional analysis of molecules and support or even replace NOE information due to their r^{-3} dependence. For this alignment one needs an anisotropic medium, which orients itself and hence the dissolved analyte.

The first approach of Murali Dama was to synthesise low molecular weight organogelators (LMOG) with several aromatic rings attached. The hope was that due to the anisotropy of the aromatic rings these systems should orient themselves

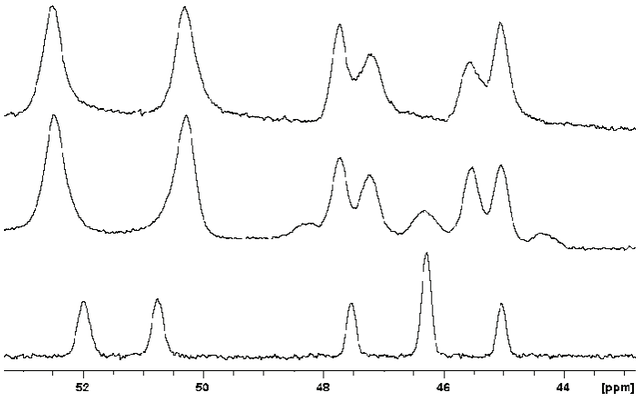
slightly in the NMR spectrometer. However, we had to realise that these LMOG's would not fulfil our wishes.

In a second approach Murali Dama has synthesised new liquid crystal systems such as polyisocyanides Poly-L-1, and indeed, these compounds perform the desired job. This system will even offer the possibility to test the chirality of organic compounds.

In his very recent third approach Murali Dama has synthesised a polyacetylene **1** and could show that this class of molecules is even better suited for our purpose.



⇐ Deuterium quadrupolar splitting of CDCl3 induced by polyacetylene **1**



⇐ Gated decoupled ^{13}C NMR spectra of the two enantiomers of menthol (top) in the presence of **1** and of menthol in $CDCl_3$ only (bottom)

⇒ *Polyisocyanides as a New Alignment Medium to Measure Residual Dipolar Couplings for Small Organic Molecules*
M. Dama, S. Berger / Organic. Letters (2012) **14** 241

⇒ *Polyacetylenes as a New Alignment Medium to Measure Residual Dipolar Couplings for Chiral Organic Molecules*
M. Dama, S. Berger / Tetrahedron Letters (2012) **53** 6439

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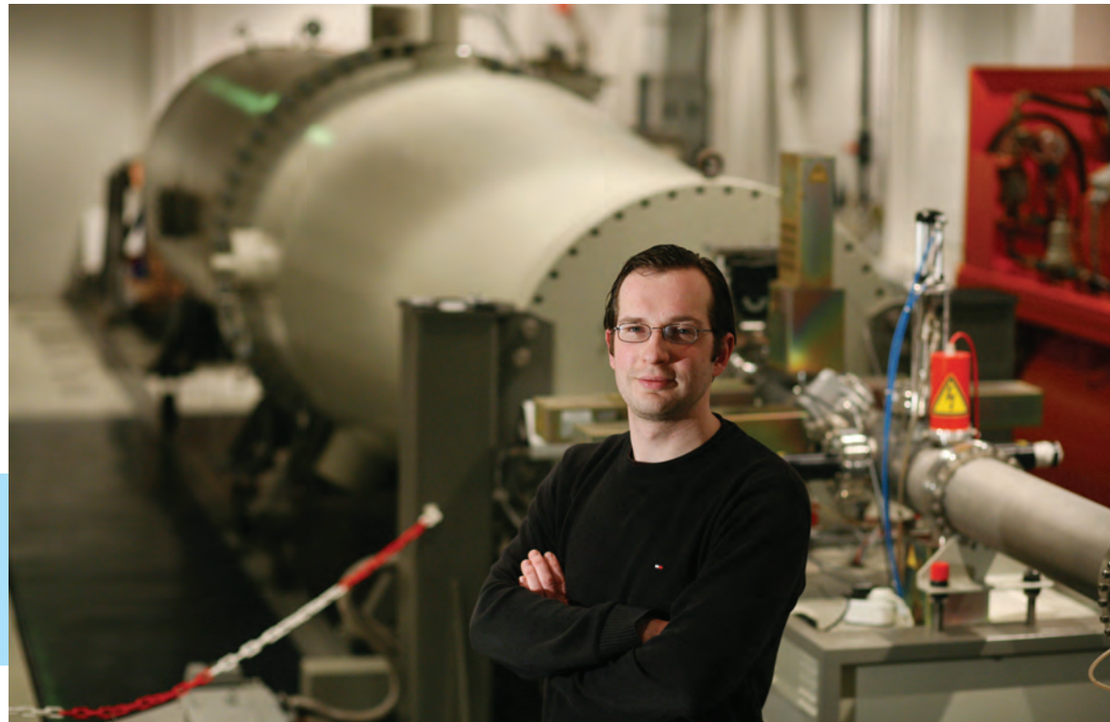
The focused ion beam at LIPSION – a versatile research tool for 2D and 3D analysis, imaging and materials modification

Prof. Dr. Tilman Butz
Dipl.-Phys. Tobias Andrea, Dipl.-Phys. Martin Rothermel

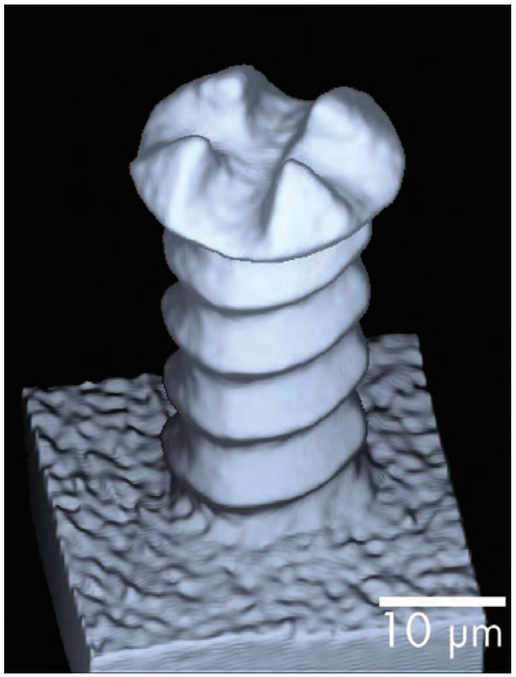
The LIPSION high energy nanoprobe enables BuildMoNa doctoral candidates to pursue a variety of research projects.

The element-sensitive technique of PIXE (particle induced X-ray emission) tomography with submicron resolution has the potential to be widely used for a number of applications. However, long measurement and reconstruction times restrain potential users from making demand of this technique. Martin Rothermel's research thus focuses on enhancing ion beam characteristics and reconstruction software performance. Due to the complex probe-sample-interactions a highly sophisticated



reconstruction algorithm is needed, which is able to accurately model the effects of particle deceleration and X-ray attenuation within the sample.

Tobias Andrea is investigating the potential of ion beam tomography for the three-dimensional characterisation and elemental mapping of single cells and for the creation of 3D micro- and nanostructures. 3D reconstructions of several cell samples could be obtained using limited-angle tomography which combined STIM (scanning transmission ion microscopy) and PIXE. Also, the technique of proton beam sculpting has been developed in which insights from tomography are applied in the field of proton beam writing. Using patterned proton irradiation from multiple angles several PMMA microsculptures have been created which show potential for micromachining applications.



⇐ STIM tomogram of PMMA microscrew created using gray-scale proton beam irradiation from two angles

⇒ *Comment on: "Revealing Common Artifacts due to Ferromagnetic Inclusions in Highly Oriented Pyrolytic Graphite", by M. Sepioni, R.R. Nair, I.-Ling Tsai, A.K. Geim and I.V. Grigorieva*
D. Spemann, M. Rothermel, P. Esquinazi, M. Ramos, Y. Kopelevich, H. Ohldag / EPL (2012) **97** 47001

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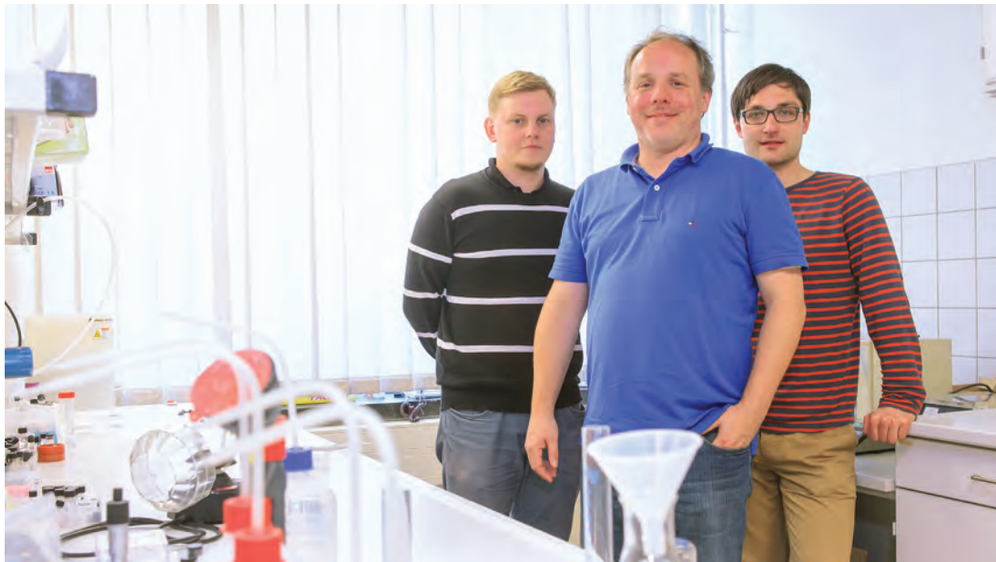
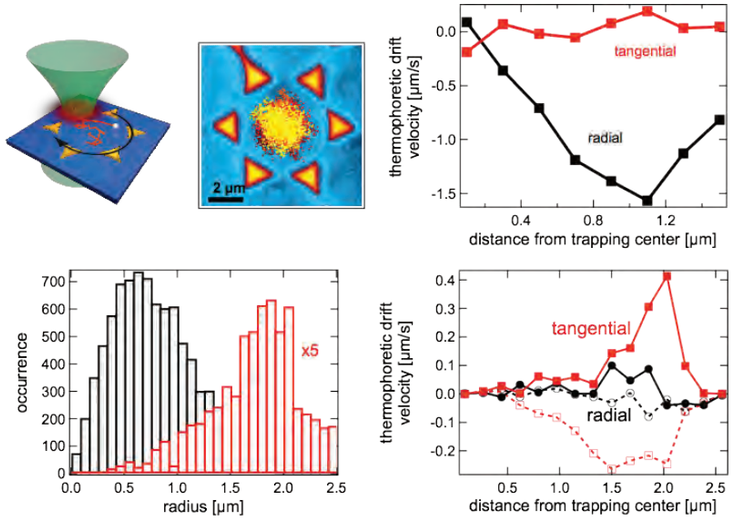
Gold nanostructure assisted thermophoretic trapping of single nano-objects

Prof. Dr. Frank Cichos
Dipl.-Phys. Marco Braun, Dipl.-Phys. Nils Neubauer

The manipulation and trapping of nano-objects that undergo Brownian motion are of great interest in soft-matter sciences. Optical tweezing is the most common technique for the trapping of individual particles in solution and is based on the optical gradient force. Hence, a sufficiently high polarisability of the particle in the solution is required. While it is thus easy to trap single dielectric particles larger than 100 nm, a trapping of smaller objects such as single molecules by means of optical tweezers can hardly be realised. Molecular trapping can be achieved by a technique called Anti-Brownian Electro-kinetic trap (ABEL trap), which exploits the feedback controlled electric field of four electrodes. The latter technique requires electrical contacts, which introduce difficulties when fabricating multiple traps. The molecular nanophotonics group has developed an all-optical technique which replaces the electric fields by highly localised thermal fields. The so-called thermophoretic trap exploits thermophoretic forces that act on a particle placed in a temperature gradient, which e.g. locally distorts the screening of the surface charges and by that induce a particle drift. In our approach the temperature field is gener-



ated by an optically heated gold nanostructures on a substrate surface. Due to the small dimensions of the heat sources, even a small temperature increase introduces large temperature gradients causing a strong thermophoretic drift by which the motion of a diffusing particle can by manipulated. Our experiments demonstrate that single polymer particles with a diameter below 100 nm can be trapped with modest temperature increases at the gold nanostructure. The trapping can be carried out by static or dynamic temperature fields. The latter one introduces even the possibility to control the motion of the particles in the trap. The obtained results reveal that in current experiments only the temperature gradients and no other thermoosmotic flows are responsible for the trapping. Thus, the trapping efficiency scales with the Soret coefficient characterising the thermodiffusive mobility. As our approach is relying on a very easily created periodic gold nanostructure, the system can be scaled up to a nanofluidic manipulation scheme, which is capable of trapping and moving single nano-objects.



⇑ (left) Principle of the thermophoretic trap with a gold nanostructure created by colloidal lithography. (right) Trajectory of a single polymer particle (100 nm diameter) in the trap

⇒ *Nanolens Diffraction around a Single Heated Nanoparticle*
M. Selmke, M. Braun, F. Cichos / Optics Express (2012) **7** 8055

⇒ *Gaussian Beam Photothermal Single Particle Microscopy*
M. Selmke, M. Braun, F. Cichos / JOSA A (2012) **29** 2237

⇒ *Photothermal Microscopy: Detection of a Nanolens*
M. Selmke, M. Braun, F. Cichos / ACS Nano (2012) **6** 2741

⇒ *Twin-Focus Photothermal Correlation Spectroscopy*
M. Selmke, R. Schachoff, M. Braun, F. Cichos / RSC Advances (2012) **3** 394

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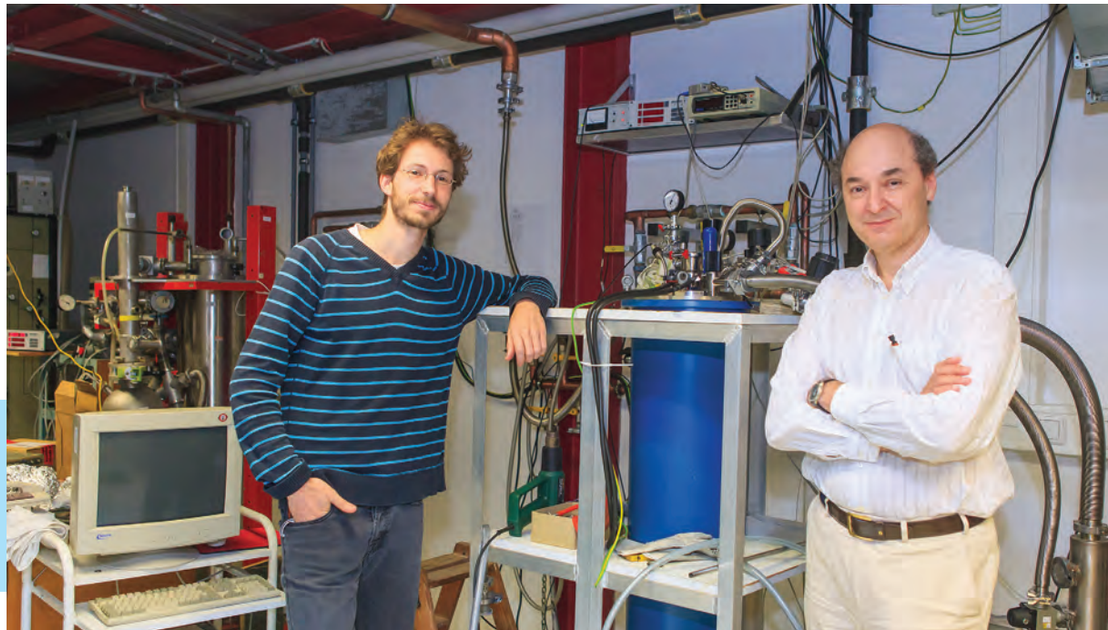
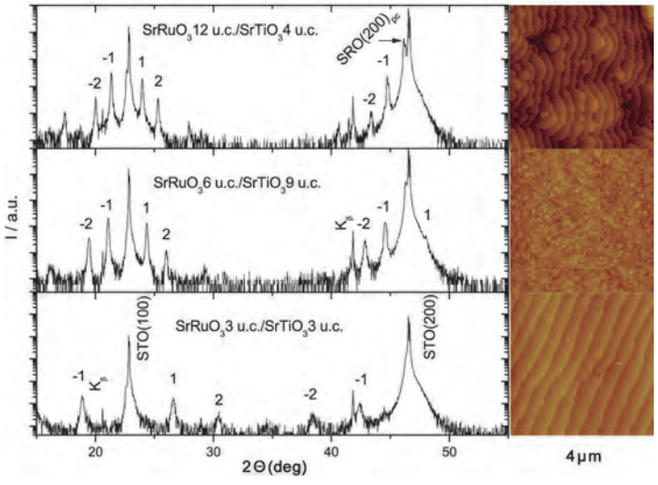
Emergent phenomena at oxide interfaces: magnetic and electronic properties

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

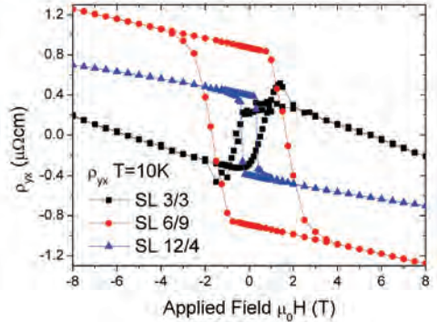
Good epitaxial growth characteristics make oxide heterostructures of the perovskite family a model system for the study of emerging phenomena at interfaces. Superlattices (SL) of oxides with a variety of electronic (isolating, half metal, metallic) and magnetic (dia-, para-, and ferromagnetic) properties have been grown by pulsed laser deposition.

Transport measurements on a rotatable stage in magnetic fields up to 8T provide further insights. Symmetries in magnetotransport reveal structural information for layers to thin to be probed by the aforementioned techniques. Special attention is dedicated to the study of the normal and anomalous Hall effect (AHE). While $SrRuO_3$ single layers as thin as three unit cells and SL with individual layer thicknesses above 4 unit cells show an AHE similar to the bulk and a temperature independent high field Hall slope, the ultrathin SL shows a temperature dependence in the high field Hall slope and opposite sign in the AHE.





⇐ X-Ray Diffraction data (left) and Atomic Force Microscopy (right) images of three $SrRuO_3/SrTiO_3$ superlattices. The satellite peaks in the XRD-patterns confirm smooth interfaces and homogeneous thicknesses of the 15 stacked bilayers. The absence of a clear terrace structure in the surface morphology of the second AFM image indicate a different growth mechanism for SL 6/9.



⇐ Off-diagonal resistivity vs. applied magnetic field at 10 K for the three $SrRuO_3/SrTiO_3$ superlattices. In the thinnest SL (3/3) the non-linear (anomalous) contribution is reversed in sign indicating changes in the electronic structure.

⇒ *An Alternative Route towards Micro- and Nano-patterning of Oxide Films*
G. Bridoux, J. Barzola-Quiquia, F. Bern, W. Böhlmann, I. Vrejoiu, M. Ziese, P Esquinazi / Nanotechnology (2012) **23** 085302

⇒ *Can Doping Graphite Trigger Room Temperature Superconductivity? Evidence for Granular High-Temperature Superconductivity in Water-Treated Graphite Powder*
T. Scheike, W. Böhlmann, P. Esquinazi, J. Barzola-Quiquia, A. Ballestar, A. Setzer / Advanced Materials (2012) **24** 5826

⇒ *Stabilization of Ferromagnetic Order in $La_{0.7}Sr_{0.3}MnO_3$–$SrRuO_3$ Superlattices*
M. Ziese, F. Bern, E. Pippel, D. Hesse, I. Vrejoiu / Nano Letters (2012) **12** 4276

⇒ *Revealing the Origin of the Vertical Hysteresis Loop Shifts in an Exchange biased Co/YMnO3 Bilayer*
J. Barzola-Quiquia, A. Lessig, A. Ballestar, C. Zandalazini, G. Bridoux, F. Bern, P. Esquinazi / Journal of Physics: Condensed Matter (2012) **24** 366006

⇒ *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

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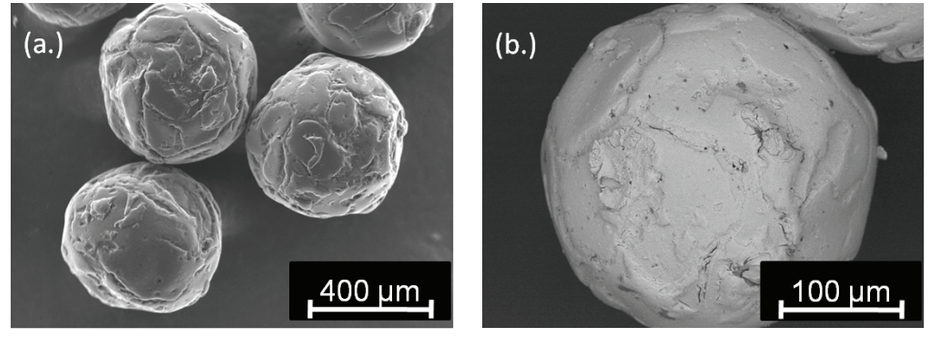
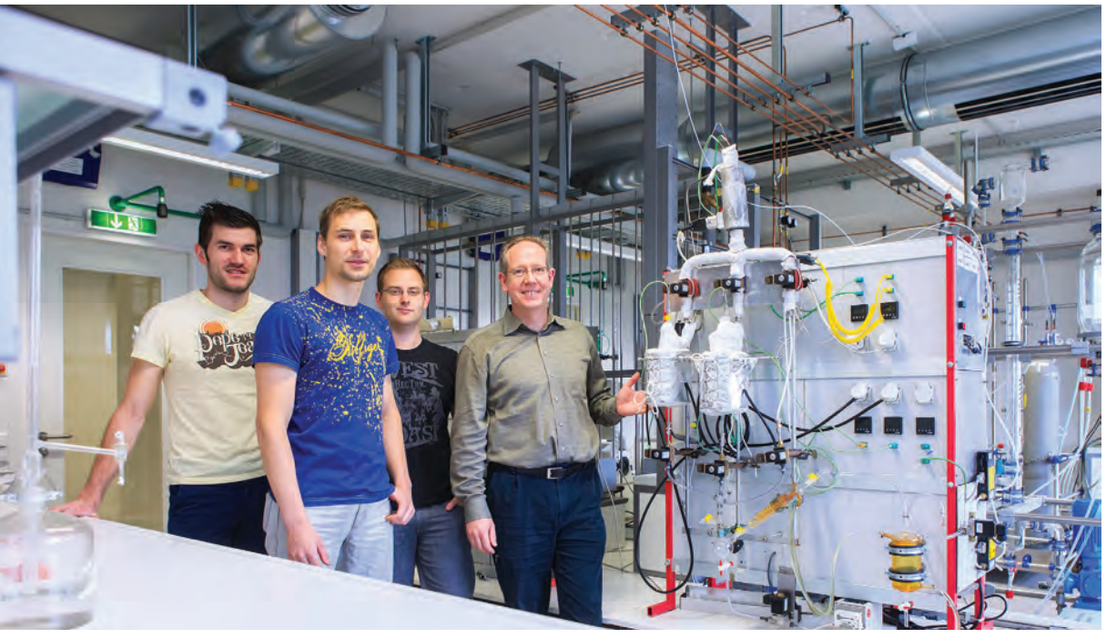
Building complex nanomaterials for applied catalysis

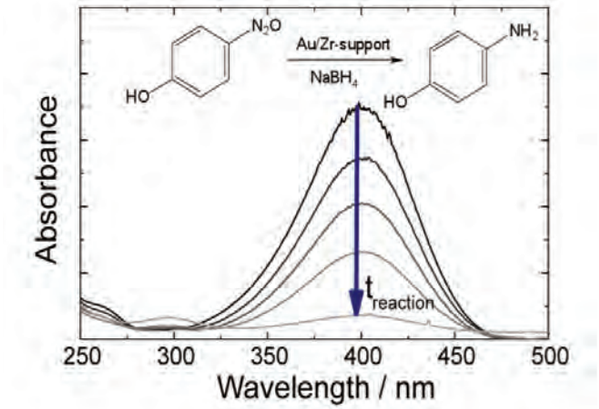
Prof. Dr. Roger Gläser
M.Sc. Chem. Thomas Heinze, M.Sc. Chem. Michael Marx, M.Sc. Chem. Dennis Richter, M.Sc. Chem. Patrick With

Heterogeneously catalysed reactions are not only at the heart of producing most chemicals and materials, but also play a central role in energy applications. Our research combines the design of nanoporous materials with defined porosity and function with the application in applied catalysis. Thus, we follow the principles of the graduate school by using templating strategies and scaffolding approaches to synthesise novel materials for the use as catalyst and catalyst supports. For instance, supercritical fluid reactive deposition of metals by reduction of complexes dissolved in supercritical carbon dioxide represents an innovative approach for catalyst preparation. Another approach is the covalent bonding of Ionic Liquid-functionalities on SiO_2-based nanoporous supports. Highly selective oxidation catalyst can be obtained by exchanging the anion of the ionic liquid with ruthenium or manganese containing species. Furthermore, we investigate applications in environmental catalysis such as selective catalytic reduction of nitrogen oxides by catalysts transport-optimised pore systems. Also, energy-related catalysis such as high-temperature conversions or photocatalysed water splitting for hydrogen production play an important role. One example are porous carbon nitrides modified with different sensitisers to enhance the harvest of solar energy and, thus, enlarge their activity for the hydrogen formation in the overall water splitting with visible light.



⇑ Carbon sphere used as an exotemplate (a.) for the preparation of zirconia, ceria, vanadia or titania spheres with hierarchically structured pore systems (b.) as porous support for Au-catalyst from supercritical fluid reactive desposition





⇐ Schematic UV-Vis spectra during the catalytic reduction of p-nitrophenol to p-aminophenol over Au-catalysts using $NaBH_4$

⇒ *Poröse Materialien auf Basis von metallischen Mischoxiden sowie deren Herstellung und Verwendung*
R. Gläser, M. Lutecki, P. With, A. Heinrich, S. Fichtner, B. Böhringer, Blücher GmbH, Universität Leipzig / Offenlegungsschrift DE 10 2012 011 764 A1, 20 December 2012

⇒ *Poröse Materialien auf Basis von Oxiden des Titans und/oder des Vanadiums sowie deren Herstellung und Verwendung*
R. Gläser, M. Lutecki, P. With, A. Heinrich, S. Fichtner, B. Böhringer, Blücher GmbH, Universität Leipzig / Offenlegungsschrift DE 10 2012 011 778 A1 20. December 2012

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Quantum optics and round corners in Leipzig

Prof. Dr. Marius Grundmann
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The “Runde Ecke” is an (in)famous landmark in the city of Leipzig, back in GDR times home of the Stasi (state security) headquarter, now a museum. As it turns out round corners are also important to explain the properties of wire-shaped resonators, building blocks for miniature lasers. Typical zinc oxide microwire resonators exhibit the shape of a prism with hexagonal cross-section, deviating from an ideal geometry in two aspects: surface roughness and a finite curvature radius of several hundred nanometers of the 60° corners. Both effects lead to a reduction of cavity quality. Using optimised microwires from a carbothermal evaporation process, zinc oxide cavities with atomically smooth side facets and sharp corners (radius smaller than ten nm) have been fabricated. The initial demonstration that whispering gallery modes (WGM) entertain lasing in such structures was reported from our BuildMoNa team in 2008 for optical pumping at low temperatures (about 10 K) (C. Czekalla et al. / Appl. Phys. Lett. (2008) **92** 241102). The latest, improved cavities

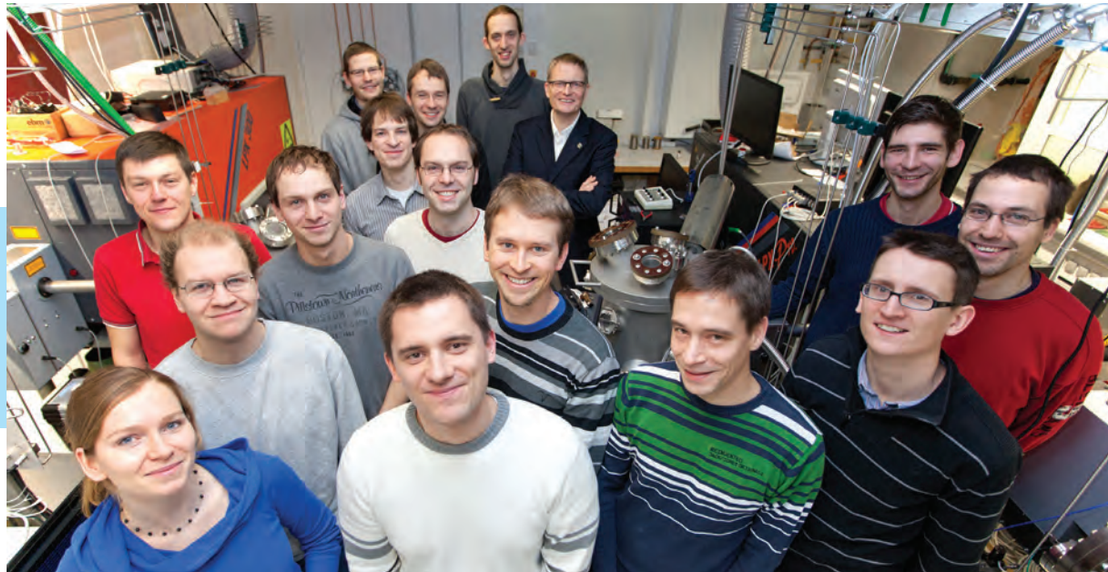
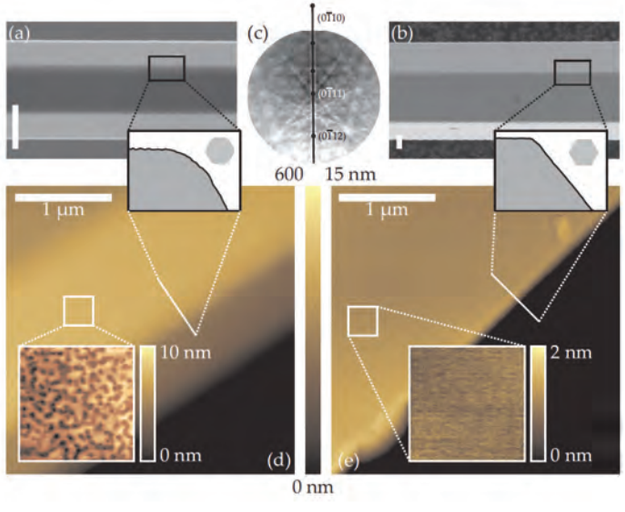
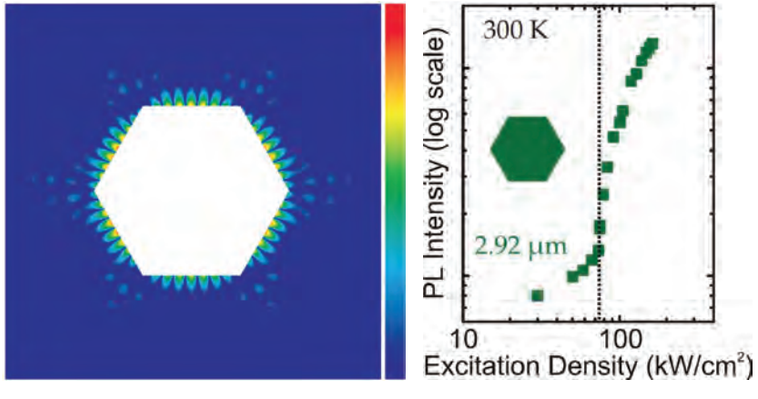


exhibit lasing also at room temperature with the lowest reported thresholds of 73 kW/cm², a value about a factor of ten smaller than previous reports in the literature. Such cavities are investigated towards coupling oft the whispering gallery modes with electronic excitations (excitons) in order to form polaritons and their condensates. Such macroscopically coherent condensates up to 250 K and their ballistic transport have been found this year by us in ZnO planar cavities with oxide Bragg mirrors. Using ZnO nanowires as core, the spectral and spatial overlap of quantum well excitons and whispering gallery modes could already we demonstrated, paving the way for studying light-matter coupling in such systems.



⇑ (a, b) Geometry of ZnO microwire with (a) blunt and (b) sharp corners (SEM images). (d, e) AFM images of facet surfaces. (c) EBSD micrograph recorded on a ZnO microwire facet. The main crystallographic index family (0-11i) is indicated by a vertical black line.



⇑ left: Intensity (log scale) of optical field of WGM outside a ZnO microwire with sharp corners. right: Optically pumped lasing characteristic of ZnO microwire with 2.92 µm diameter at room temperature

⇒ *The Corner Effect in Hexagonal Whispering Gallery Microresonators*
C.P. Dietrich, M. Lange, T. Böntgen, M. Grundmann / Appl. Phys. Lett. (2012) **101** 141116

⇒ *Ballistic Propagation of Exciton-Polariton Condensates in a ZnO-based Microcavity*
H. Franke, C. Sturm, R. Schmidt-Grund, G. Wagner, M. Grundmann / New J. Phys. (2012) **14** 013037

⇒ *Microwire (Mg,Zn)O/ZnO and (Mg,Zn)O/(Cd,Zn)O Non-polar Quantum Well Heterostructures for Cavity Applications*
C.P. Dietrich, M. Lange, M. Stölzel, M. Grundmann / Appl. Phys. Lett. (2012) **100** 031110

⇒ *(Zn,Cd)O Thin Films for the Application in Heterostructures: Structural and Optical Properties*
M. Lange, C.P. Dietrich, K. Brachwitz, T. Böntgen, M. Lorenz, M. Grundmann / J. Appl. Phys. (2012) **112** 103517

⇒ *ZnO-based n-channel Junction Field-effect Transistor with Room-temperature Fabricated p-type $ZnCo_2O_4$-gate*
F.-L. Schein, H. von Wenckstern, H. Frenzel, M. Grundmann / IEEE Electron Device Letters (2012) **33** 676

⇒ *The (Mg,Zn)O Alloy*
H. von Wenckstern, R. Schmidt-Grund, C. Bundesmann, A. Müller, C.P. Dietrich, M. Stölzel, M. Lange, M. Grundmann / Handbook of Zinc Oxide and Related Materials, Vol. 1 Materials, 251, Z.C. Feng, ed. (Taylor and Francis/CRC Press, Florida, USA, 2012), ISBN 978-1439855706

⇒ *Design Rules of (Mg,Zn)O-based Thin-film Transistors with high-κ WO_3 Dielectric Gates*
M. Lorenz, A. Reinhardt, H. von Wenckstern, M. Grundmann / Applied Physics Letters (2012) **101** 183502

⇒ *Optical and Defect Properties of Hydrothermal ZnO with Low Lithium Contamination*
R. Heinhold, H.-S. Kim, F. Schmidt, H. von Wenckstern, M. Grundmann, R.J. Mendelsberg, R.J. Reeves, S.M. Durbin, M.W. Allen / Applied Physics Letters (2012) **101** 062105

⇒ *On the Radiation Hardness of (Mg,Zn)O PLD Thin Films*
F. Schmidt, H. von Wenckstern, D. Spemann, M. Grundmann / Applied Physics Letters (2012) **101** 012103

⇒ *Exchange Bias and Magnetoelectric Coupling Effects in $ZnFe_2O_4$-$BaTiO_3$ Composite Thin Films*
M. Lorenz, M. Ziese, G. Wagner, J. Lenzner, C. Kranert, K. Brachwitz, H. Hochmuth, P. Esquinazi, M. Grundmann / CrystEngComm (2012) **14** 6477

⇒ *Microscopic Identification of Hot Spots in Multi-barrier Schottky Contacts on Pulsed Laser Deposition Grown Zinc Oxide Thin Films*
S. Müller, H. von Wenckstern, O. Breitenstein, J. Lenzner, M. Grundmann / IEEE Transactions on Electron Devices (2012) **59** 536

⇒ *Electronic and Optical Properties of ZnO/(Mg,Zn)O Quantum Wells with and without a Distinct QCSE*
M. Stölzel, J. Kupper, M. Brandt, A. Müller, G. Benndorf, M. Lorenz, M. Grundmann / Journal of Applied Physics (2012) **111** 063701

⇒ *Excitonic Transport in ZnO*
M. Noltemeyer, F. Bertram, Th. Hempel, B. Bastek, A. Polyakov, J. Christen, M. Brandt, M. Lorenz, M. Grundmann / Journal of Materials Research (2012) **27** 2225

⇒ *Exciton Localization and Phonon Sidebands in Polar ZnO/MgZnO Quantum Wells*
M. Lange, J. Kupper, C.P. Dietrich, M. Brandt, M. Stölzel, G. Benndorf, M. Lorenz, M. Grundmann / Physical Review B (2012) **86** 045318

⇒ *Whispering Gallery Modes in Deformed Hexagonal Resonators*
M. Grundmann, C.P. Dietrich / physica status solidi (b) (2012) **249** 871

⇒ *Electrical Transport in Strained $Mg_xZn_{1-x}O$:P Thin Films Grown by Pulsed Laser Deposition on ZnO (000-1)*
M. Brandt, M. Bonholzer, M. Stölzel, G. Benndorf, D. Spemann, M. Lorenz, M. Grundmann / physica status solidi (b) (2012) **249** 82

⇒ *Persistent Layer-by-layer Growth for Pulsed-laser Homoepitaxy of (000-1) ZnO*
J. Zippel, M. Lorenz, G. Benndorf, M. Grundmann / physica status solidi RRL (2012) **6** 433

⇒ *Visible Emission from ZnCdO/ZnO Multiple Quantum Wells*
M. Lange, C.P. Dietrich, K. Brachwitz, M. Stölzel, M. Lorenz, M. Grundmann / physica status solidi RRL (2012) **6** 31

⇒ *Modal Gain and its Diameter Dependence in Single ZnO Micro- and Nanowires*
J.P. Richters, J. Kalden, M. Gnauck, C. Ronning, C.P. Dietrich, H. von Wenckstern, M. Grundmann, J. Gutowski, T. Voss / Semiconductor Science and Technology (2012) **27** 015005

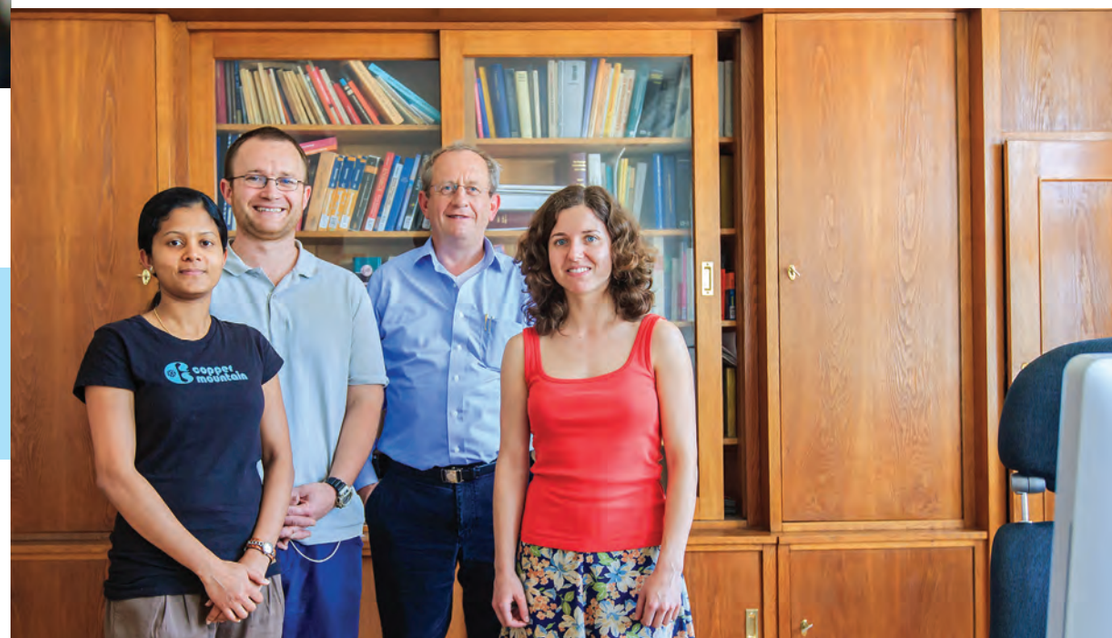
Electronic structure investigation of modern materials with magnetic resonance techniques

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, Dr. Benno Meier

Our research deals with the investigation of the electronic 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).

Our expertise lies in the work at extreme conditions like in the highest magnetic fields (up to 100 T, in cooperation with the Helmholtz-Zentrum Dresden-Rossendorf) and at highest pressures (up to 4 GPa). These extreme conditions are needed to induce changes to the electronic structure of solid materials like metals or superconductors.

In pulsed field NMR, after we showed that signal averaging is possible, we were able to run multi-pulse experiments.



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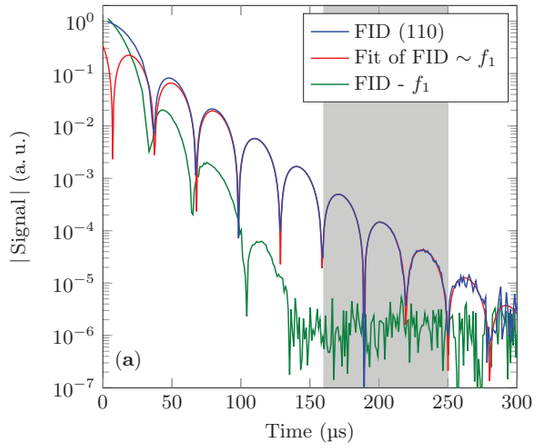

⇐ Extraction of two decay modes from the FID for B parallel to (110) in CaF_2. After subtracting the fit or first Mode f_1 as determined by fitting the tail of the FID, a second mode f_2 becomes apparent.

In static fields, we studied the long-time behaviour of the free induction decay of ^{19}F in a CaF_2 high-quality single crystal. Here, it was possible to increase the sensitivity by two orders of magnitude compared with previous measurements allowing to verify a theory by Boris Fine, a theoretical physicist at the University of Heidelberg.

On a novel MOF with a Zn_4O cluster with triazole ligands we were able with different ^{13}C NMR techniques to verify the presence of mobile guest molecules (DMF) in the pores which is complicated with X-ray diffraction.

⇒ *Eigenmodes in the Long-Time Behavior of a Coupled Spin System Measured with Nuclear Magnetic Resonance*
B. Meier, J. Kohlrautz, J. Haase / Phys. Rev. Lett. (2012) **108** 177602

⇒ *Implementation of Specific-heat and NMR Experiments in the 1500 ms Long-pulse Magnet at the Hochfeld-Magnetlabor Dresden*
F. Weickert, B. Meier, S. Zherlitsyn, T. Herrmannsdörfer, R. Daou, M. Nicklas, J. Haase, F. Steglich, J. Wosnitza / Meas. Sci. Technol. (2012) **23** 105001

⇒ *Nuclear Magnetic Resonance Apparatus for Pulsed High Magnetic Fields*
B. Meier, J. Kohlrautz, J. Haase, M. Braun, F. Wolff-Fabris, E. Kampert, T. Herrmannsdörfer, J. Wosnitza / Rev. Sci. Instrum. (2012) **83** 083113

⇒ *A Novel Zn_4O-based Triazolyl Benzoate MOF: Synthesis, Crystal Structure, Adsorption Properties and Solid State ^{13}C NMR Investigations*
J. Lincke, D. Lässig, K. Stein, J. Moellmer, A.V. Kuttatheyil, C. Reichenbach, A. Moeller, R. Staudt, G. Kalies, M. Bertmer, H. Krautscheid / Dalton Trans. (2012) **41** 817

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Molecular simulations of ion effects on structural and thermodynamical properties of biopolymers

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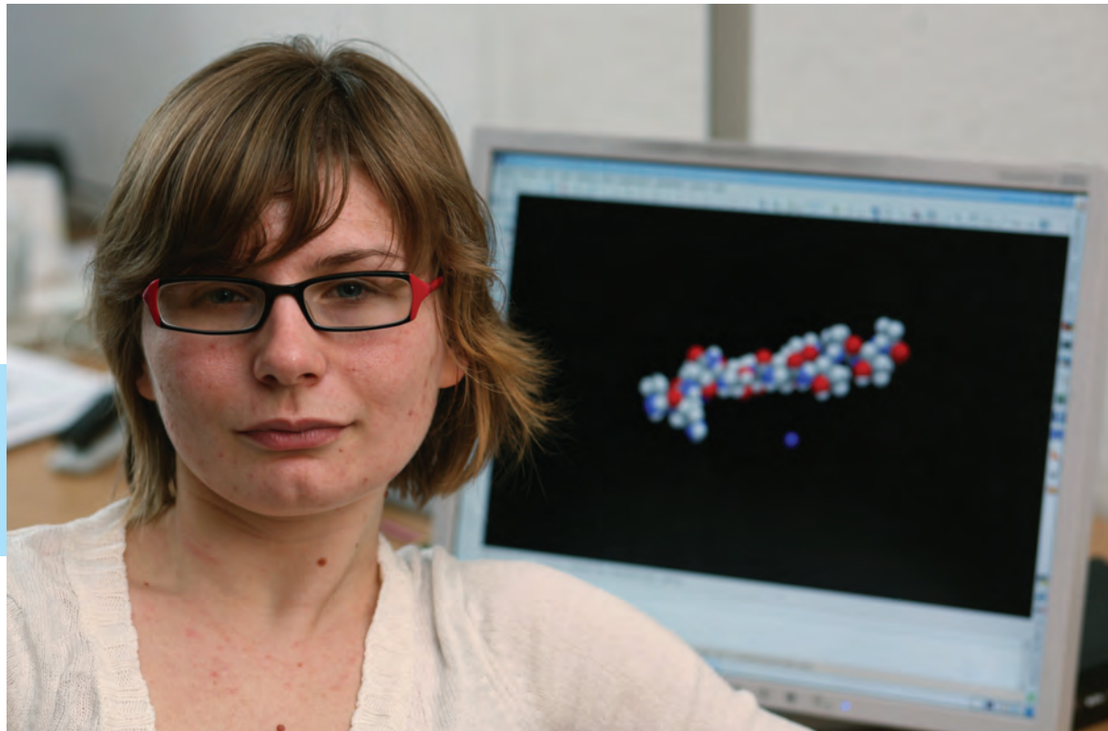
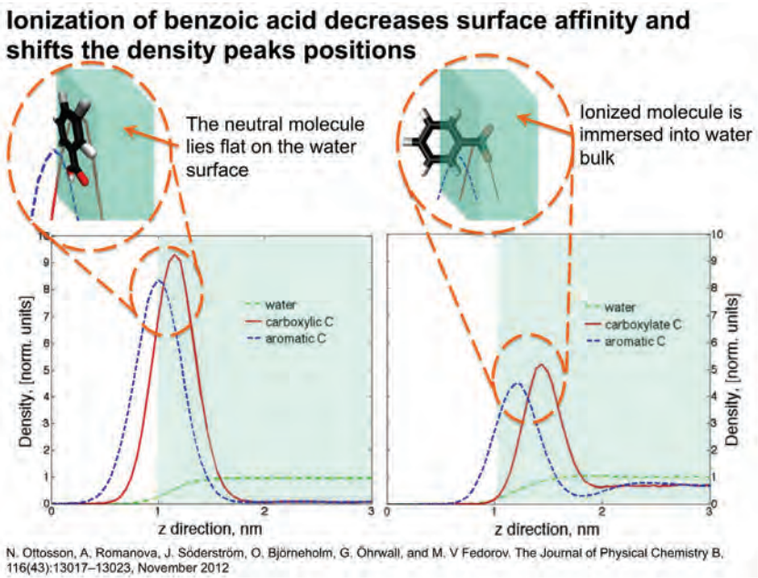
M.Sc. Chem. Anastacia Romanova

Proteins are the basic building blocks for all living organisms. Proteins work efficiently and selectively as catalysts, sensors, controllers etc. Proteins are biodegradable and are not hazardous for the environment. This makes protein-based devices one of the most prospective and sustainable technologies of the 21st century.

However, there is a large lack in our understanding of the molecular-level mechanisms of how proteins work. Particularly, mechanisms of ion effects on protein structure and activity are not well explored. Understanding of these mechanisms could be a significant step forward to controllable and sustainable production of peptide/protein-based devices. Unfortunately, even smaller oligoproteins are quite





N. Ottosson, A. Romanova, J. Söderström, O. Björneholm, G. Öhrwall, and M. V Fedorov. The Journal of Physical Chemistry B, 116(43):13017–13023, November 2012

complicated systems to study. This is why to reach better level of understanding of the basic mechanisms of protein interactions with ions in water we studied interactions of carboxylic group of benzoic acid with ions and a hydrophobic interface. We have found that strength of ion binding to the carboxylic group significantly affects orientation of benzoic acid at the interface as well as its surface affinity.

⇒ *Molecular Mechanisms of Salt Effects on Carbon Nanotube Dispersions in an Organic Solvent (N-methyl-2-pyrrolidone)*
A.I. Frolov, R.N. Arif, M. Kolar, A.O. Romanova, M.V. Fedorov, A.G. Rozhin / Chemical Science (2012) **3** 541

⇒ *Molecular Sinkers: X-ray Photoemission and Atomistic Simulations of Benzoic Acid and Benzoate at the Aqueous Solution/Vapor Interface*
N. Ottosson, A.O. Romanova, J. Söderström, O. Björneholm, G. Öhrwall, M.V. Fedorov / Journal of Physical Chemistry B (2012) **116** 13017

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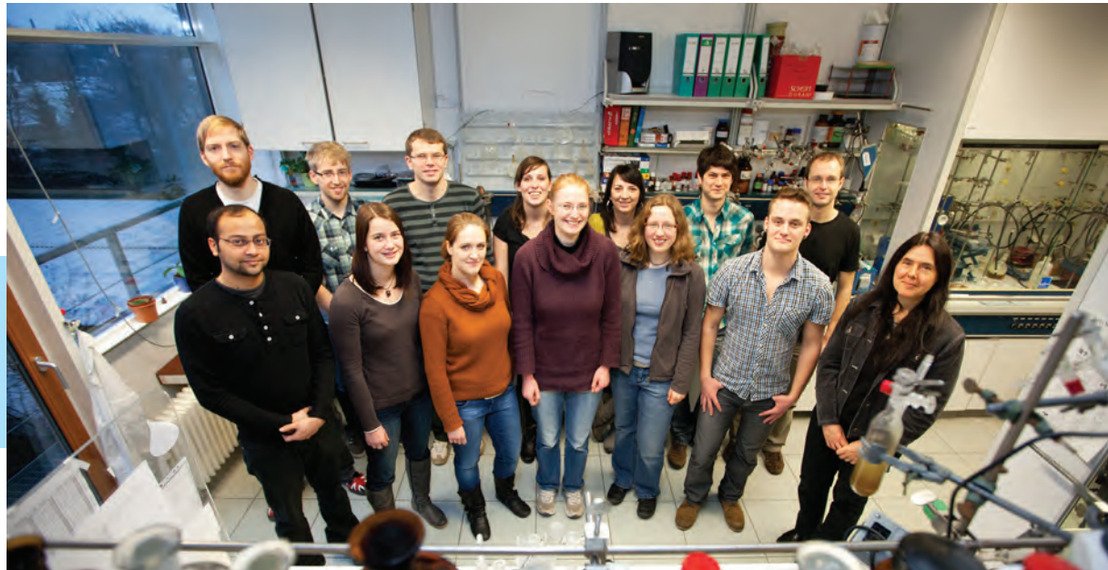
The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carbaborane clusters and antitumour drugs).

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

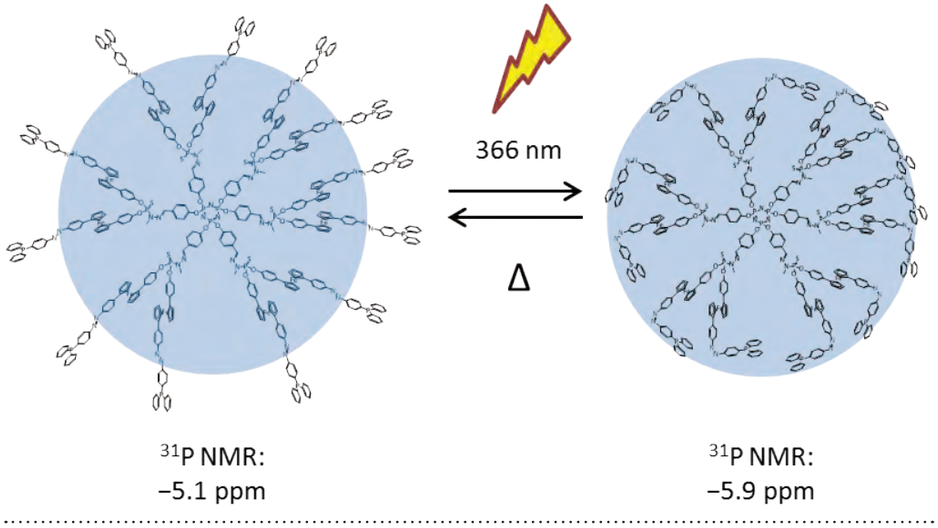


in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way "switchable" phosphines for catalytic applications (M. Madalska, P. Neumann).

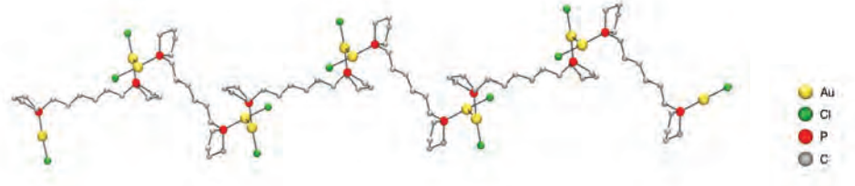
Another approach focuses on the use of selective phosphorus-based macrocycles (J. Haushälter), nano-frames (M. Streitberger), containers, or cavities (functionalised (*S*)-BINAP as linkers) in metal-organic frameworks (MOFs) with well-defined structures and porosity. These compounds can be used as receptors for catalytically active transition metals, generating molecular nanosized reactors that should allow specific interactions of the cavity with substrates during a catalytic process. Variation of the coordinated metal atom or the size of the cavity will influence the selectivity in catalytic processes.

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 [LnM=PR] (A. Grundmann), strained inorganic (A. Kreienbrink) or organic (T. Möller) phosphorus-based rings, alkylene-bridged bis(phospholanes) (M. Streitberger) or planar-chiral ferrocenylphosphinoboranes (S. Pandey).
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 a novel approach to this class of compounds starting with volatile phosphorus-rich metal complexes as molecular precursors.

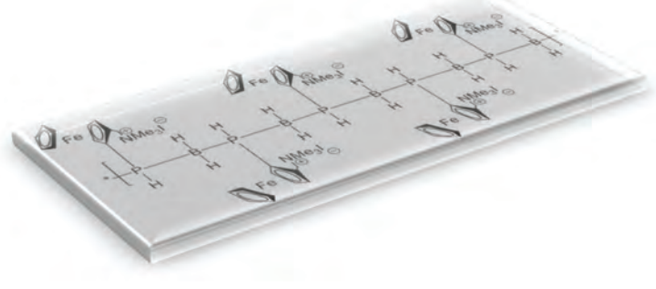
Inorganic Building Blocks in Medicinal Chemistry: Carbaboranes are highly hydrophobic and extremely stable icosahedral carbon-containing boron clusters. The cage framework of these clusters can easily be modified with a variety of substituents, both at the carbon and at the boron atoms and can either 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 Y1-receptor-selective neuropeptide Y (NPY) derivative (R. Frank, 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).



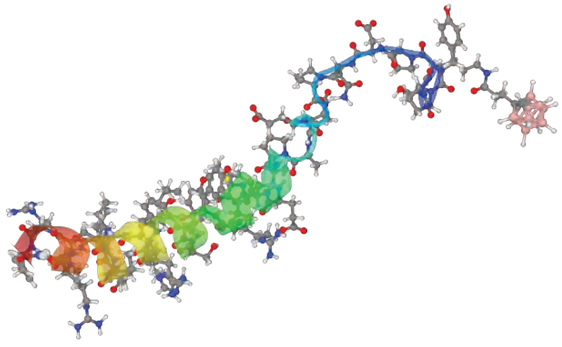
⇑ UV-switchable ferrocenylphosphine-based dendrimer



⇑ Gold(I)-based polymer via aurophilic interaction in gold(I)-chloride 1,7-bis(1-phospholano)hexane



⇑ Ionic inorganic polymer from ferrocenylphosphinoborane as molecular building block



⇐ Carbaborane-conjugate of breast-tumour selective neuropeptide Y ([Phe^{7},Pro^{34}]-NPY)

⇒ *Imitation and Modification of Bioactive Lead Structures via Integration of Boron Clusters*
S. Stadlbauer, R. Frank, M. Scholz, S. Boehnke, V. Ahrens, A.G. Beck-Sickinger, E. Hey-Hawkins / IMEBORON-XIV: Invited Manuscript, Pure and Applied Chemistry (2012) **84** 2289

⇒ *Electrophilic Sulfenylation of 7,8-Dicarba-nido-dodecahydroundecaborate(1–), 7,8-nido-$C_2B_9H_{12-}$*
R. Frank, T. Grell, M. Hiller, E. Hey-Hawkins / Dalton Trans. (2012) **41** 6155

⇒ *ortho-Carbaborane Derivatives of Indomethacin as Cyclooxygenase (COX)-2 Selective Inhibitors*
M. Scholz, A.L. Blobaum, L.J. Marnett, E. Hey-Hawkins / Bioorg. Med. Chem. (2012) **20** 4830

⇒ *Synthesis and Thermolysis of the Phosphorus-rich Manganese(I) Complex [Mn_2(μ-Br){cyclo-(P_4tBu_3)PtBu}$(CO)_6$]: From Complexes to Metal Phosphides*
A. Kircali, R. Frank, S. Gómez-Ruiz, B. Kirchner, E. Hey-Hawkins / ChemPlusChem (2012) **77** 341
Cover; article was highlighted in ChemistryViews

⇒ *From ortho-Carbaborane-9-thiol Towards New Building Blocks*
R. Frank, S. Boehnke, A. Aliev, E. Hey-Hawkins / Polyhedron (2012) **39** 9

⇒ *Endocyclic P–P Bond Cleavage in Carbaborane-substituted 1,2-diphosphetane: A new Route to Secondary Phosphinocarbaboranes*
A. Kreienbrink, P. Lönnecke, M. Findeisen, E. Hey-Hawkins / invited contribution, Chem. Commun. (2012) **48** 9385

⇒ *Asymmetric Phospha-Diels-Alder Reaction: A Stereoselective Approach towards P-chiral Phosphanes via Diastereotopic Face Differentiation*
T. Möller, M.B. Sárosi, E. Hey-Hawkins / Chem. Eur. J. (2012) **18** 16604

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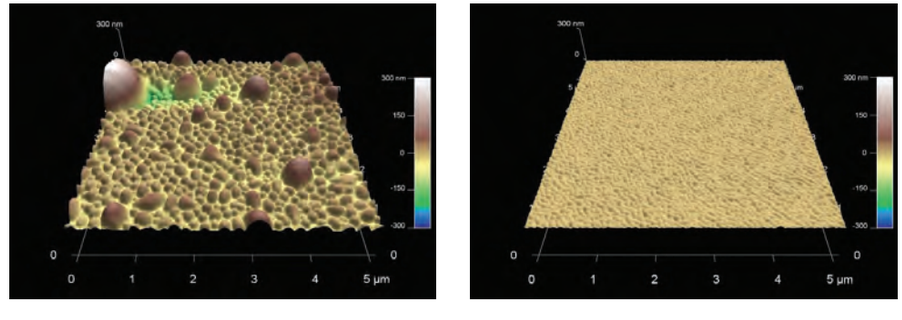
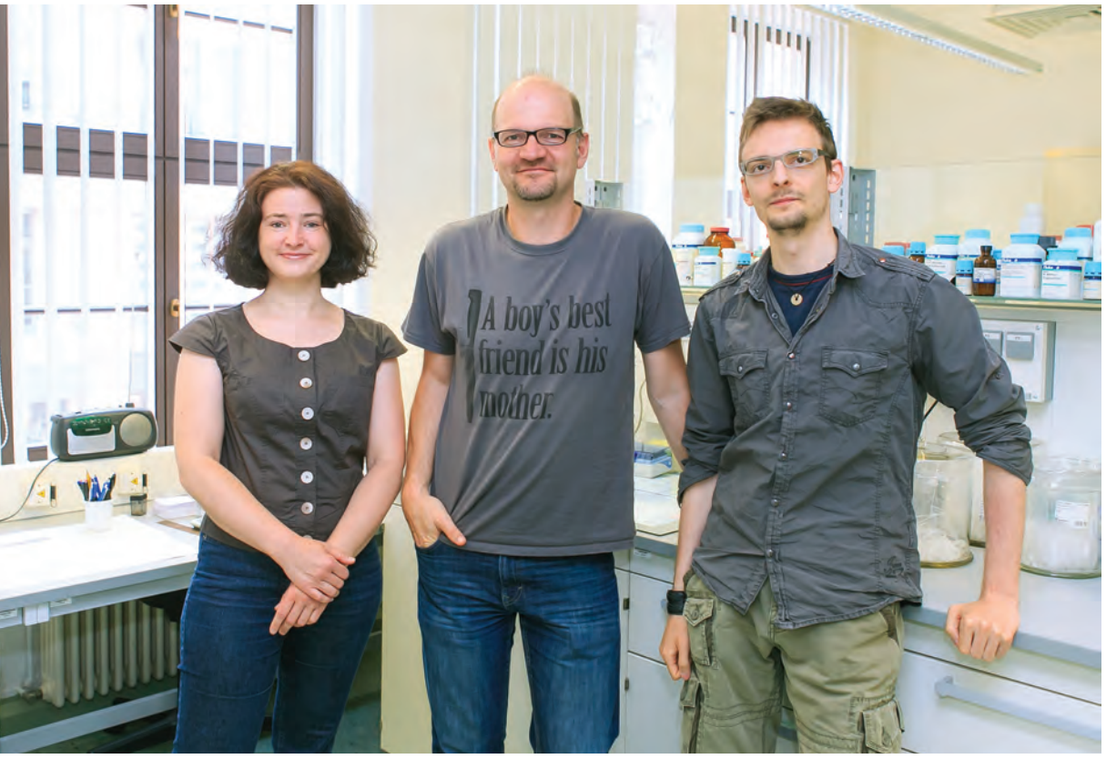
Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake

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

Layer-by-Layer (LbL) biopolymer coated micro-particles and capsules provide the opportunity to design highly effective and specific drug delivery systems. The modular principle of construction, based on the step-by-step adsorption of oppositely charged polyelectrolytes, allows the defined integration of active agents as well as additional modifications for local application, specific cell uptake and time-controlled administration. An interesting point in the design of such carriers is the outer carrier layer since many different functions can be controlled by a defined surface modification. In this project, Martin Göse is involved in the design of a specific surface modification, the adsorption of modifiable lipid membranes. Besides providing high biocompatibility, a homogeneous lipid layer also inhibits binding of serum proteins and offers a basis for specific binding of antibodies to address the desired cells. Adapted polymer coating, efficient liposome spreading and successful antibody binding with high specificity are focused in the project. The investigations also require the application of different techniques to investigate the quality of the lipid and antibody coating. Direct surface topology methods as AFM and SEM as well as methods to detect the surface properties as CLSM, scattering and fluorescence parameters of Flow Cytometry complete the research spectrum.



⇑ Influence of different polyelectrolyte coating conditions on multilayer structures. Left: polymer coating with 9 layers of protamin and dextran after dipping the slide into the solution, right same coating but achieved by spreading onto the slide



Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
Dipl.-Phys. Niklas Fricke, Dipl.-Phys. Martin Marenz, Dr. Monika Möddel,
Dipl.-Phys. 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 techniques based on stochastic series expansions, and thermostated Molecular Dynamics simulations. These methods are adapted by us to the problems at hand and constantly further improved in order to cope with the complexity of the considered problems:

⇒ *Inhibition of Human Neutrophil Elastase by alpha1-antitrypsin Functionalized Colloidal Microcarriers*
U. Reibetanz, M. Schönberg, S. Rathmann, V. Strehlow, M. Göse, J. Leßig / ACS Nano (2012) **6** 6325

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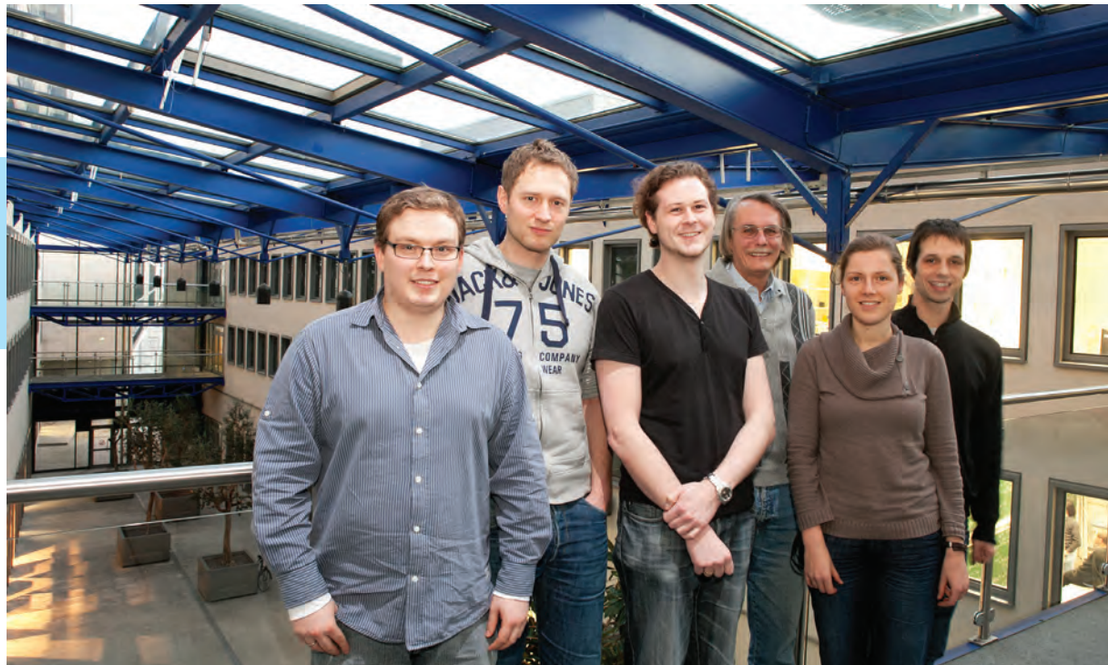
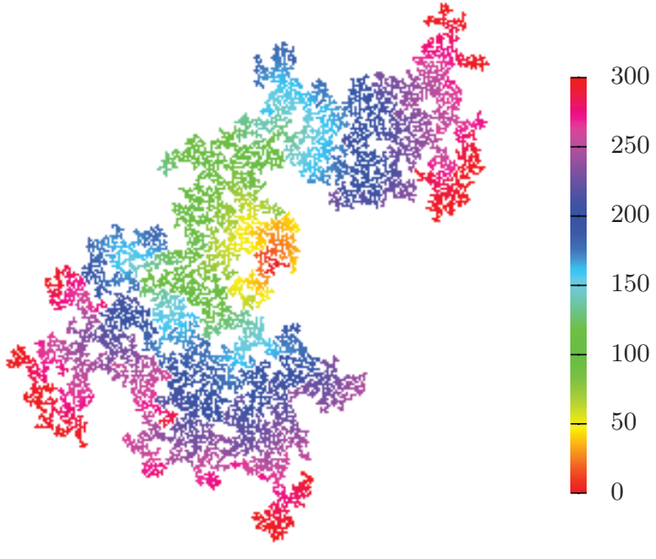


Monika Möddel employs Monte Carlo computer simulations in generalized ensembles for investigations of the conformational mechanics of polymer adsorption transitions and the associated structure formation at attractive, patterned solid substrates. In June 2012 she has very successfully defended her PhD Thesis on this topic with the grade "summa cum laude".

Sebastian Schöbl and Johannes Zierenberg consider polymers in disordered environments and compare their configurational statistics obtained with chain-growth algorithms and multicanonical simulation methods. This is an important basic building block for an understanding of, e.g., the universal properties of the cyclo-skeleton investigated by several other BuildMoNa groups. In July 2012 Sebastian Schöbl has submitted his PhD Thesis.

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.

Johannes Zierenberg builds on Micha Wiedenmann's work and studies the aggregation properties of a number of polymers, with emphasis on the distinguishing differences between flexible and semiflexible macromolecules.



⇑ Example for a critical percolation cluster on which the behaviour of self-avoiding random walks has been studied. Colours show the chemical distance to the origin, which is in the red centre.

Martin Marenz aims at developing 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. Similar to our previous studies of a generic bead-stick polymer model, the adsorption propensity and structure formation processes are in the focus of interest.

Niklas Fricke extended our recently proposed novel renormalization group inspired complete enumeration method for self-avoiding random walks on a percolation cluster, modelling polymers in disordered environments, to up to seven space dimensions. This method allows us to enumerate walks of about 1000 steps in a couple of minutes which with standard techniques would take over 10^{170} years.

⇒ *Grafted versus Non-Grafted Polymer Adsorption*
M. Möddel, M. Bachmann, W. Janke / Forschungszentrum Jülich NIC Series (2012) **45** 277

⇒ *Exact Enumeration of Self-Avoiding Walks on Percolation Clusters*
N. Fricke, W. Janke / Physics Procedia (2012) **34** 39

⇒ *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*
N. Fricke, W. Janke / Europhysics Letters (2012) **99** 56005

⇒ *Influence of Lattice Disorder on the Structure of Persistent Polymer Chains*
S. Schöbl, J. Zierenberg, W. Janke / Journal of Physics A (2012) **45** 475002

⇒ *Simple Flexible Polymers in a Spherical Cage*
M. Marenz, J. Zierenberg, H. Arkin, W. Janke / Condensed Matter Physics (2012) **15** 43008

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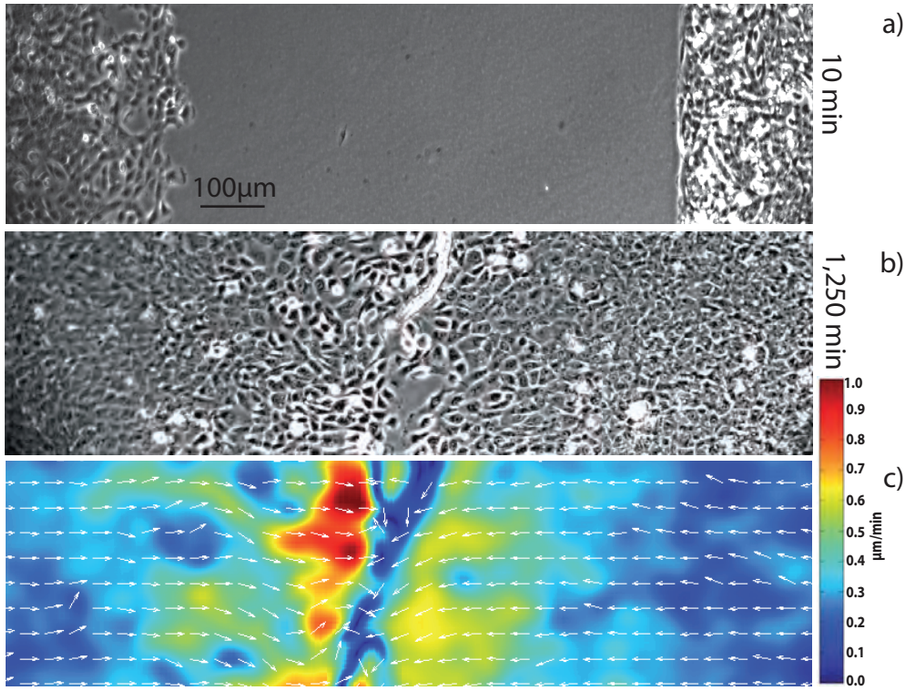
Impact of cell migration and mechanical properties on tumour formation and cancer progression

Prof. Dr. Josef Alfons Käs
Dipl.-Phys. Anatol Fritsch, M.Sc. Phys. Markus Gyger, Dipl.-Phys. Chris Händel, Dipl.-Phys. Tina Händler, Dr. Florian Huber, Dipl.-Phys. Tobias Kießling, Dipl.-Math. Melanie Knorr, M.Sc. Phys. 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

BuildMoNa students in the group of Prof. Käs investigated the dynamics and mechanical properties of eukaryokic cells to gain a better understanding of their function and the impact on diseases. In detail, collective cell migration is an important feature of wound healing, embryonic and tumour development. Previous studies suggested that cellular interactions cause a line tension which holds the cells back if they try to escape the monolayer. BuildMoNa students could show that even weakly interacting cells can form constant cell boundaries and intact monolayers. Furthermore, directed motion of the cells not only results in the formation of a constant cell front, but also leads to jamming of cells when two monolayers meet. During such events, cellular motion becomes undirected in the first step and finally comes to a halt when cells from the back of the monolayer continue to push against the front. Such jamming stabilises the borders and no mixing of cells from different monolayers – even of the same cell type – occurs: A stable border establishes.

A better understanding of the underlying mechanisms why cells jam or can escape the monolayer and the connection to the cellular viscoelastic properties can provide deeper knowledge in the formation of metastasis during cancer progression since here single cells leave the host tumour and start to migrate freely. In contrast, in early stages of cancer tumour cells remain within their host tissue and only major changes of the cellular mechanisms such as variations in cell-cell coupling must occur that an escape becomes possible.

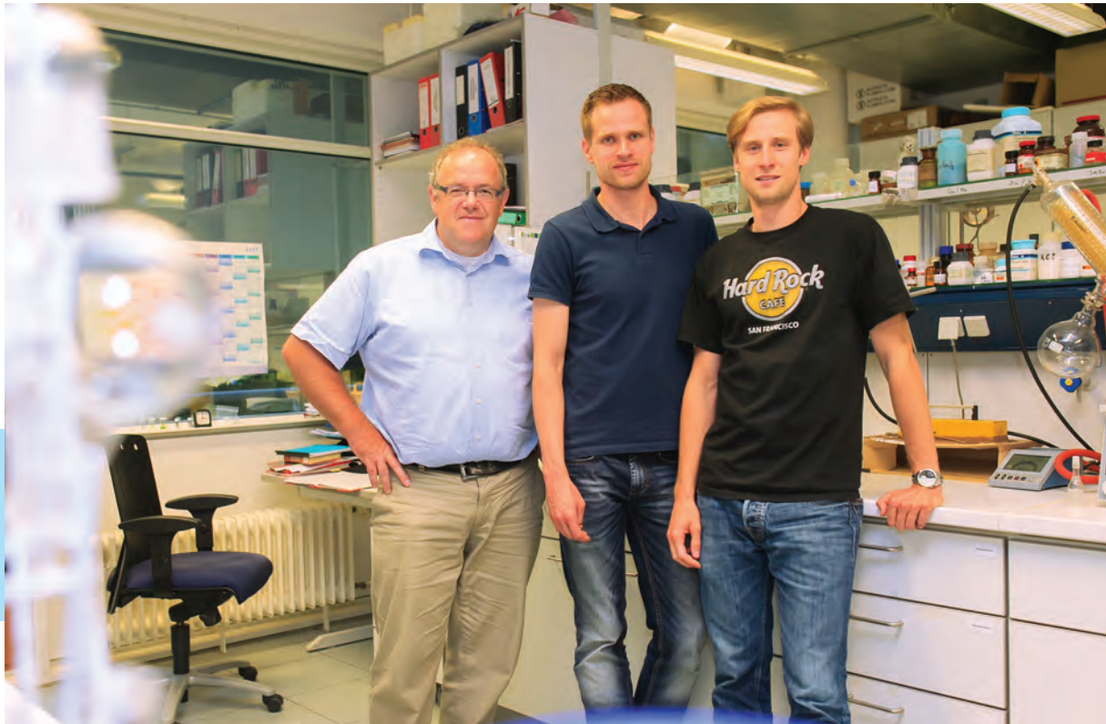


⇑ Phase contrast images of two oppositely migrating cell monolayers at times 10 min (a) and 1,250 min (b), respectively. At the lower cell density (left monolayer), single cells escape the monolayer. Colour-coded spatial velocity distribution of the monolayers after 1,250 min (c). The velocities are both spatially heterogeneous, while single cells migrate uni-directionally.

Coordination compounds in supramolecular chemistry and molecular magnetism

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

One of our main research areas deals with supramolecular chemistry. Recently, we have focused our attention on the host guest chemistry of container molecules incorporating two Lewis-acidic metal ions. Thus, the ability of the cavitand $[Ni_2(L^{Me2H4})]^{2+}$ to act as a selective receptor for small spherical anions has been investigated. The cavitand binds fluoride and chloride ($K_a \sim 10^4\ M^{-1}$) in acetonitrile/ethanol by two converging Lewis-acid/base interactions, exhibits little affinity for bromide ($K_a < 10^2\ M^{-1}$), and no affinity for iodide or polyatomic anions (ClO_4^-, NO_3^-, HCO_3^-, $H_2PO_4^-$, HSO_4^-, SO_4^{2-}). This binding selectivity can be attributed to the high degree of preorganisation of the $[Ni_2(L^{Me2H4})]^{2+}$ receptor, and a size fit mis-



⇒ *The Impact of Jamming on Boundaries of Collectively Moving Weak-interacting Cells*
K.D. Nnetu, M. Knorr, J.A. Käs, M. Zink / New Journal of Physics (2012) **14** 115012

⇒ *Directed Persistent Motions Maintain Sheet Integrity During Multi-cellular Spreading and Migration*
K.D. Nnetu, M. Knorr, D. Strehle, M. Zink, J.A. Käs / Soft Matter (2012) **8** 2913

⇒ *ERBB2 Overexpression Triggers Transient High Mechanoactivity of Breast Tumor Cells*
M. Martin, K. Müller, C. Cadenas, M. Hermes, M. Zink, J.G. Hengstler, J.A. Käs / Cytoskeleton (2012) **69** 267

⇒ *Tuning Liver Stiffness against Tumours: An in vitro Study using Entrapped Cells in Tumour-like Microcapsules*
A. Leal-Egaña, A. Fritsch, F. Heidebrecht, A. Díaz-Cuenca, M. Nowicki, A. Bader, J. Käs / Journal of the Mechanical Behavior of Biomedical Materials (2012) **9** 113

⇒ *Counterion-induced Formation of Regular Actin Bundle Networks*
F. Huber, D. Strehle, J.A. Käs / Soft Matter **8** 931

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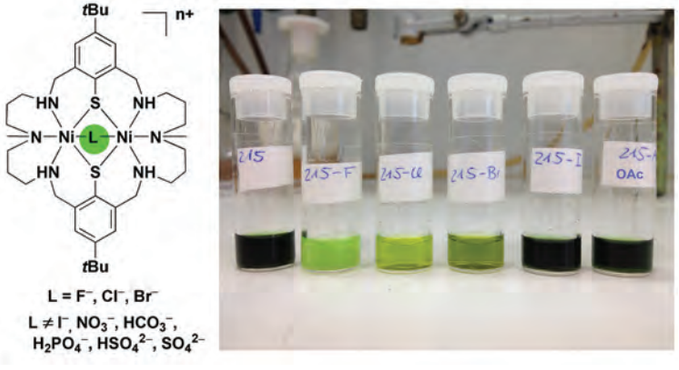
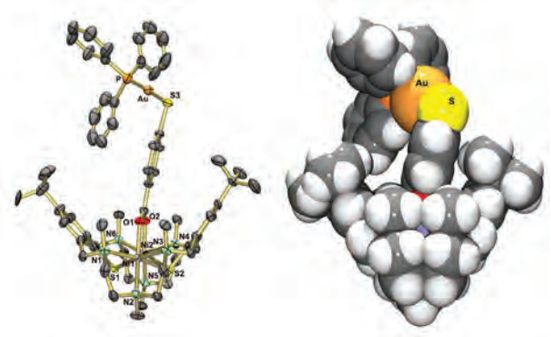
match of the receptors binding cavity for anions larger than Br^-. The colour changes accompanying the binding events allow a discrimination of the halide ions by the naked eye in the mM range in the visible, and the mM range in the UV.

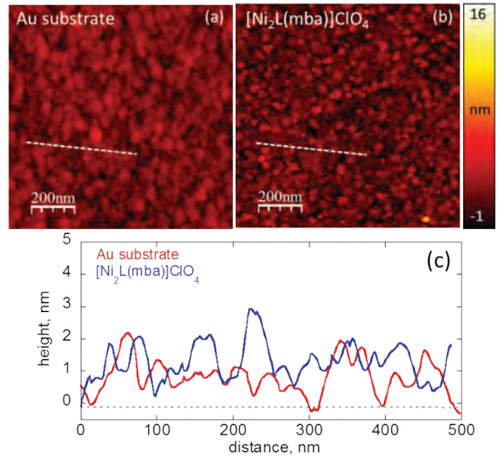
Our other main research area is focused on the synthesis and characterisation of molecular based magnetic materials. Here, we have set out to explore the possibility of constructing switchable molecular devices based on magnetically bistable molecules. One step in the preparation of such devices consists of the chemisorption of switchable molecules on surfaces. In this context we have developed macrocyclic transition metal polyaza-dithiophenolate complexes with switchable spin ground states and a method which allows their chemisorption from solution on gold surfaces. The strategy makes use of ambidentate ligands with a hard donor group for attachment to the $[M_2L]^{2+}$ complexes and a soft donor function (thiol or phosphine) for chemisorption to metal surfaces. The chemisorption of the macrocyclic Ni_2 complex to the gold surface has been studied by contact angle measurements, X-ray photoelectron spectroscopy, ellipsometry, atomic force microscopy, and scanning tunneling microscopy using a discrete trinuclear $Ni^{II}{}_2Au^{I}$ complex $[Ni_2L(O_2CC_6H_4S)AuPPh_3]^+$ as a spectroscopic and structural probe. In future studies we will improve the first generation models such that they can be deposited onto surfaces with a high-level of long-range order.



⇑ Structure of the macrocyclic $[Ni_2L^{Me2H4}(L)]^{n+}$ receptor and accompanying colour changes upon anion binding



⇐ Ortep (left) and van der Waals plot (right) of the molecular structure of the Ni_2Au complex $[Ni_2L(mba)Au(PPh_3)]+$ in the crystal.



⇐ AFM topography characteristics considering a 1×1 μm² area, (a) Au substrate as grown with a roughness of 0.6 (1) nm (rms), (b) Au substrate after deposition of $[Ni_2L(mba)]ClO_4$ with a roughness of 0.9 (1) nm (rms), (c) AFM profiles following the white-dotted line in (a) and (b)

⇒ *Stabilization of Hypophosphite in the Binding Pocket of a Dinuclear Macrocyclic Complex: Synthesis, Structure and Properties of $[Ni_2L(u\text{-}O_2PH_2)]BPh_4$ ($L = N_6S_2$ Donor Ligand)*
J. Lach, A. Jeremies, V. Lozan, C. Loose, T. Hahn, J. Kortus, B. Kersting / Inorg. Chem. (2012) **51** 12380

⇒ *Pd-mediated Cleavage of S–C Bonds: Preparation and Characterization of Pd(II) Complexes of 2,6-difor-myl-4- tert-butylthiophenol Dioxime*
S. Gruschinski, M. Handke, B. Kersting / Z. Anorg. Allg. Chem. (2012) **638** 1274

⇒ *Peparation and Characterization of Dinuclear Nickel(II) Complexes Containing $N_3Ni(u\text{-}1,3\text{-}SO_3R)_2(u\text{-}O_2CR)NiN_3$ Cores: Crystal Structures and Magnetic Properties of $[Ni_2(L_2)(O_2CCH_3)]BPh_4$ and $[Ni_2(L_2)(O_2CPh)]BPh_4$ (where H_2L_2 = Macrocyclic Ligand with $N_6(SO_3)_2$ Donor Set)*
J. Lach, T. Hahn, B. Kersting, J. Kortus / Eur. J. Inorg. Chem. (2012) 2381

⇒ *Synthesis, Structure and Reactivity of Dinuclear Nickel Amino-Thiophenolate Complexes bearing bridging $VO_2(OH)_2-$ and $VO_2(OR)_2-$ Coligands*
V. Lozan, J. Lach, B. Kersting / Inorg. Chem. (2012) **51** 5213

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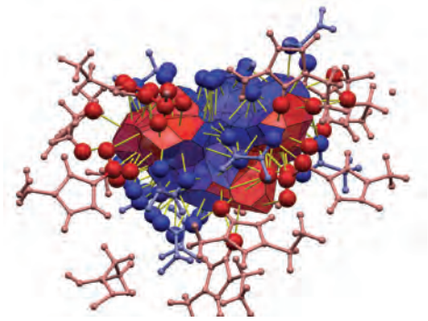
Complex systems from theoretical methods – development and applications

Prof. Dr. Barbara Kirchner
M.Sc. Chem. Martin Brehm, M.Sc. Chem. Eva Perlt

The prediction of technically relevant properties of complex systems sometimes goes beyond the scope of theoretical methods. Especially the theoretical investigation of associated liquids is a demanding task. Often, molecular dynamics simulations are applied for this purpose due to their capability of describing dynamics as well as the manifold kinds of inter particle interactions. The output of such calculations is in most cases limited to the time dependent coordinates of the particles. In order to obtain relevant information and properties out of these trajectories and to visualize them Martin Brehm has been developing his TRAVIS – TRAjectory Analyzer and VISualizer, which is freely available via www.travis-analyzer.de. This project is continuously improved and extended by further analyses. Furthermore, it has been applied to studies on Ionic Liquids resulting in numerous publications.

Another development project being concerned with the floating orbitals molecular dynamics method, i.e., the release of orbital centres from the respective nuclear centres during molecular dynamics, has been treated by Eva Perlt. The advantage of moving the orbital centres away from the nuclei is in the description of chemical bonding as well as the computation of properties related to polarizability.



⇐ Voronoi cell of one [EMIM] cation together with neighbouring cations (shown in red) and anions (shown in blue) as obtained with the TRAVIS programme

⇒ *A One-Parameter Quantum Cluster Equilibrium Approach*
M. Brüssel, E. Perlt, M. v. Domaros, M. Brehm, B. Kirchner / The Journal of Chemical Physics (2012) **137** 164107

⇒ *On the Ideality of Binary Mixtures of Ionic Liquids*
M. Brüssel, M. Brehm, A.S. Pensado , F. Malberg, M. Ramzan, A. Stark, B. Kirchner / Physical Chemistry Chemical Physics (2012) **14** 13204

⇒ *Short Time Dynamics of Ionic Liquids in AIMD Based Power Spectra*
K. Wendler, M. Brehm, F. Malberg, B. Kirchner, L. Delle Site / The Journal of Chemical Theory and Computation (2012) **8** 341

⇒ *Proton Transfer and Polarity Changes in Ionic Liquid-Water Mixtures: A Perspective on Hydrogen Bonds from ab initio Molecular Dynamics at the Example of 1-Ethyl-3-methylimidazolium Acetate-Water Mixtures. Part 1*
M. Brehm, H. Weber, A.S. Pensado, A. Stark, B. Kirchner / Physical Chemistry Chemical Physics (2012) **14** 5030

⇒ *Effect of Dispersion on the Structure and Dynamics of the Ionic Liquid 1-Ethyl-3-methylimidazolium Thiocyanate*
A.S. Pensado, M. Brehm, J. Thar, A.P. Seitsonen, B. Kirchner / ChemPhysChem (2012) **13** 1845

⇒ *Simulationen auswerten*
M. Brehm / Nachrichten aus der Chemie (2012) **60** 552

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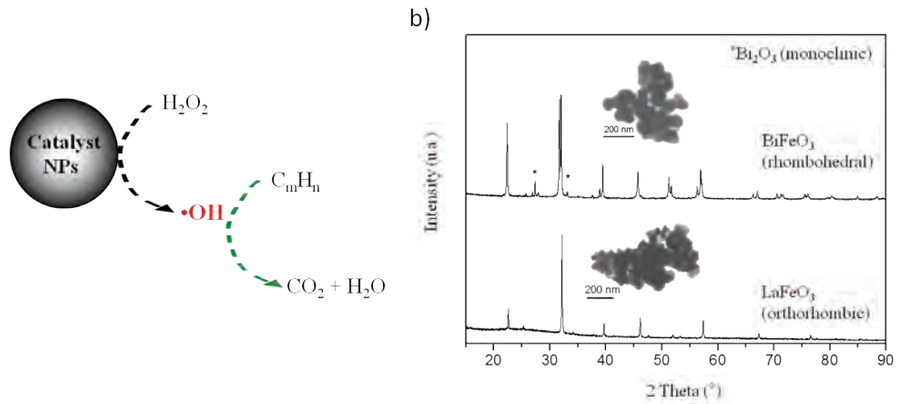
Nanocatalysts for water treatment

Prof. Dr. Frank-Dieter Kopinke
Dr. Klara Rusevova, Dr. Jens Schneider, Dr. Ksenia J. Surudo

A novel promising trend in environmental research such as on water decontamination processes is the application of nano-reagents (e.g. zero-valent iron) and nanocatalysts (e.g. metallic Pd, iron oxides).

The work of Klara Rusevova was basically dealing with the integration of colloidal catalysts and reagents in chemical oxidation processes. She was mainly focused on the synthesis, characterisation and testing of various nanoparticulate iron-containing oxides (e.g. magnetite, perovskites) in so called heterogeneous Fenton-like reactions, whereby $BiFeO_3$ perovskite revealed as the most promising catalyst material. By studying isotope fractionation effects during the degradation of model compounds, she was able to deduce insight into the type of reactive species formed on the catalyst surface, confirming a dominant role of hydroxyl radicals.

She defended her doctoral work entitled as "Novel colloidal catalysts and reagents for oxidation of organic pollutants in water" in December 2012. The thesis was written in a cumulative form, i.e. it consists of four scientific publications accepted for publication in highly ranked journals.



⇑ A simplified scheme of reaction pathways in heterogeneous Fenton-like reactions using non-supported Fe-containing catalysts, leading to the destruction of organic contaminants to final products CO_2 and water

⇑ XRD patterns and TEM images of synthesised $BiFeO_3$ and $LaFeO_3$ perovskites

⇒ *Sorption-induced Effects of Humic Substances on Mass Transfer of Organic Pollutants through Aqueous Diffusion Boundary Layers: The Example of Water/Air Exchange*
K. Ramus, F.-D. Kopinke, A. Georgi / Environ. Sci. Technol. (2012) **46** 2196

⇒ *Critical Evaluation of the 2D-CSIA Scheme for Distinguishing Fuel Oxygenate Initial Reaction Mechanisms*
M. Rosell, R. González-Olmos, T. Rohwerder, K. Rusevova, A. Georgi, F.-D. Kopinke, H. Richnow / Environ. Sci. Technol. (2012) **46** 4757

⇒ *Nano-sized Magnetic Iron Oxides as Catalysts for Heterogeneous Fenton-like Reactions – Influence of Fe(II)/Fe(III) Ratio on Catalytic Performance*
K. Rusevova, F.-D. Kopinke, A. Georgi / Journal of Hazardous Materials (2012) **241–242** 433

⇒ *Influence of Dissolved Humic Substances on the Mass Transfer of Organic Compounds across the Air-Water Interface*
K. Ramus, F.-D. Kopinke, A. Georgi / Chemosphere (2012) **86** 138

⇒ *Stabilization of Potassium Permanganate Particles with Manganese Dioxide*
K. Rusevova, F.-D. Kopinke, A. Georgi / Chemosphere (2012) **86** 783

⇒ *Nanostructured Catalysts for Contaminant Oxidation in Water by Heterogeneous Fenton-like Reactions*
A. Georgi, K. Rusevova, R. Gonzalez-Olmos, K. Mackenzie / In: Nanotechnology for Water Treatment, Universal Publishers, Boca Raton (USA, 2012)

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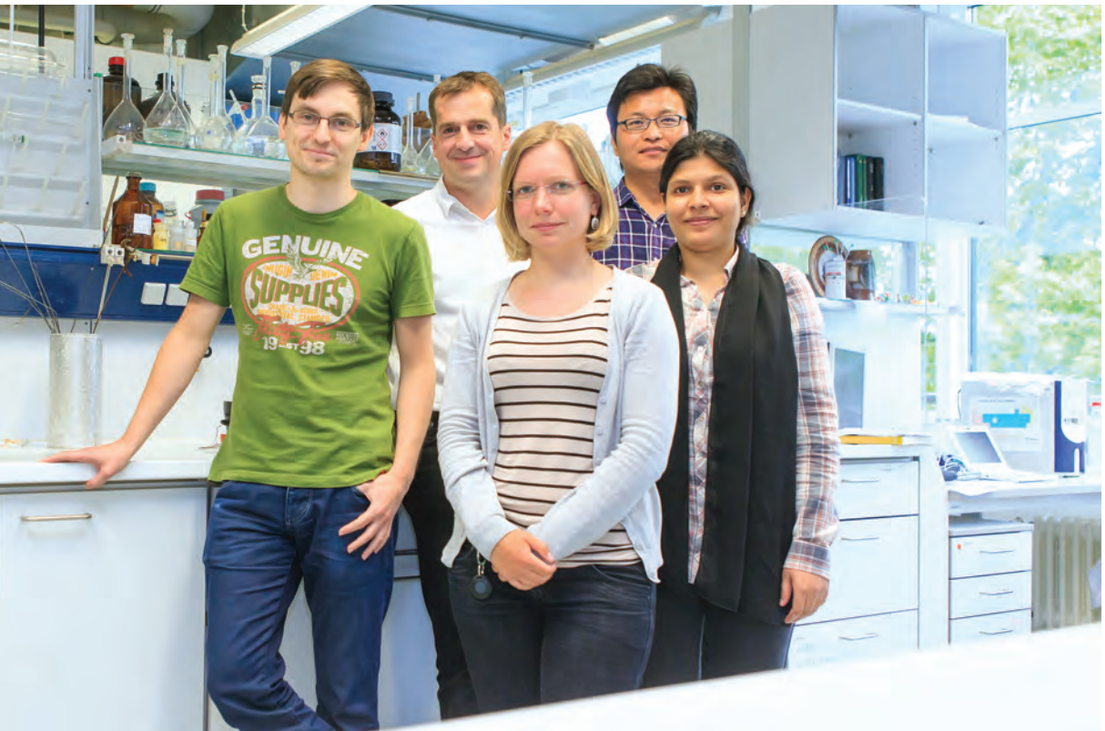
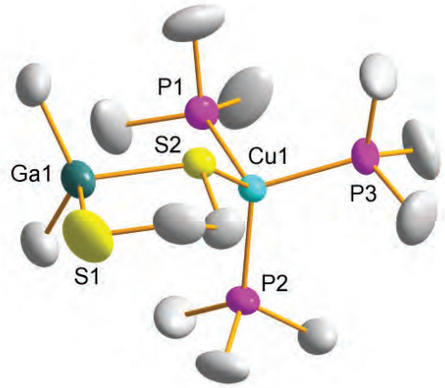
$CuMS_2$ Single-source precursors (M = Ga, In)

Prof. Dr. Harald Krautscheid
M.Sc. Chem. Salma Begum, B.Sc. Chem. Jorge Luis Cholula Díaz,
M.Sc. Chem. Dirk Friedrich, M.Sc. Chem. Marcel Handke, Dr. Jörg Lincke,
M.Sc. Chem. Zhaoyang Wang

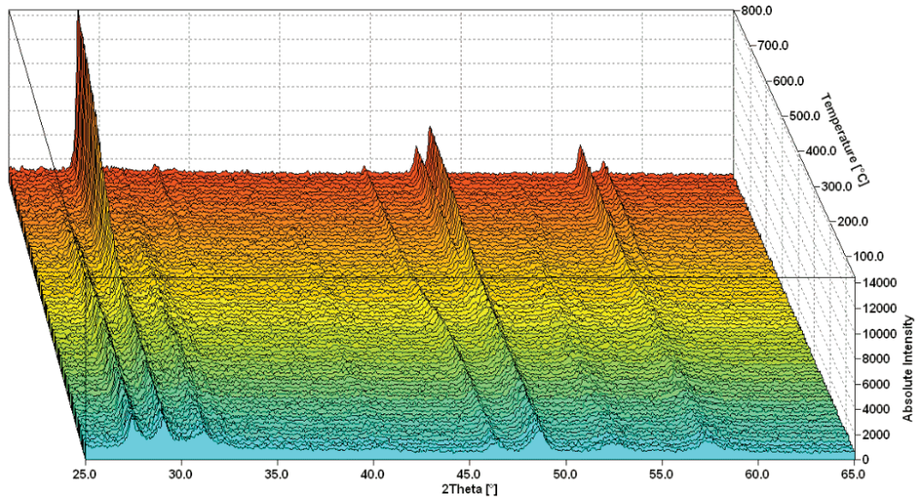
The ternary semiconductors $CuGaS_2$ (bandgap 2.5 eV) and $CuInS_2$ (1.5 eV) can be used for manufacturing flexible thin film solar cells. For such photovoltaic applications, these materials are typically used in their tetragonal chalcopyrite type structure. We developed a series of organometallic complexes that are capable of forming $CuMS_2$ upon pyrolysis at moderate temperatures below 500 °C. As an example, the structure of $[(Me_3P)_3Cu(SCH_2CH_2S)GaMe_2]$ is illustrated below. Unexpectedly, thermolysis of several of our precursor complexes produce hexagonal $CuMS_2$, which is related to the hexagonal ZnS structure (wurtzite) by statistical replacement of zinc atoms by copper and gallium or indium atoms. This is an interesting feature since this nano-structured wurtzite type $CuMS_2$ was discovered just recently for M = In and Ga. As shown by temperature dependent powder X-ray diffraction for the low temperature thermolysis residue of $[(Me_3P)_3Cu(SCH_2CH_2S)GaMe_2]$, the as-produced wurtzite type $CuGaS_2$ is transformed into chalcopyrite structured $CuGaS_2$ at higher temperature. An HRTEM image of a $CuGaS_2$ particle with hexagonal and cubic domains is presented below.

Solutions of the precursor complexes are investigated in spray pyrolysis experiments for the formation of $CuMS_2$ films; the nanoparticles might be useful in ink printing processes for the production of photovoltaic devices based on $CuMS_2$ semiconductors.

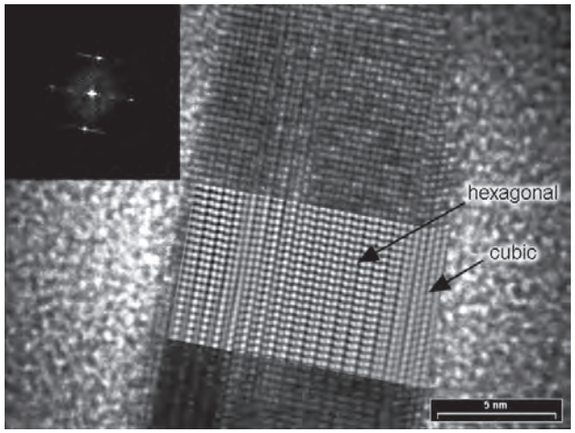




⇐ Molecular structure of the single-source precursor $[(Me_3P)_3Cu(SCH_2CH_2S)GaMe_2]$



⇑ Temperature dependent PXRD of a thermolysis (350 °C) residue of $[(Me_3P)_3Cu(SCH_2CH_2S)GaMe_2]$; broad reflections at low temperature belong to nano-structured wurtzite type $CuGaS_2$; at temperatures above 600 °C the material is transformed into chalcopyrite structured $CuGaS_2$



⇐ HRTEM lattice image of a $CuGaS_2$ particle (Beam direction perpendicular to [0001])
Insets: FFT and Bragg-filtered portion of the crystal

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

Prof. Dr. Friedrich Kremer
Dr. Ciprian-Ghiorghita Iacob, Dipl.-Phys. Wilhelm Kossack, M.Sc. Phys. Ilya Semenov, Dipl.-Phys. Tim Stangner, Dipl.-Phys. Martin Treß, Dipl.-Phys. Olaf Ueberschär, Dipl.-Phys. Carolin Wagner

Glassy dynamics of condensed isolated polymer coils: The glassy dynamics of randomly distributed, condensed isolated and semi-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 40 nm. This geometry presents a pioneering opportunity to investigate both the structure (by Atomic Force Microscopy (AFM)) and the dynamics (via BDS) of exactly the same

⇒ *An Isomorphous Series of Cubic, Copper Based Triazolyl Isophthalate MOFs: Linker Substitution and Adsorption Properties*
J. Lincke, D. Lässig, M. Kobalz, J. Bergmann, M. Handke, J. Möllmer, M. Lange, C. Roth, A. Moeller, R. Staudt, H. Krautscheid / Inorganic Chemistry (2012) **51** 7579

⇒ *New Organometallic Single-Source Precursors for $CuGaS_2$ – Polytypism in Gallite Nanocrystals Obtained by Thermolysis*
O. Kluge, D. Friedrich, G. Wagner, H. Krautscheid / Dalton Transactions (2012) **41** 8635

⇒ *Assessment of Hydrogen Storage by Physisorption in Porous Materials*
M. Bastos Neto, C. Patzschke, M. Lange, J. Möllmer, A. Möller, S. Fichtner, C. Schrage, D. Lässig, J. Lincke, R. Staudt, H. Krautscheid, R. Gläser / Energy & Environmental Science (2012) **5** 8294

⇒ *Solid State Syntheses of Coordination Polymers by Thermal Conversion of Molecular Building Blocks and Polymeric Precursors*
D. Lässig, J. Lincke, R. Gerhardt, H. Krautscheid / Inorganic Chemistry (2012) **51** 6180

⇒ *Pure and Mixed Gas Adsorption of CH_4 and N_2 on the Metal-Organic Framework Basolite® A100 and a Novel Copper-based 1,2,4-Triazolyl Benzoate MOF*
J. Moellmer, A. Moeller, C. Patzschke, K. Stein, D. Lässig, J. Lincke, R. Gläser, H. Krautscheid, R. Staudt, Journal of Materials Chemistry (2012) **22** 10274

⇒ *A Novel Zn_4O-Based Triazolyl Benzoate MOF: Synthesis, Crystal Structure, Adsorption Properties and Solid State ^{13}C NMR Investigations*
J. Lincke, D. Lässig, K. Stein, J. Moellmer, A. Viswanath Kuttatheyil, C. Reichenbach, A. Moeller, R. Staudt, G. Kalies, M. Bertmer, H. Krautscheid / Dalton Transactions (2012) **41** 817

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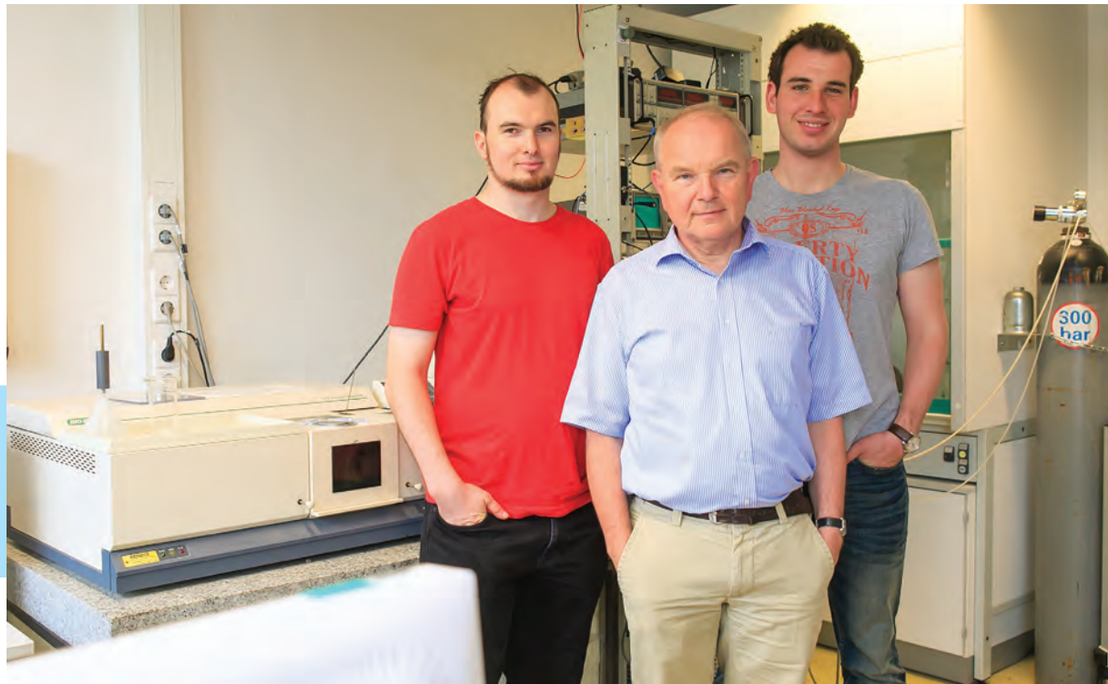
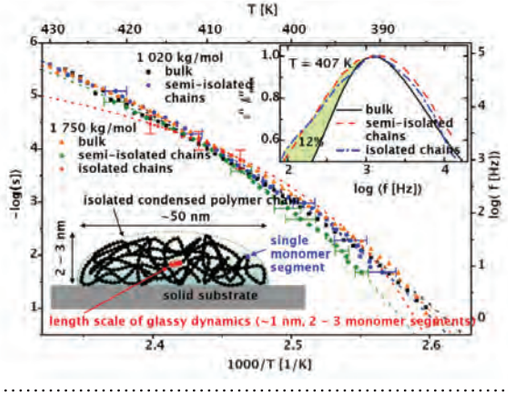


sample. Herein, the former technique reveals that the mean volume of the coils is 1 to 2 times the volume expected for a single chain, while the latter experiments demonstrate that (i) even single polymer chains exhibit VFT temperature dependence, being the characteristic feature for the dynamic glass transition; (ii) for P2VP coils on silicon, the mean relaxation time is bulk-like; and (iii) the relaxation time distribution is broadened especially in the low frequency range – a finding which we assign to interactions between the solid substrate and the first layer of chain segments in the direct vicinity of the interface.

Amino acid sequence dependent interactions between receptors and ligands studied with optical tweezers: For diagnostic procedures that rely on monoclonal antibodies (mAb), it is imperative to know whether the antibody (e.g. HPT-101) recognise the epitope of its target peptide/protein (e.g. tau-protein) specific or whether possible cross-reactivity may occur with other forms of the protein. In Wagner et al. / Soft Matter (2011) **7** 4370 non-specific interactions of two antibodies with the tau-peptide were detected. Based on this result, an epitope mapping was generated. By means of the so called alanine-scan, it is possible to identify essential as well as secondary amino acids for the interaction between the tau-peptide and four different monoclonal. It is apparent that the specificity of the antibody refers not only to a specific isolated phosphorylation site, but to the surrounding amino acid sequence in the tau peptide. First optical tweezers assisted measurements show that the dynamic force spectroscopy approach can make qualitative statements about the existence of essential amino acids and secondary amino acids and identify them, respectively.

Investigating the interactions between GPCRs and ligands on a single-contact level: Optical tweezers provide an extraordinary technique for the investigation of the interactions between biological macromolecules on a single-molecule level as they

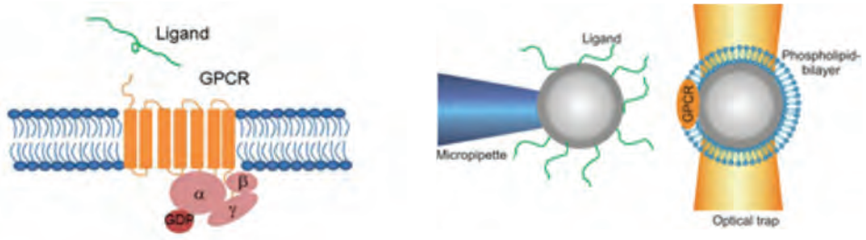


⇑ Mean relaxation time of the segmental dynamics vs. inverse temperature for P2VP bulk, semi-isolated and isolated condensed polymer coils of different molecular weight as indicated. Inset: Corresponding spectra of the dielectric loss demonstrate the broadening in the (semi-)isolated chains at lower frequencies. The scheme visualises why a single polymer chain can still exhibit glassy dynamics.

allow for positioning a micron-sized particle with nanometer resolution and measuring the forces acting on it with an accuracy of ~50 fN. In this project, the system of interest is the interaction between G-protein coupled receptors (GPCRs) and ligands. GPCRs are receptors, which transduce signals through the cell membrane. They consist of extra- and intracellular loops as well as transmembrane segments. The binding of a ligand causes a structural change of the receptor. To measure the binding between the Y2 receptor and its ligand neuropeptide Y by means of optical tweezers, the colloid held in the optical trap is covered with phospholipid bilayers mimicking the cell membrane. The GPCRs will then be inserted into this membrane. Also, the ligand will be immobilised on the surface of a microparticle, which is attached to the tip of a micropipette. In a first step, control experiments have to be carried out to investigate the interaction between membrane-covered particles as well as between a membrane covered particle and a blank one.

Decoupling of ionic conduction from structural dynamics in polymerised ionic liquids: Polarised IR-spectroscopic and mechanical measurements are combined to analyse the ionic conduction and structural dynamics in neat and polymerised bis(trifluoromethyl-sulfonyl)imide-based ionic liquids (IL) are investigated by a combination of Broadband Dielectric Spectroscopy, dynamic mechanical spectroscopy and differential scanning calorimetry. While in the low-molecular weight IL rotational and translational diffusion follow Einstein and Einstein-Smoluchowski equations, for the polymerised system a decoupling between charge transport and structural dynamics by up to two orders of magnitude at low temperatures is found. If rescaled to the calorimetric glass transition temperature T_g, charge transport is more efficient for the polymeric IL.

The interaction between HPT-101 and tau-peptides with different phosphorylation patterns investigated by optical tweezers: Optical tweezers-assisted dynamic force spectroscopy is employed to investigate specific receptor/ligand bindings on the level of single binding events. Here, the specific binding of the anti-human tau monoclonal antibody (mAb) HPT-101 to synthetic tau-peptides with 2 potential phosphorylation (Thr231 and Ser235) sites is analysed. The binding parameters bond lifetime τ_0, the characteristic length x_{ts} and the free energy of activation ΔG are determined for the interactions to the biphosphorylated as well as to the two monophosphorylated peptides. It is shown that the specific binding to the biphosphorylated peptide is much stronger than expected from the summation of the interactions to each monophosphorylated peptide. Calculating the relative affinity from the single-molecule data reveals a significantly higher value for the binding to the biphosphorylated peptide.



⇑ Left: The G-protein coupled receptor consists of extra-, intracellular and transmembrane domains. A ligand binding from the extracellular side causes a structural change of the receptor. Right: Experimental setup to measure the interaction between GPCRs and ligands on a single-contact level. The colloid in the optical trap is covered by phospholipid bilayers containing GPCRs. The ligands are immobilised on the surface of the colloid in the micropipette.

⇒ *Enhanced Charge Transport in Nano-confined Ionic Liquids*
C. Iacob, J.R. Sangoro, W.K. Kipnusu, J. Kärger, F. Kremer / Soft Matter (2012) **8** 289

⇒ *A Novel Video-based Microsphere Localozation Algorithm for Low Contrast Silica Particles Under White Light Illumination*
O. Ueberschär, C. Wagner, T. Stangner, C. Gutsche, F. Kremer / Optics & Lasers in Engineering (2012) **50** 423

⇒ *Molecular Dynamics and Morphology in Confined 4-heptyl-4-isothiocyanoatobiphenyl Liquid Crystals*
M. Jasiurkowska, W. Kossack, R. Ene, C. Iacob, W.K. Kipnusu, P. Papadopoulos, J.R. Sangoro, M. Massalska-Arodz, F. Kremer / Soft Matter (2012) **8** 5194

⇒ *Brownian Dynamics Determine the Universality of Charge Transport in Ionic Liquids*
J.R. Sangoro, M. Mierzwa, C. Iacob, M. Paluch, F. Kremer / RSC Adv. (2012) **2** 5047

⇒ *Molecular Order and Dynamics of Tris(2-ethylhexyl)phosphate Confined in Uni-Directional Nanopores*
W.K. Kipnusu, W. Kossack, C. Iacob, M. Jasiurkowska, J.R. Sangoro, F. Kremer / Z. Phys. Chem. (2012) **226** 797

⇒ *Structure Changes in Nephila Dragline: The Influence of Pressure*
R.C. Ene, R. Krywka, S.-G. Kang, P. Papadopoulos, M. Burghammer, E. Di Cola, M. Müller, F. Kremer / Polymer (2012) **53** 5507

⇒ *Molecular Dynamics of Polymers at Nanometric Length Scales: From Thin Layers to Isolated Coils*
F. Kremer, E.U. Mapesa, M. Treß, M. Reiche / In: Recent Advances in Broadband Dielectric Spectroscopy, Y.P. Kalmykov (Eds.), NATO Science for Peace and Security Series B: Physics and Biophysics, Chapter 12, Springer (2012), ISBN: 978-9-400-75011-1

⇒ *Electrophoretic Mobility and Charge Inversion of a Colloidal Particle Studied by Single-colloid Electrophoresis and Molecular Dynamics Simulations*
I. Semenov, S. Raafatnia, M. Sega, V. Lobaskin, C. Holm, F. Kremer / Phys. Rev. E (2012) **87** 022302

⇒ *Microfluidic Mobility of Single (DNA-grafted) Colloids in Dilute DNA Suspensions*
O. Ueberschär, M. Krüger, C. Gutsche, T. Stangner, C. Wagner, K. Kühne, F. Kremer / Polymer (2012) **53** 5760

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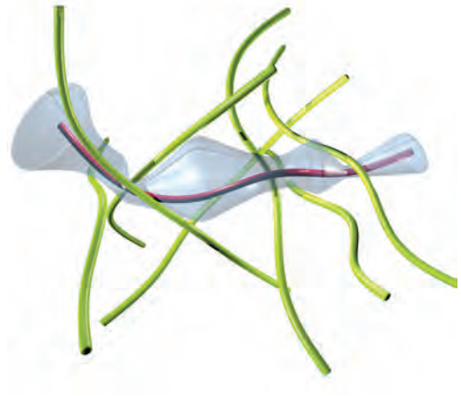
Biopolymers in solutions and transient networks

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

Due to their unique blend of mechanical stability and malleability "on demand", crosslinked polymer networks fill a wide range of biological and industrial needs in the form of plastics, gels or the cell cytoskeleton. Locally, the static and dynamic properties of a polymeric network largely depend on steric crowding effects; based on recent improvements to the phenomenological tube model, where network effects are self-consistently incorporated by a confinement cage on the single polymer level, we discuss the heterogeneous packing structure of biopolymer networks and its bearing on microstructure measurements. In particular, we analyse–motivated by experiments with actin solutions, where the network filaments become shear aligned upon sample preparation–the influence of imposed nematic order on the tube geometry and quantify its widening due to the polymer alignment.

On large timescales, or under extreme conditions such as strong external forces, crosslink remodelling tends to dominate the overall material behaviour, a phenomenon we have previously been able to explain in the context of cell mechanics using



⇐ A test polymer (red) in the network is sterically confined to a tube-like cage (blue) by its impenetrable neighbor filaments

the newly developed “Inelastic GWLC”; we now aim to extend our model to strong temperature variations. We furthermore contribute to the quantitative understanding of crosslink remodelling itself by extending established theories of force-induced unbinding to non-instantaneous intramolecular relaxation and by providing quantitative estimates for the strong frictional forces generated within polymeric force actuators, both of which should become relevant as dynamic force spectroscopy methods evolve towards ever higher loading rates.

⇒ *Resolving the Stiffening-Softening Paradox in Cell Mechanics*
L. Wolff, P. Fernandez, K. Kroy / PLoS ONE (2012) **7** e40063

⇒ *Minimal Model for the Inelastic Mechanics of Biopolymer Networks and Cells*
L. Wolff, K. Kroy / Phys. Rev. E (2012) **86** 040901(R)

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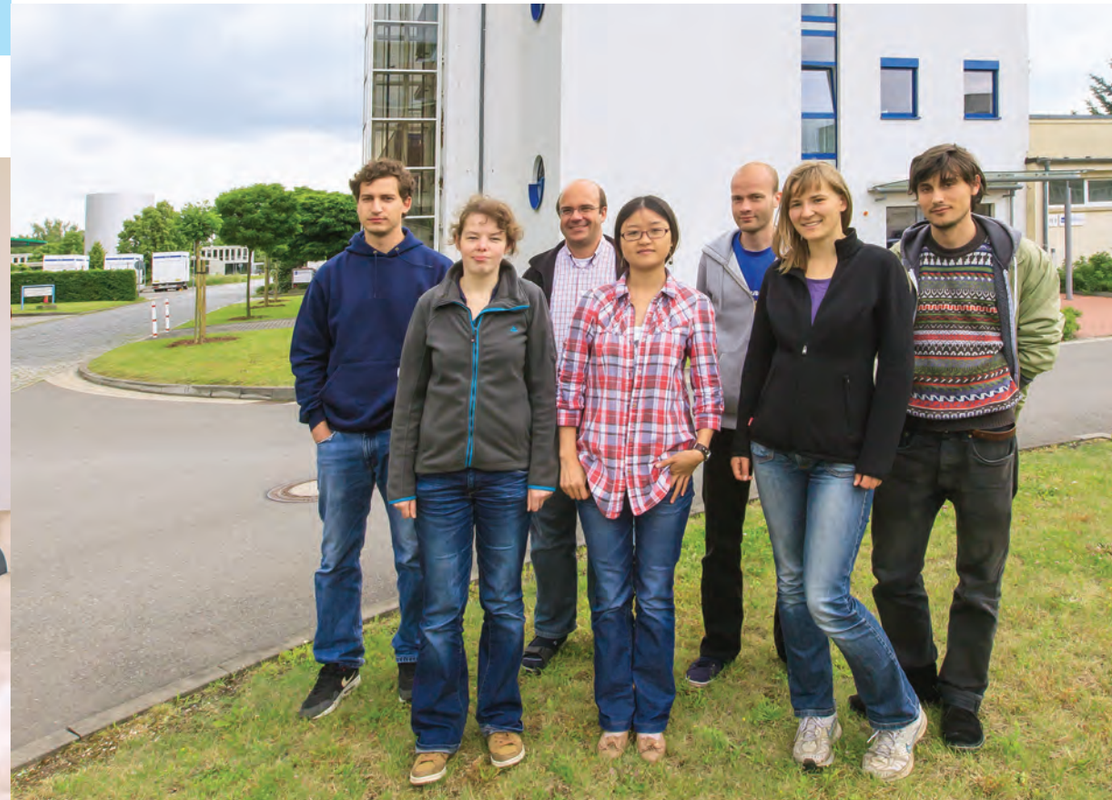
New functional materials for biomedical applications

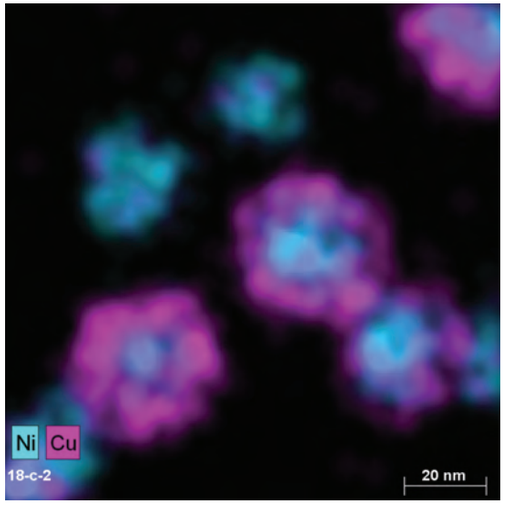
Prof. Dr. Stefan G. Mayr
M.Sc. Phys. Uta Allenstein, Dipl.-Phys. Ariyan Arabi-Hashemi, Dipl.-Phys. Jörg Buchwald, Dipl.-Phys. Anja Graumann, Dipl.-Phys. Marcel Hennes, M.Sc. Phys. Chem. Yanhong Ma

Inorganic-organic interfaces play a central role in different areas of science and engineering. The evaluation of new application purposes requires a detailed understanding of the underlying physical concepts and processes occurring at the nanoscale and their impact on meso- and macroscopic scales. Especially within the field of regenerative medicine, functional materials (e.g. ferromagnetic shape memory materials and core shell nanoparticles) possess useful properties for the realisation of new therapies. Prerequisite requirements for these kind of applica-tions are biocompatibility and external controllability. Within BuildMoNa we currently investigate:



The influence of ion-irradiated on FMSM materials: Using molecular beam epitaxy 500 nm thick single crystalline Fe_7Pd_3 were synthesised and subsequently irradiated with 1.8 MeV Kr^+ ions of different fluences. XRD Theta/2Theta and pole figure measurements show a fluence dependent phase transformation from fcc austenite to different martensite phases ending in the Nishiyama-Wassermann orientation relation. The reason for this process is found in point defect induced stress fields, which increase the austenite-martensite transformation temperature according to Clausius-Clapeyron.

Synthesis of magnetic core-shell (CS) nanoparticles: Magnetic nanoparticles can be employed in a variety of fields in medicine and biodiagnostics, e.g. as contrast enhancer in magnetic resonance imaging or as colloidal mediator for cancer therapy. Corrosivity and cytotoxicity of most magnetic materials can be overcome by synthesising heterostructured magnetic particles, with a thin noble metal shell covering the magnetic core. We therefore explored the possibility to obtain these highly desired CS-structures by self-organisation through phase separation and surface segregation at the nanoscale. As computer simulation results, based on a hybrid Molecular-Dynamics/Metropolis Monte-Carlo approach, indicate absence of rotationally symmetric equilibrium structures, a gas phase condensation setup with additional coating stage has been designed and successful production of CS particles could be demonstrated, paving the way for future biocompatibility tests.



⇐ Cu/Ni core shell nanoparticles

The simulation of mechanical properties of surfaces at the nanoscale: CR-AFM (Contact-Resonance Atomic Force Microscopy) is a new experimental technique that allows resolving mechanical properties at the nanoscale. To get a better understanding of this new measurement technique, we performed "ab-initio" (DFT-) simulations to calculate the surface elastic constants. Due to the computational limits of DFT, we are only able to simulate a few atom layers. As materials, we simulated silicon and strontiumtitanate, which were also measured by the CR-AFM technique and used as reference samples. In combination with a conjugate gradient method, we can extrapolate the elastic constants to almost the entire film thickness range. Additionally, we began to study the dissipative behaviour of a periodic indentation on a silicon thin film using classical molecular dynamics.

⇒ *Freestanding Single Crystalline Fe–Pd Ferromagnetic Shape Memory Membranes – Role of Mechanical and Magnetic Constraints Across the Martensite Transition*
Y. Ma, A. Setzer, J.W. Gerlach, F. Frost, P. Esquinazi, S.G. Mayr / Adv. Funct. Mater. (2012) **22** 2529

⇒ *Ion-Irradiation-Assisted Phase Selection in Single Crystalline Fe_7Pd_3 Ferromagnetic Shape Memory Alloy Thin Films: From fcc to bcc along the Nishiyama-Wassermann Path*
A. Arabi-Hashemi, S.G. Mayr / Phys. Rev. Lett. (2012) **109** 195704

⇒ *Structural Defects in Fe-Pd-based Ferromagnetic Shape Memory Alloys: Tuning Transformation Properties by Ion Irradiation and Severe Plastic Deformation*
S.G. Mayr, A. Arabi-Hashemi / New J. Phys. (2012) **14** 103006

⇒ *Structural Properties of Spherical Cu/Ni Nanoparticles*
M. Hennes, J. Buchwald, S.G. Mayr / CrystEngComm (2012) **14** 7633

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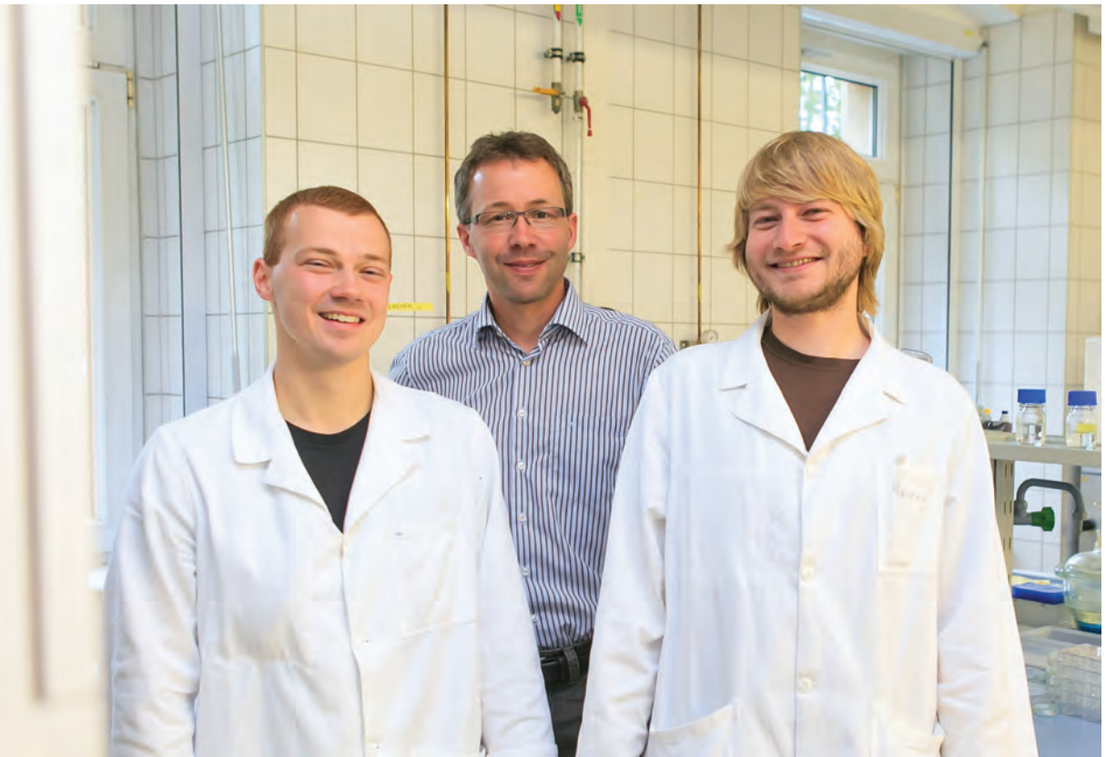
Engineering biomimetic microenvironments for *in vitro* cell studies

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

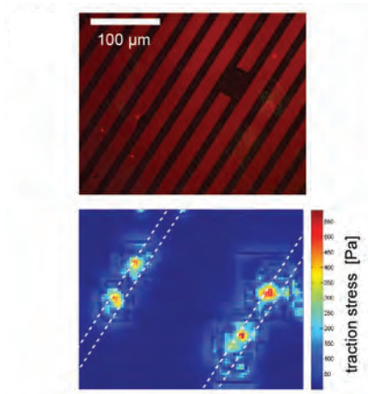
The extracellular microenvironment controls many cellular processes including cell growth, differentiation and apoptosis. In order to better understand these regulating cues biomimetic systems are used for in-depth analysis in high-resolution *in vitro* studies. We design and construct materials scaffolds 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, which are considered to be important in the bone marrow stem cell niche. Using polymeric microparticles with glycosaminoglycan functionalisation a controlled and slow release of SDF-1, Dkk-1 and Wnt3a microscale gradients are established in 2D and 3D cell culture scaffolds.

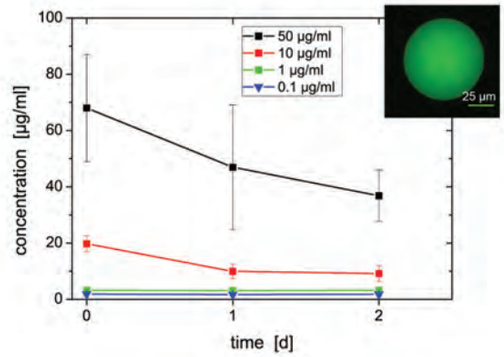


A. Müller uses synthetic hydrogel layers to model the impact of materials stiffness, ligand affinity and spatial constraints on cell adhesion. Synthetic peptide ligands as well as polymer coatings allow a control of ligand affinity, which subsequently affects ligand mobility under dynamic force load of cellular adhesion receptors. In combination with these cues spatial constraints are modelled as well by introducing micropatterns on top of the polymer-coated hydrogel layers.

Overall these systems allow us to investigate the dynamic cell behaviour in vitro at defined microenvironmental conditions for a number of cell types including hematopoietic stem cells, endothelial cells, fibroblasts and macrophages.



⇑ Traction force microscopy of endothelial cells on micropatterned hydrogel substrates (red: fibronectin ligand, green: displaced fluorescent beads of traction force microscopy)



⇑ Loading-dependent (concentration in legend), slow release of a protein (i.e. lysozyme) from heparin-functionalised agarose microparticles (inset, green: heparin-FITC)

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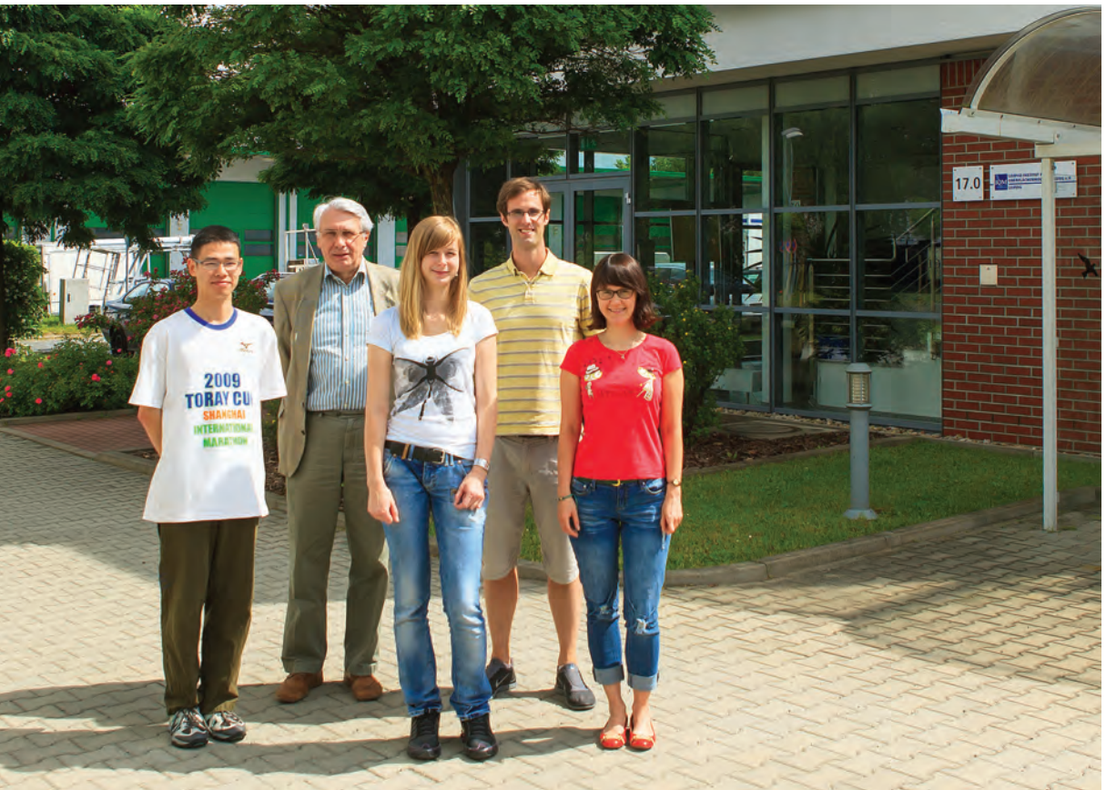
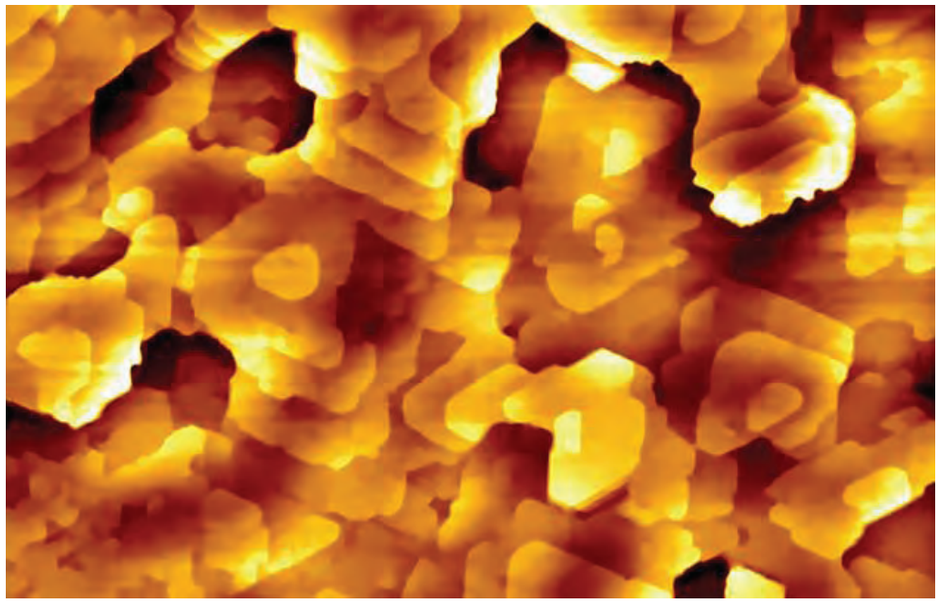
Ion beam assisted thin films and nanostructure deposition

Prof. Dr. Dr. h.c. Bernd Rauschenbach
Dr. Chinmay Khare, Dipl.-Phys. Lena Neumann, M.Sc. Phys. Marina Sarmanova, M.Sc. Chem. Eng. Erik Thelander

The studies to preparation and characterisation of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium were continued. The research was focused on the application of ion and laser beam assisted techniques. 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 induced by the additional low-energy ion bombardment and pulsed laser irradiation, respectively. A main emphasis of this research was the preparation of ultra-thin GaN films (< 50 nm) on different substrates by ion beam assisted molecular beam epitaxy. These films are characterised by ultra-smooth surfaces, a strong defect reduction and a perfect interface between the substrate silicon carbide and the gallium nitride layer. Scanning tunnelling microscope studies demonstrate a terrace-step structure which is evidence for a two-dimensional growth mode.



Either in nanolectronics or nanoelectromechanical systems, mechanical property characterisation of the constituent building blocks in the form of ultrathin films and one-dimensional nanostructures (nanotubes, nanowires, nanobelts, etc.) is a necessary step for their assembly and functionality. It is thus imperative to develop techniques capable of providing easy and reliable mechanical property measurements at the nanoscale. Benefiting from the nanoscale spatial resolution of atomic force microscopy, contact-resonance atomic force microscopy (CR-AFM) provides direct measurements of the elastic responses of materials at the nanoscale. We have used the capabilities of CR-AFM to study the local mechanical properties on surfaces.



⇑ Two-dimensional growth of ultra-thin GaN film on ^{6}H-SiC substrate prepared by ion beam assisted molecular beam epitaxy and measured by scanning tunnelling microscopy

⇒ *Initial Stages of the Ion-beam assisted Epitaxial GaN Film Growth on 6H-SiC(0001)*
L. Neumann, J.W. Gerlach, B. Rauschenbach / Thin Solid Films (2012) **520** 3936

⇒ *Hyperthermal Ion-beam assisted Droplet Epitaxy of Gallium Nitride Thin Films*
J.W. Gerlach, T. Ivanov, L. Neumann, Th. Höche, D. Hirsch, B. Rauschenbach / J. Appl. Phys. (2012) **111** 113521

⇒ *Microspot Sensing based on Surface Enhanced Fluorescence from Nanosculptured Thin Films*
A. Karabchevsky, C. Khare, B. Rauschenbach, I. Abdulhalim / J. of Nanophotonics (2012) **6** 061508

⇒ *$Ge_2Sb_2Te_5$ Phase-change Films on Polyimide Substrates by Pulsed Laser Deposition*
H. Lu, E. Thelander, J.W. Gerlach, D. Hirsch, U. Decker, B. Rauschenbach / Appl. Phys. Lett. (2012) **101** 031905

⇒ *Effects of Annealing on Arrays of Ge Nanocolumn formed by Glancing Angle Deposition*
C. Khare, J.W. Gerlach, T. Höche, B. Fuhrmann, H.S. Leipner, B. Rauschenbach / Appl. Surf. Sci. (2012) **258** 9762

⇒ *Ion Beam Sputter Deposition of Epitaxial Ag Films on Native Oxide Covered Si(100) Substrates*
C. Khare , J.W. Gerlach, C. Patzig, B. Rauschenbach / Appl. Surf. Sci. (2012) **258** 9617

⇒ *Detailed Study of Surface Enhanced Raman Scattering from Metallic Nano Sculptured Thin Films and their Potential for Biosensing*
A. Shalabney, C. Khare, B. Rauschenbach, I. Abdulhalim / J. of Nanophotonics (2012) **6** 48

⇒ *Influence of Burst Pulses on Film Topography on Picosecund Pulsed Laser Deposition of $LaAlO_3$*
E. Thelander, B. Rauschenbach / J. of Phys. Conference Series (2012) **365** 012015

⇒ *Non-periodic Nanostructure Templates by Diffraction Mask Projection Laser Ablation*
M. Mäder, T. Höche, B. Rauschenbach / Phys. Stat. Sol. A (2012) **209** 2208

⇒ *Ordered Si-Ge Nanostructures by Glancing Angle Deposition via Ion Beam Sputtering*
J. Bauer, M. Weise, C. Khare, B. Rauschenbach / Proceed. MRS Symp. (2012) **1329** 81

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

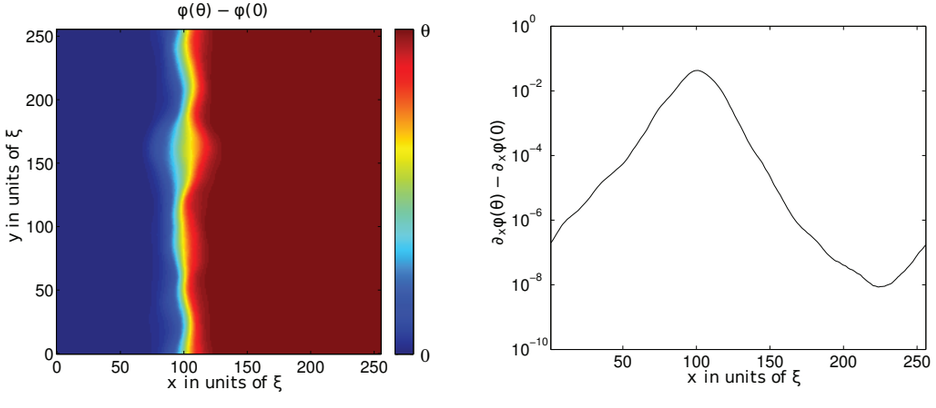
Prof. Dr. Bernd Rosenow
Dipl.-Phys. Alexander Janot, M.Sc. Phys. Martin Treffkorn

In our research we study low-energy excitations of quantum condensates, e.g. superfluid exciton-polariton condensates, quantum Hall fluids, and superconductors. All these systems are characterized by collective quantum dynamics which can be attributed to the excistence of a macroscopic wave function. Recent experimental obeservation of these remarkable phenomena are the coherent emission of light from exciton-polariton condensates, and the dissipationless counterflow and Josephson-like interlayer current for exciton condensates in quantum Hall double layers.

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 generalization 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. An important building block of such interferometers are quantum point contacts, which allow tunnelling between counter-propagating edge states.

With our recursive Green function algorithm we try to study transport through quantum point contacts as they are used in experiments. To that end we attempt to implement a realistic self-consistent model of a gate induced quantum point contact build from specific semi-conductor heterostructures. From such a model we may obtain an effective two-dimensional description of the potential landscape inside the 2D electron gas, which we can use in our transport algorithm. The results obtained in this way, might be used to design experiments in such a way that they can either achieve or avoid conductance oscillations inside a single quantum point contact.

For the case of the exciton-polariton condensate we have investigated the superfluid stiffness in a disordered environment taking into account a non-equilibrium pumping mechanism. We found that on short length scales the disorder is screened by fluctuations of the condensate density, while on longer scales the quantum mechanical phase starts to fluctuate, too, which destroys the long range correlation of the quantum wave function. In order to calculate the condensate superfluid stiffness we have studied the response of the system to an externally imposed phase twist. We found that for sufficiently large non-equilibrium system the response occurs by formation of a domain wall, which is randomly pinned. Our calculations predict that the superfluid stiffness vanishes for condensates which are larger than a critical 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.



⇑ Domain wall formation in an externally driven and disordered quantum condensate as response to an imposed phase-twist, θ, along the x-direction. We show a snap shot of the phase (left panel) and current (right panel) response for one disorder realization. We observe a randomly pinned local response with exponentially decaying tails, which is characteristic of a domain wall. The decay length decreases with increasing disorder strength and particle depletion.

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Experiences

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

Prof. Dr. Bernd Abel

BuildMoNa has passed very successful years now – making Leipzigs University and the connected scientific institutions very visible within Germany and outside. It has been a very important tool and platform to combine excellent research and excellence in teaching. It is very clear that the students as well as the teachers and scientists benefitted and still benefit much more from it than anticipated at the beginning and as one may actually 'feel' as a member of BuildMoNa. The community of scientists within BuildMoNa has become a family now and all participate with enthusiasm – also those who entered the 'family' quite late, such as myself in 2008.

Unfortunately, the BuildMoNa extension proposal was not successful in the recent round of the German Excellence Initiative. This BuildMoNa a serious issue and this will certainly limit the possibilities in the future. Nevertheless, it is strong enough to continue its way as a very important and successful graduate school – with much support from other sources. University and non-university institutions – as well as colleagues from all participating institutions – are strong enough to

BuildMoNa has passed very successful years now – making Leipzigs University and the connected scientific institutions very visible within Germany and outside. It has been a very important tool and platform to combine excellent research and excellence in teaching. It is very clear that the students as well as the teachers and scientists benefitted and still benefit much more from it than anticipated at the beginning and as one may actually 'feel' as a member of BuildMoNa. The community of scientists within BuildMoNa has become a family now and all participate with enthusiasm – also those who entered the 'family' quite late, such as myself in 2008.

Unfortunately, the BuildMoNa extension proposal was not successful in the recent round of the German Excellence Initiative. This BuildMoNa a serious issue and this will certainly limit the possibilities in the future. Nevertheless, it is strong enough to continue its way as a very important and successful graduate school – with much support from other sources. University and non-university institutions – as well as colleagues from all participating institutions – are strong enough to continue the important and successful concept of BuildMoNa in the future.

As a BuildMoNa member with centres of gravity and roots at the university and in a non-university institute I really look with a 'loving eye' on our BuildMoNa graduate school. It enhances discussions with colleagues, it enables recruiting excellent students, and it seems to be a nice 'glue' for very different institutions, which otherwise compete for resources and students. This was one of the most important benefits of BuildMoNa in the past and it will be in the future.

So, all the best and much further success for BuildMoNa in the future, also as a continuously living platform of teaching, excellence, scientific exchange, and further growth! BuildMoNa is – and will be – strongly embedded in the Research Academy Leipzig, the overall framework for graduate research training at our University and it is strongly connected to and important for future Top-Level Research Areas and the planned Collaborative Research Centres of our University.

Prof. Dr. Bernd Abel

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

M.Sc. Chem. Wilma Neumann

The fifth year of BuildMoNa was probably the most emotional year since the implementation of the graduate school in 2007. After all these years the built-up structures and programmes were well established. However, the renewal proposal for the second round of the German Excellence Initiative played the central role this year and took a lot of effort from the PIs and the coordinators. After the official presentation of the graduate school in Bonn in February 2012, a long time of waiting followed for the final decision of the reviewers on 15th of June. The application process, including the evaluation of the graduate school, stimulated all members to strengthen the interdisciplinary and collaborative environment and to improve the concepts. Although funding of the graduate school by the DFG as part of the Excellence Initiative was not prolonged, the graduate school received a positive review which should encourage its members to continue this interdisciplinary project and to implement some of the newly elaborated concepts. Some have already been realised, such as the introduction of basic modules trying to bring students from dif-

ferent scientific backgrounds to a similar level of fundamental knowledge. This is important to increase the efficiency of the interdisciplinary scientific modules and has also been very well received by the doctoral candidates (DCs).

As the largest class of the Research Academy Leipzig (RALeipzig), BuildMoNa has set new standards for the structured doctoral qualification at Universität Leipzig. Especially the module programme of transferable skills has offered many opportunities for the DCs to improve their soft skills, which are also important for interdisciplinary research. BuildMoNa has established a programme in English also available for international students, which will now be organised together with the RALeipzig.

Especially now after funding by the DFG will only continue until October 2014, the Universität Leipzig and RALeipzig should support these established structures of the graduate school and should promote its interdisciplinarity. They should help to propagate that BuildMoNa will continue as a class at the RALeipzig and offer to build up new collaborative structures.

The RALeipzig could also be inspired by BuildMoNa in the communication between the PIs and the DCs. The Steering Committee of the graduate school has always been open to ideas and comments of the DCs and has tried to support or implement them, such as the fusion of the Scientific Symposium in autumn and the Doctoral Candidates' Workshop in spring to one joint meeting, the Annual BuildMoNa Conference, which will take place in March each year.

However, the DCs should even more communicate their needs and concerns to allow further improvement of the graduate school, which serves as an inspiring and supporting platform for young scientists. On the other hand, BuildMoNa should further encourage and support the DCs to develop interdisciplinary, collaborative research and should communicate the advantages of a structured doctoral qualification whenever possible, especially now after reorientation of the graduate school.

M.Sc. Chem. Wilma Neumann

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
Workshop for doctoral candidates	R								W					
Scientific symposium	R/E		SY											
Literature seminars	R/E			S		S		S		S		S		S
Guest lectures/colloquia	E	5	L	L	L	L	L	L	L	L	L	L	L	L
Tutoring	R/E			T	T	T	T			T	T	T	T	
Research stays abroad	E		flexible during the whole year (1 week up to a few months)											
Summer/winter schools	E													
Industrial training	E													
Active participation in conferences/workshops	R/E		flexible during the whole year (1 up to a few days)											
Transferable (generic) skills	R/E	5		S	S	S	S			S	S	S	S	
					M		M				M		M	

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

Scientific and methods modules

Basic concepts in chemistry (2012-B1)

22 / 23 March 2012,
written exam, 2 credit points, yearly recurrence, 31 participants

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

Responsible Scientists/Lecturers:
Prof. Dr. B. Abel, Prof. Dr. B. Kersting, Prof. Dr. B. Kirchner,
Prof. Dr. H. Krautscheid

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

⇒ The chemical bond: 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 com-position 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

⇒ Theoretical chemistry: introduction to computational chemistry, basic concepts, intermolecular forces, basic quantum chemistry of electronic structure and diversity of methods, density functional theory, force fields, molecular dynamics simulations, applications and examples from the computer

Basic concepts in biochemistry (2012-B2)

7 / 8 March 2012,
written exam, 2 credit points, yearly recurrence, 26 participants

Doctoral researchers without a background in biochemistry or biology will be brought up to a level necessary to understand the thematic and advanced modules (T1–T6, A2, A1). The module introduces basics in bioactive molecules and biomacromolecules, including their structure and (bio)chemical properties, as well as cell biology. The doctoral researchers will learn 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:
Prof. A.G. Beck-Sickinger, Universität Leipzig, Germany; Dr. C. Berger, Universität Leipzig, Germany; Dipl.-Biochem. S. Berndt, Universität Leipzig, Germany; Dr. A. Chatzinotas, UFZ, Leipzig, Germany; Prof. Dr. H. Harms, UFZ, Leipzig, Germany; Prof. Dr. D. Huster, Universität Leipzig, Germany; Prof. Dr. S. Müller, UFZ, 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 (2012-B3)

13 / 14 / 21 February 2012,
written exam, 2 credit points, yearly recurrence, 6 participants

Doctoral researchers without a physics background will be brought up to a level necessary to understand the thematic and advanced modules (T1–T6, A3, A2). The doctoral researchers will gain 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 will also be exposed to fundamental concepts of statistical physics and thermodynamics. Moreover, they will gain 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:
⇒ Fundamentals of matter
⇒ Solid-state physics (charge transport, band structure, Bloch oscillation, point contacts, tunnelling, magnetotransport)
⇒ Diffusion (Brownian motion, mass transport, random motion, ballistic motion, dissipation)
⇒ Hydrodynamics
⇒ Nanoconfinement (electrons, photons, phonons, structured dielectric media/ photonic crystals, plasmons, metallic nanostructures)
⇒ 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)

Smart molecules: Synthesis, properties, and applications of macrocycles and cage compounds (2012-T1)

28 / 29 June 2012,
written exam, 2 credit points, yearly recurrence with modification, 19 participants

The module aimed at 1. Understand how macrocycles and cage compounds are obtained by conventional synthesis or self-assembly processes; 2. Understand the chemical properties, spectroscopic and structural features of cyclic or cage compounds; 3. Understand the properties and applications of these host compounds.

Responsible Scientists:
Prof. Dr. E. Hey-Hawkins, Prof. Dr. B. Kersting

Lecturers:
Jun.-Prof. Dr. Guido Clever, Universität Göttingen, Germany; Prof. Dr. Peter Comba, Universität Heidelberg, Germany; Prof. Dr. Peter G. Edwards, Cardiff University, UK; Prof. Dr. Evamarie Hey-Hawkins, Universität Leipzig, Germany; Prof. Dr. Jennifer Hines, Ohio University, Athens, USA; Prof. Dr. Berthold Kersting, Universität Leipzig, Germany; Dr. Jonathan Nitschke, University of Cambridge, UK; Dr. Milosz Pawlicki, University of Wroclaw, Poland; Prof. Dr. Christoph Schalley, FU Berlin, Germany

Contents:
⇒ RNA molecular switches and springs
⇒ Container molecules
⇒ Coordination cages
⇒ Modelling macrocycles
⇒ Mass spectrometry of cages and capsules
⇒ Basic and modern aspects of porphyrin chemistry
⇒ Facially capping phosphorus macrocycles
⇒ PN-based macrocycles and cages
⇒ Basics of macrocyclic chemistry

Methods:
⇒ Synthesis
⇒ Synthesis of macrocycles
⇒ Cages and capsules
⇒ Handling and characterisation of cyclic and cage compounds

Multifunctional scaffolds (2012-T2)

27 / 28 September 2012,
written exam, 2 credit points, yearly recurrence with modification, 17 participants

The module aims at providing the scientific background required to study and manipulate biopolymers, biopolymer networks, proteins and protein networks and aggregates, to understand the stability and mechanical actuation of cells and tissues, and its dependence on the architecture of protein aggregates, cell membranes and characteristic cytoskeletal structures, as well as tissue architecture.

Responsible Scientists:
Prof. Dr. W. Janke, Prof. Dr. F. Kremer, Prof. Dr. K. Kroy, Prof. Dr. T. Pompe

Lecturers:
Dr. John Dunlop, MPI Golm, Germany; Dr. Claus Heussinger, Universität Göttingen, Germany; Prof. Dr. Anders Irbäck, Lund University, Sweden; Dr. Martin Steinhauser, FRIAS Freiburg, Germany; Norman Wagner, University of Delaware, USA

Contents:
⇒ Physical, biochemical & biological perspective on various multifunctional scaffolds and modern experimental techniques
⇒ General soft matter properties, statistical physics and simulation approaches, protein aggregates, complex interactions in aqueous media, complex suspension flows, biopolymers, biopolymer bundles and networks, and lipid bilayers
⇒ Computational approaches to assess the stability, nucleation, and growth of aggregate structures (e.g. amyloid fibrils), protein folding and misfolding, theoretical and experimental techniques to assess biopolymer bundle formation and bundle mechanics, and the mechanical stability of lipid bilayers and cell membranes
⇒ Role of confining geometries on tissue growth and the role of tissue architecture on hygroscopic actuation in plant cells

Methods:
⇒ Rheology
⇒ Micro-rheology
⇒ In-vitro and in-situ ultrasound techniques
⇒ Tissue engineering
⇒ Statistical mechanics
⇒ Theoretical modeling
⇒ Monte Carlo and Molecular Dynamics computer simulations

Complex nanostructures (2012-T3)

9 / 10 July 2012,
oral exam, 2 credit points, yearly recurrence with modification, 23 participants

The module aims at deepen the understanding of physics and materials properties at the nanoscale as accessible by direct imaging and quantification of materials properties using scanning tunneling (STM) and atomic force microscopy (AFM), atomic force acoustic microscopy (AFAM) as well as scanning electron (SEM) and high resolution transmission electron microscopy (TEM).

Responsible Scientists:
Prof. Dr. B. Rauschenbach, Prof. Dr. S. Mayr

Lecturers:
Prof. Dr. O. Eibl, Universität Tübingen, Germany; Dr. W. Erfurth, MPI Halle/S., Germany; Prof. Dr. T. Höche, Fraunhofer Halle/S., Germany; Prof. Dr. L. Kienle, Universität Kiel, Germany; Dr. B. Köhler, Fraunhofer IZFP Dresden, Germany; PD Dr. S. Wirth, MPI CPFS Dresden, Germany

Contents:
⇒ Understanding of physics behind high resolution imaging techniques, and state-of-the art capabilities for spatially-resolved materials characterisation
⇒ Impact of dimensionality, open surfaces and interfaces on physical and materials properties
⇒ Relation of global properties to macroscopic response

Methods:
⇒ Introducing the most prominent direct imaging-techniques (STM, AFM, SEM, TEM) – from the fundaments to their technical realisation
⇒ Practical training / instrument demonstration in the laboratory

From molecules to materials (2012-T4)

5 / 6 July 2012,
oral exam, 2 credit points, yearly recurrence with modification, 7 participants

This module links molecular science and materials science, teaches how materials with optimised properties such as fluidity, liquidcrystallinity, catalytic activity and adjustable magnetic, electronic, or mechanical properties are obtained from molecules, and provides an understanding of the properties and applications of these materials.

Responsible Scientists:
Prof. Dr. R. Gläser, Prof. Dr. F. Kremer, Prof. Dr. H. Krautscheid

Lecturers:
Prof. Dr. R. Gläser, Universität Leipzig, Germany; Prof. Dr. H. Krautscheid, Universität Leipzig, Germany; Prof. Dr. F. Kremer, Universität Leipzig, Germany; Prof. Dr. Arne Thomas, TU Berlin, Germany; Prof. Dr. Brigitte Voit, Leibniz-Institut für Polymerforschung Dresden e.V., Germany

Contents:
⇒ Synthesis of metallic and polymeric materials and coordination polymers
⇒ Basic properties of the liquid and the liquid crystalline state
⇒ Catalytic supports from “hard” (synthetic molecules and crystalline nanostructures) and/or “soft” (polymers) building blocks, which include: polymers, hybrid materials, supramolecular arrangements; modifications to improve the material qualities
⇒ Properties of these materials: porosity, pore size distribution, specific surface area, functionality, thermal properties, mechanical properties
⇒ Application of these materials in catalysis (heterogeneous/immobilised catalysts), for gas separation or gas storage (MOFs), as sensors etc.

Methods:
⇒ Seminars

Hybrid systems (2012-T6)

26 / 27 June 2012,
oral exam, 2 credit points, yearly recurrence with modification, 8 participants

Strengthening the understanding of cell/substrate interfaces concerning complex neuronal organotypic tissues. Neurogenesis and synaptogenesis depenedent on substrate topology and cellular adherence will be the focus of the teaching programme. Processes of directed axonal outgrowth dependent on guidance molecules in combination with subcellular changes and cytoskeleton architecture can be monitored in real time using microelectrode arrays. Therefore some basics of microelectrode configuration and surface topology will be presented in a tutorial. The principles field potential recording, impedance spectroscopy in correlation with high resolution microscopy in a nanoscale on various biochips will be trained in theory and practice. Finally some applications of miniaturised recording devices regarding injury and degenerative progress of neurons and their neuritis will be demonstrated.

Responsible Scientists:
Prof. Dr. A. Robitzki

Lecturers:
Dr.-Ing. Ulf-Dieter Braumann, IZBI Leipzig, Germany; Dr. Heinz-Georg Jahnke, BBZ Leipzig, Germany; Prof. Dr. W. Janke, Universität Leipzig, Germany; PD Dr. Uwe Pliquett, IBA Heiligenstadt, Germany; Prof. Dr. A. Robitzki, BBZ Leipzig, Germany

Contents:
⇒ Neuronal cell biology, guidance molecules and axonal out growth
⇒ Microarrays, various microelectrode configurations and electrode surface topologies
⇒ Brain slices and neurospheres on microarrays for impedance spectroscopy and field potential recording in combination with modeling & imaging microscopic anaylsis
⇒ Electrodes – the challenge in electrical characterisation of biological material
⇒ Computer simulation of polymers in disordered media
⇒ Work stations for brain slice recording on a chip (demonstration / practical course)

Methods:
⇒ Impedance spectroscopy
⇒ Field potential recording
⇒ High resolution microscopy of cells and tissues
⇒ Imaging of microscopic analysis

Smart and Active Assemblies (2012-A1)

18 / 19 October 2012,
written exam, 2 credit points, yearly recurrence with modification, 12 participants

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

Responsible Scientists:
Prof. Dr. G. Gläser, Prof. Dr. E. Hey-Hawkins

Lecturers:
Dr. M. Armbrüster, MPI für Chemische Physik fester Stoffe, Dresden, Germany; Prof. Dr. M. Bertau, TU Freiberg, Germany; Prof. Dr. R. Gläser, Universität Leipzig, Germany; Prof. Dr. M. Hartmann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Prof. Dr. E. Hey-Hawkins, Universität Leipzig, Germany; Prof. Dr. P.C.J. Kamer, St. Andrews, UK; Prof. Dr. S. Kureti, TU Freiberg, Germany

Contents:
⇒ Complex assemblies (specific synthesis, modification, structure and catalytic properties, various environments with optimised catalytic activity, selectivity and stability)
⇒ Complex catalysts (functionalised mixed metal (oxide) nanoparticles, metal complexes, MOFs, immobilisation of catalysts (on solid or in liquid supports))
⇒ Complex biocatalysts (developing of engineered enzymes, immobilisation of enzymes, surface modification, improved tailor-made biocatalysts, biomimetic catalyst assemblies (zeozymes, artizymes))
⇒ Catalytic activation by smart assemblies (activation of unreactive molecules or solids, enantioselective catalysis)
⇒ Theory (novel modelling tools, large-scale computations of real-world applications of complex structures and their properties, local and electronic structure of active sites)

Methods:
⇒ Active site assemblies (synthesis, characterisation of electronic and structural properties by molecular spectroscopy)
⇒ Catalysts (spectroscopy under working conditions, advanced testing, e.g., via high-throughput experimentation)
⇒ Theoretical methods

Chemical biology and biophysics of cancer (2012-A2)

13 / 14 November 2012,
written exam, 2 credit points, yearly recurrence with modification, 16 participants

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

Responsible Scientist:
Prof. Dr. J. Käs

Guest Lecturers:
Prof. Dr. Gabriela Aust, Universität Leipzig, Germany; Prof. Dr. Ben Frabry, Universität Erlangen-Nürnberg, Germany; Dr. Jörg Galle, IZBI Leipzig, Germany; Prof. Dr. Josef Käs, Universität Leipzig, Germany; Prof. Dr. Claudia Mierke, Uni-

versität Leipzig, Germany; Prof. Dr. Torsten Remmerbach, Universität Leipzig, 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)
⇒ Diagnostics and screening (cytobrushes, imaging [CT, MRI], tumour markers, histology, tumour staging)
⇒ Therapy (surgery, radiation, chemotherapy [antineoplastic drugs, cytostatic molecules, protein kinase inhibitors])
⇒ Targeted tumour therapy (specific and unspecific shuttles, specific expression of cell surface proteins, internalisation of biomolecules into tumour cells, linkers for controlled release, etc.)
⇒ Personalised medicine and better tumour staging (single cell analysis, high throughput and content, genetic networks, tumour specific tracers and their application by PETimaging or fMRI-scanning, tumour cell biomechanics and adhesion)
⇒ Models of tumour growth (finite element-based models, differential adhesion hypothesis, glass-like behaviour)
⇒ Relapse (selective pressure and resistant tumour cells, dormant cancer cells, cancer stem cells)

Methods:

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

Scientific minisymposium

Quantum coherence in nanostructures (2012-A3)

4 / 5 October 2012

The third BuildMoNa Minisymposium was organised by the research groups of Prof. Dr. M. Grundmann and Prof. Dr. Bernd Rosenow.

The symposium dealt with macroscopic coherent quantum states such as superfluids, superconductors or Bose-Einstein condensates that hold great promise for applications such as frictionless, dissipationless transport or ultralow hreshold lasers, if brought to room temperature. It also elucidated the role of spins (“spintronics”) and light-matter interactions (nanophotonics) in nanoscience. The field is partly a challenge in materials physics, partly a challenge in theoretical understanding. The fundamentals of the field and several practical examples were considered.

Internationally renowned speakers covered three aspects of the minisymposium: Bose-Einstein condensation of exciton-polaritons, topological insulators and hybrid structures, and coherent transport in graphene. The speakers were:

⇒ Dr. J. Bloch, CNRS LPN, Paris, France:
Polariton condensates in semiconductor microcavities: Propagation and localisation
⇒ Prof. Dr. H. Buhmann, Universität Würzburg, Germany:
HgTe, a topological insulator
⇒ Prof. Dr. P. Eastham, Trinity College,Dublin, UK:
Semiclassical and quantum models of polariton condensates
⇒ Prof. Dr. K. Ensslin, ETH Zürich, Switzerland :
Scanning gate experiments on quantum point contacts and cavities
⇒ Prof. Dr. N. Grandjean, EPF Lausanne, Switzerland:
Polariton condensation in III-nitride based microcavities
⇒ Prof. Dr. C.M. Marcus, Niels Bohr Institute, Copenhagen, Denmark:
Proximity effect in nanowires
⇒ Prof. Dr. G. Refael, Caltech, Pasadena, USA:
Unconventional magnetic and electric Josephson signatures of Majorana bound states in quantum wires
⇒ Dr. J. Smet, MPI f. Festkörperforschung, Stuttgart, Germany:
Higher order fractional quantum Hall states in graphene
⇒ Prof. Dr. B. Trauzettel, Universität Würzburg, Germany:
Transport properties of helical Tomonaga-Luttinger liquids

Transferable skills workshops

Speaking with confidence

Millie Baker,
9 / 10 January 2012, 10 participants

This workshop aimed at improving the experience of speaking to groups – whether to have more impact, or simply to be able to relax when presenting. Perhaps participants already feel comfortable presenting and would like to strengthen their confidence – be more authentic or have more professional impact during speaking. Or participants may experience some form of anxiety when standing before and speaking to a group. Without seeking to eliminate 'nerves', the workshop looked at new ways of managing them.

Presenting your strengths convincingly: Effective strategies for applying for academic jobs

Dr. Gudrun A. Schwegler, uni-support,
23 / 24 April 2012, 12 participants

This training provided an opportunity to systematically learn how to apply for postdoc positions at universities and research institutions. In addition to receiving concrete information and tips about how to structure applications documents, participants were also able to practice presenting their academic profile and get feedback about the impression they make. Participants learned argumentation strategies for dealing with difficult questions as a preparation for interviews.

In addition, during one year following the seminar, participants have the option to submit one current application for individual feedback and evaluation.

Scientific writing and publishing research, part I

Dr. Dorothea Sommerfeldt,
26 / 27 April 2012, 12 participants

This workshop aimed to: built up and enhance English speaking and writing skills,

accordingly this course was held entirely in English; to run through a morning session of practical English writing skills (common pitfalls, grammar, punctuation, abbreviations) and how to achieve good writing (accuracy, brevity, clarity and style); help in gaining practice and confidence in actually organising and getting first words onto paper, using pieces of own writing (redraft and work on the abstract as an example); demonstrate the process of publication, targeting writing for a specific journal, addressing the cover letter.

Career planning

Uni support,
5 / 6 June 2012, 10 participants

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

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

Presentation workshop

Dr. Frank Lorenz, Rhetoric Excellence,
17 / 27 September 2012 within the Workshop for doctoral candidates, 12 participants

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

Work organisation and time management during the doctoral process

Dr. Gudrun A. Schwegler, uni-support,
19 September 2012, 12 participants

The workshop offered learning opportunities on three levels:

1. The aim at this level was to gain a clear overview of the doctoral project from a top-down perspective. Participants learned to structure their project sensibly and to formulate goals that are not only appropriate, but also concrete and achievable. The individual steps and tasks could then be deduced from these goals. These measures provided a basis for realistically planning both long-term for the overall project and middle-term for the next 3–6 months.

2. Because even promising project plans can fail when implemented under everyday working conditions, this level of the workshop focused on the bottom-up perspective, i.e. on the organisation and management of day-to-day jobs and tasks. Participants identified what type of worker they are and the conditions they work under best. Keeping the difference between effective and efficient work in mind, they learned effective methods of setting priorities and guidelines for handling tasks effectively. Using practical exercises, these principles were applied to create realistic daily and weekly schedules.

3. This level took a look at the framework conditions for academic work in terms of both personal and outside influences. With these factors in mind, a kind of survival kit has been assembled to help deal with the difficulties, stumbling blocks and challenges that may appear during the course of the doctoral process including loss of motivation, delays due to technical problems, and teamworkcomplications.

Scientific writing and publishing research, part II

Dr. Dorothea Sommerfeldt,
1 / 2 October 2012, 10 participants

This workshop included: more on the "perfection" of writing skills, more on how to make text more fluent (paragraphing, coherence, transitions, emphasis), more on the specific parts of a paper (title, introduction, materials and methods, results, discussion), with more extensive practical sessions on the introduction and discussion.

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. M. Lisa Manning	*Syracuse University, NY, USA*	Emergent mechanical properties in embryonic tissues	10 April 2012	*Faculty of Physics and Earth Sciences*
Prof. Dr. Thisbe K. Lindhorst	*Universität Kiel, Germany*	New concepts to ellucidate carbohydrate-specific bacterial adhesion	12 June 2012	*Faculty of Biosciences, Pharmacy and Psychology*
Prof. Dr. Thomas Schleid	*Institut für Anorganische Chemie, Universität Stuttgart, Germany*	Geo-inspired phosphors based on rare-earth metal(III) fluorides with complex oxoanions	13 June 2012	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Hilbert von Löhneysen	*Karlsruhe Institute of Technology (KIT), Physics Institute, Institute of Nanotechnology, and DFG Center for Functional Nanostructures, Germany*	Superconductors and ferromagnets in contact: from thin films to nanostructures	19 June 2012	*Faculty of Physics and Earth Sciences*
Prof. Dr. Jose L. Toca-Herrera	*Universität für Bodenkultur, Wien, Austria*	Success and limitations of biophysical measuring methods	26 June 2012	*Faculty of Biosciences, Pharmacy and Psychology*

Events

5th Scientific symposium

The fifth scientific symposium of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held on 12 March 2012 at the Helmholtz Centre for Environmental Research (UFZ). Interdisciplinary topics from the current research on the development and investigation of new materials were presented. Renowned guest speakers from science gave talks on current topics of BuildMoNa. During the poster session, as one part of the symposium, doctoral candidates presented their scientific topics and discussed them with the international guests, receiving further inspiration for their work at the Graduate School BuildMoNa.

Invited speakers were:

⇒ Prof. Dr. Horst Kessler, Technische Universität München, Germany:
Structure and function of proteins by NMR: spider silk
⇒ Prof. Dr. Ferdinand Hofer, Technische Universität Graz, Austria:
Analytical electron microscopy of complex nanostructured materials
⇒ Prof. Dr. Hans-Ulrich Demuth, Probiodrug AG, Halle/Saale, Germany:
Inhibition of glutaminyl cyclases targeting neurodegeneration and neuroinflammation in Alzheimer's disease
⇒ Prof. Dr. Dave H.A. Blank, University of Twente, The Netherlands:
Materials science on a nanoscale

⇑ Participants of the 5th scientific symposium

5th Workshop for doctoral candidates

25 doctoral candidates presented their scientific results with short talks at the 5th BuildMoNa Workshop on 24 and 25 September 2012 in Burgstädt. About 100 BuildMoNa participants followed the lectures in the conference room 7/8, the conference venue of the Center Hotel Alte Spinnerei. 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 Wilma Neumann for her presentation “Cisplatin-COX inhibitor conjugates for the treatment of cancer”, the second to Jakob Tómas Bullerjahn for his presentation “Improved modelling of forced Kramers escape” and the third to Solveig Boehnke for “Boron neutron capture therapy: Linking boron-rich building blocks with tumour-selective compounds”.

⇐ Participants of the workshop

⇑ Winners of the presentation awards at the 5th Workshop: Wilma Neumann, Jakob Bullerjahn, Solveig Boehnke (from left to right)

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

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