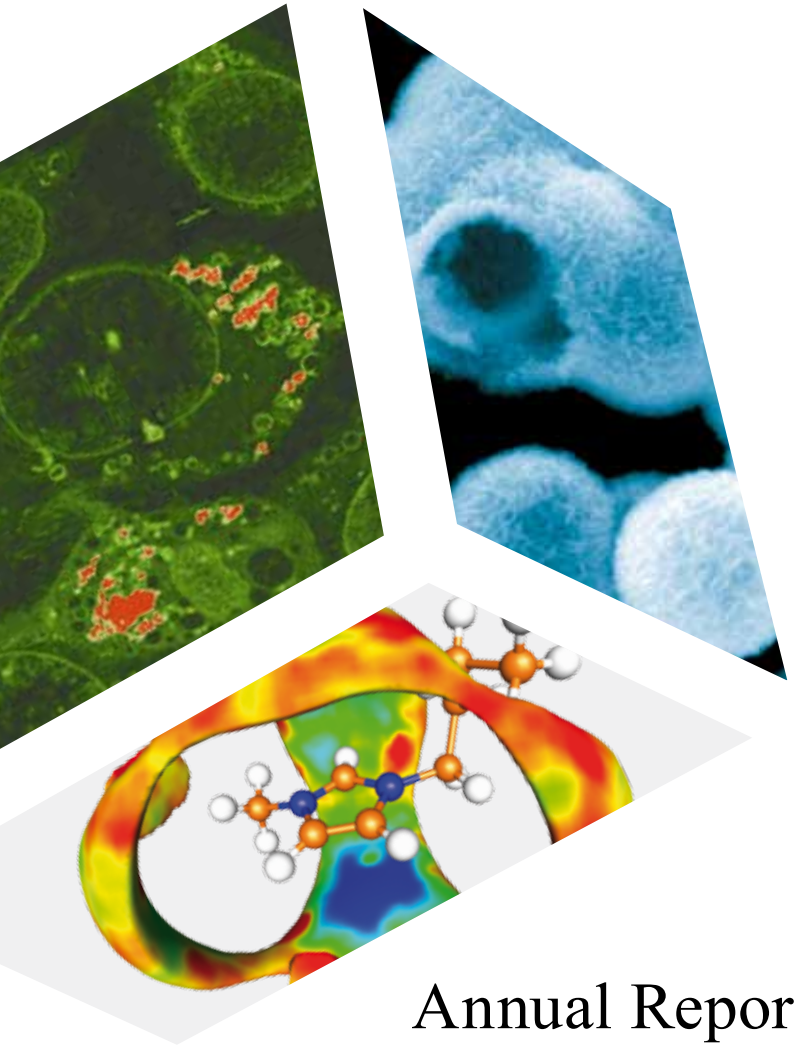
UNIVERSITÄT LEIPZIG

BuildMoNa

Graduate School

Building with Molecules and Nano-objects



Annual Report 2009

Cover image:
⇒ Left: Scanning electron microscopy image of epoxy resin embedded HaCaT cells incubated with Pd/Mag particles; the particles are visible as red spots due to the strong back scatter electron signal (false colour image)
⇒ Right: Zirconia hollow spheres with mesoporous walls as supports for metal catalysts in high-temperature conversions
⇒ Bottom: Spatial distribution function of [SCN] – around imidazolium with mapped velocities of the anions

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Annual Report 2009

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

Preface Prof. Dr. Evamarie Hey-Hawkins

The Graduate School *Leipzig School of Natural Sciences – Building with Molecules and Nano-objects* (BuildMoNa) focuses on interdisciplinary education of young scientists based on excellent research. The latter follows the "bottom-up" strategy for the development of new materials: From suitable building blocks, such as nano-objects, adaptable molecules, polymer grids, peptides and proteins, new materials are designed, preferably by processes like self-organisation.

Building with molecules and nano-objects is a scientific strategy which is not only reflected in the research projects, but equally in the development and application of new methods in the training programme.

After eight calls for proposals, altogether 97 doctoral candidates were enrolled as members of BuildMoNa by the deadline 31 December 2009. Of these, 40 doctoral candidates are financed by means of third-party funds and 24 candidates were awarded a BuildMoNa scholarship, which is included in the budget of the Graduate School. Additionally, 19 doctoral candidates are funded by "ESF-Landesinnovationspromotionen".

On 18 May 2009 two young researchers groups were implemented at the Graduate School BuildMoNa. The aim of these ESF-funded projects is to enable young academics to be involved in knowledge and technology transfer and to establish a network between universities and companies within the context of their research work. Five male and three female doctoral candidates and the post-doctoral researcher Dr. Mike Hildebrand are involved in the young researchers group "Supported catalysts for innovative bio-, nano- and environmental technology" (coordination Prof. Dr. Evamarie Hey-Hawkins). The interdisciplinary programme of this project unifies the excellence existing at the Universität Leipzig in the area of catalysis and is based on existing knowledge and facilities to produce selective homogeneous, heterogeneous and bio-catalysts in a specific manner, to characterise them extensively and to test their catalytic activity, selectivity and stability also under application-relevant conditions. The main emphasis lies in the development of new catalysts that are especially interesting for industrial partners in Saxony and Germany. The young researchers group "Functional multiscale structures" (coordination Prof. Dr. Marius Grundmann) is led by the post-doctoral researcher Dr. Holger von Wenckstern and consists of five male and one female doctoral candidates. Nano-objects and micro-dimensional structures are to be synthesised or produced and analysed with respect to structural, chemical, mechanical, electronic and optical qualities. It is planned to optimise the structures with regard to their application-relevant qualities and to process them in component structures. The young researchers group is based on third-party funded projects in the area of excellent basic research (FOR522), projects with direct reference to applications and projects with Saxon industrial participation. Collaborative projects have already been conducted with the Solarion AG Leipzig and Q-Cells AG Thalheim.

In the course of the future development of the Graduate School the number of the participating "principal investigators" was further extended. Prof. Bernd Abel, Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Prof. Wolfgang Hackbusch, Max Planck Institute for Mathematics in the Sciences, and Prof. Stefan G. Mayr, Leibniz Institute of Surface Modification and Faculty of Physics and Earth Sciences, were admitted as associated members of the Graduate School BuildMoNa in 2009.

The BuildMoNa programme includes the organisation and implementation of the "Scientific and Methods Modules", which reflect the interdisciplinary research orientation of the Graduate School and are completed with a graded examination. In this exam, credit points can be acquired which follow the European System. Additionally, transferable skills workshops were organised which allow the doctoral candidates to acquire additional technical and extra-curricular competences.

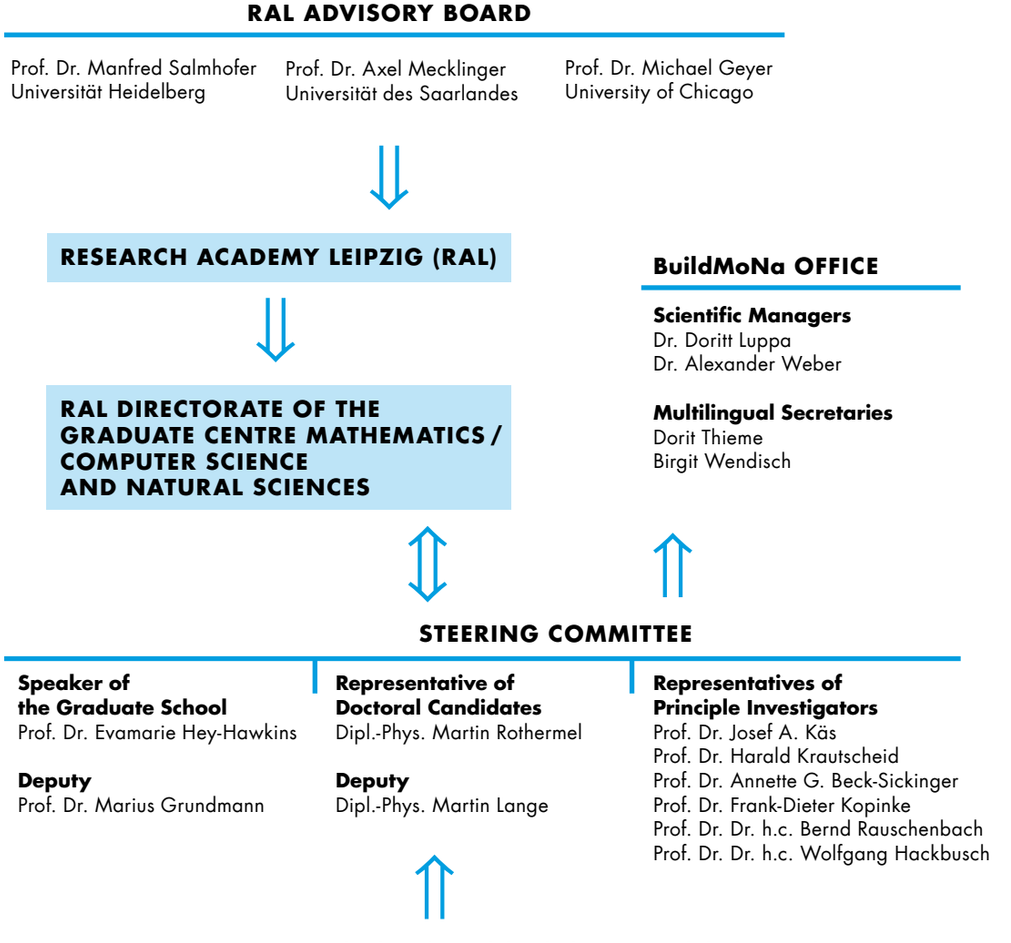
Science-related events included the "2nd BuildMoNa Symposium" and the "2nd BuildMoNa Workshop for Doctoral Candidates".

On 9 December 2009 the ceremonial event for the two-year anniversary of BuildMoNa took place. The lecture of Prof. Dietrich Hesse, MPI of Microstructure Physics, Halle dealt with "Nano-structured ferroelectric and multiferroic epitaxial perovskite heterostructures". On this occasion, the annual "BuildMoNa Awards" were presented to three doctoral candidates for their scientific publications resulting from their doctoral research.

During the next year, 2010, we will start to focus on planning the next steps for a successful application for continuation of the Graduate School in 2012.

Prof. Dr. Evamarie Hey-Hawkins

Organisation and management



The Graduate School BuildMoNa is a class of the *Research Academy Leipzig* (RAL) within the Graduate Centre for Mathematics, Computer Science and Natural Sciences, its director being Prof. Dr. S. Luckhaus. BuildMoNa is represented within the RAL by Prof. Dr. E. Hey-Hawkins as RAL Board member and by Martin Rothermel as representative of the doctoral candidates.

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

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

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

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

The BuildMoNa Office consists of 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/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.-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. Dalia Angeles-Wedler	Prof. Dr. F.-D. Kopinke	*Environmental application of palladium catalyst for hydrodechlorination reactions*
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. Abhinandan Banerjee	Prof. Dr. F.-D. Kopinke / Prof. Dr. R. Gläser	*Investigations on kinetics and mechanism of hydrodehalogenation reactions in water*
M.Sc. Chem. Eng. Neto Bastos	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	*Hydrogen purification and storage by adsorption in nanoporous materials*
Dipl.-Biochem. Lars Baumann	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. A. Robitzki	*Structure-activtiy relation of chemokines*
Dipl.-Chem. Kathrin Bellmann-Sickert	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. A. Robitzki	*Improvement of the bioavailability of neuropeptides and chemokines*
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.-Chem. Martin Brehm	Prof. Dr. B.Kirchner / Prof. Dr. R. Gläser	*Development of a program package for efficient simulation of complex chemical systems*
M.Eng. Material Marina Ines Cornejo	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Pattern formation on Si- and Ge-surfaces by low-energy ion-beam erosion*
B.Sc. Chem. Jorge Luis Cholula Díaz	Prof. Dr. Krautscheid / Prof. Dr. M. Grundmann	*Properties of novel precursor based materials*
M.Sc. Phys. Christof Peter Dietrich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Growth and charactisation of ZnO-based microstructures*
M.Sc. Chem. Marina Loredana Drob	Prof. Dr. M.R. Buchmeiser / Prof. Dr. B. Rauschenbach	*Biopolymeric materials for regenerative medicine*
M.Sc. Phys. Srujana Dusari	Prof. Dr. P. Esquinazi / Prof. Dr. H. Morgner	*Measurements of the mean free path and spin diffusion length in multigraphene*
M.Sc. Phys. Susanne Ebert	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The development of a novel technique to measure the proteomic content of biological cells by combining microfluidics, laser-based nano-manipulation and optical high-resolution tomography*
Dipl.-Phys. Roxana-Giogiana Ene	Prof. Dr. F. Kremer / Prof. Dr. M. R. Buchmeiser	*Structural levels of organisation in spider silk as studied by time-resolved polarised rheo-FTIR spectoscopy*
Dipl.-Phys. René Feder	Prof. Dr. T. Butz/ Prof. Dr. P. Esquinazi	*Defect production by single ions traversing multigraphene*
M.Sc. Chem. René Frank	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Carbaboranyl amino acids for application in BNCT*
Dipl.-Phys. Heiko Frenzel	Prof. Dr. M. Grundmann / Prof. Dr. H. Morgner	*Transport investigations on ZnO based field-effect structures*
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 tumor cells in micro- and nanostructured hard environments*
Dipl.-Phys. Jens Glaser	Prof. Dr. K. Kroy / Prof. Dr. S. Müller	*Theory of semiflexible polymers*
Dipl.-Biochem. Marco Glaß	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	*HP-Bioforce: An integrated and automated screening plattform for functional force measurement at cell and tissue layers for pharmaceutical research*
M.Sc. Chem. Michael Goepel	Prof. Dr. R.Gläser / Prof. Dr. F.-D. Kopinke	*Correlation of diffusion and phase behaviour in mesoporous materials*
M.Sc. Chem. Matthias Golecki	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	*Encapsulation of catalytically active metal complexes*
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.-Biochem. 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*
M.Sc. Chem. Tobias Hammer	Prof. Dr. H. Morgner / Prof. Dr. A.G. Beck-Sickinger	*Investigation of aqueous solutions with Ion-Scattering-Spectroscopy*
Dipl.-Biochem. Rayk Hassert	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. M. Grundmann	*Peptides for specific adhesion to hard matters*
Dipl.-Chem. Julia Haushälter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Phosphine-baskets – ligands for selective catalysis*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Helena Hilmer	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Growth and characterisation of UV microcavities*
Dipl.-Phys. Florian Huber	Prof. Dr. J. Käs / Prof. Dr. M. Grundmann	*Artificial cell motility*
M.Sc. Phys. Ciprian-Ghiorghita Iacob	Prof. Dr. F. Kremer / Prof. Dr. J. Kärger	*Molecular dynamics of organic materials confined in nano-pores*
M.Sc. Chem. Nicole Jahr	Prof. Dr. S. Berger / Prof. Dr. A.G. Beck-Sickinger	*NMR investigations at modified ubiquitines*
M.Eng. Material Xiaosong Jiang	Prof. Dr. P. Esquinazi / Prof. Dr. J. Haase	*Magnetoresistance characteristics and hydrogen NMR of single magnetic grains*
M.Sc. Chem. Cathleen Juhl	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. A. Robitzki	*Investigation of the function of adiponektin receptors by peptide segmentation*
M.Sc. Phys. Michael Jurkutat	Prof. Dr. J. Haase / Prof. Dr. W. Janke	*Investigation of the electronic properties of high-temperature superconductors by means of NMR*
M.Sc. Chem. Florian Kettner	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	*Synthesis and characterisation of porous coordination polymers*
M.Sc. Phys. Chinmay Khare	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Glancing angle deposition*
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*
M.Sc. Chem. Aslihan Kircali	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	*Phosphorus-rich complexes as precursors for binary or ternary metal phosphides M_xP_y or $M_xM'_yP_z$*
Dipl.-Math. Melanie Knorr	Prof. Dr. J. Käs	*Role of stochasticity in a moving thin polymer film*
M.Sc. Phys. Wilhelm Kossack	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	*IR-spectroscopy for the analysis of structure and dynamic of polymers*
Dipl.-Phys. Markus Kraus	Prof. Dr. F.-D. Kopinke	*Application of coupled temperature- and concentration pulses for efficient adsorptive catalytic elimination of pollutants from contaminated exhaust air*
Dipl.-Biochem. Dana Krinke	Prof. Dr. A. Robitzki / Prof. Dr. A. G. Beck-Sickinger	*Development of an impedance-based HTS screening on novel neuronal 2D and 3D cell culture models for testing drugs against neurodegenerative diseases*
Dipl.-Chem. Jochen Lach	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	*Thin films of redox-active high-spin molecules*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Daniel Lässig	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	*Synthesis and characterisation of porous coordination polymers with N-donor ligands*
Dipl.-Phys. Alexander Lajn	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	*Fabrication and characterisation of transparent field-effect transistors*
Dipl.-Phys. Martin Lange	Prof. Dr. M. Grundmann/ Prof. Dr. F. Cichos	*Growth and characterisation of quantum wire heterostructures*
M.Sc. Chem. Ulrike Lehmann	Prof. Dr. B. Kersting / Prof. Dr. E. Hey-Hawkins	*Hydrogenation of CO_2 by supported container molecules*
Dipl.-Chem. Carolin Limburg	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	*Ferrocenylphosphanides and phosphanediides as building blocks for heterometallic complexes*
M.Sc. Chem. Jörg Lincke	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	*Coordination polymers with nitrogen-rich ligands*
Dipl.-Phys. Michael Lorenz	Prof. Dr. M. Grundmann/ Prof. Dr. Mayr	*Investigations on the stability of zinc oxide based metal-semi-conductor field-effect-transistors*
Dipl.-Phys. Johanna Lutz	Prof. Dr. B. Rauschenbach	*Phase formation and diffusion behaviour for ion implanted austenitic metal alloys*
M.Sc. Chem. Martyna Madalska	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Immobilised switchable phosphine-based catalysts*
Dipl.-Phys. Marisa Mäder	Prof. Dr. B. Rauschenbach	*Substrate-bound nanostructures by diffraction mask projection laser ablation*
Dipl.-Phys. Benno Meier	Prof. Dr. J. Haase / Prof. Dr. S. Berger	*Ultra-high field magnetic resonance of modern materials*
Dipl.-Phys. Monika Möddel	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	*Modelling and computer simulations of adsorption specifity of synthetic peptides*
Dipl.-Phys. Karla Müller	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The use of scanning probe techniques and laser nanomanipulation to isolate and mechanostimulate highly potent mesenchymal stem cells*
Dipl.-Phys. Alexander Müller	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	*Investigation of carrier dynamics in ZnO films and microcavities*
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. Phys. David K. Nnetu	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	*The use of biomechanics to reduce metastatic aggressiveness*
Dipl.-Biochem. Verena Ortmann	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	*Modified peptides for biotechnology*

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Souvik Pandey	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*P-based polymers: synthesis and applications in materials science*
M.Sc. Julian Rodger Frederic Pritzwald Stegmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	*Phosphorus-based organometallic/ inorganic hybrid materials*
M.Sc. Chem. Santhosh-Kumar Podiyanachari	Prof. Dr. M. R. Buchmeiser / Prof. Dr. B. Rauschenbach	*Cyclopolymerisation of 1,6-heptadiynes*
M.Sc. Chem. / MSc. Environmental protection Ksenia Jolanta Ramus	Prof. Dr. F. D. Kopinke / Prof. Dr. R. Gläser	*Thermodynamic activity versus total concentration of xenobiotics as predictors of bioavailability*
Dipl.-Chem. Daniel Rathmann	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. A. Robitzki	*Structure activity relationships of RF-amide peptide receptors with chemical modified peptides*
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*
Dipl.-Chem. Techn. Klara Rusevova	Prof. Dr. F.-D. Kopinke / Prof. Dr. Gläser	*Iron-based nanoparticles catalysts for oxidation of pollutants in water*
M.Sc. Erica Saraçi	Prof. Dr. R. Gläser / Prof. Dr. F.-D. Kopinke	*Silicate-based molecular sieves with hierarchically structured micro-/ mesopore systems for improved heterogeneous catalysis*
Dipl.-Phys. Jens Schneider	Prof. Dr. F.-D. Kopinke / Prof. Dr. M. Grundmann	*Studies of dissociation processes of water exposed to high-frequency electromagnetic fields*
Dipl.-Phys. Sebastian Schöbl	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	*Modelling and computer simulations of molecular pattern recognition*
Dipl.-Chem. Matthias Scholz	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	*Imitiation and modification of bioactive lead structures via integration of clusters*
M.Sc. Phys. Ilya Semenov	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	*Dynamics of DNA under tension and in confinement*
M.Sc. Molek. Biotech. Lorenz Steinbock	Prof. Dr. F. Kremer	*Detection und sequencing of biopolymers by electrophoretic translocation through pores*
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. Marco Stölzel	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	*Time-resolved spectroscopy on ZnO based micro- and nanowire heterostructures and -cavities*

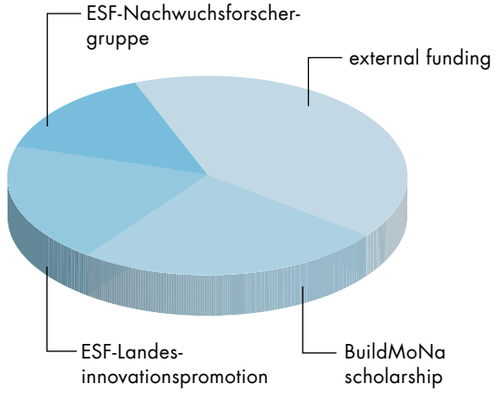
Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Dan Strehle	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Mechanical and dynamic properties of actin bundles*
M.Sc. Chem. Markus Streitberger	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	*Building catalytically active bimetallic nano-frames with flexible bis-phosphine ligands*
Dipl.-Phys. Sebastian Sturm	Prof. Dr. K. Kroy / Prof. Dr. F. Kremer	*Nonequilibrium dynamics of forced and confied semiflexible polymers*
Dipl.-Phys. Chris Sturm	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	*Investigation of the cw optical properties of ZnO cavities*
M.Sc. Chem. Mavila Sudheendran	Prof. Dr. M. Buchmeiser / Prof. Dr. H. Krautscheid	*Functional monolithic media*
Dipl.-Chem. Ronny Syre	Prof. Dr. B. Kersting / Prof. Dr. M. Buchmeiser	*Photo-induced electron tranfer in multimeric capsule complexes*
M.Sc. Chem. Eng. Erik Thelander	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	*Synthesis of nanostructures using laser ablation*
Dipl.-Phys. Olaf Ueberschär	Prof. Dr. F. Kremer	*Investigating stochastic thermodynamics by means of optical tweezers*
Dipl.-Phys. Carolin Wagner	Prof. Dr. F. Kremer	*Investigation of the interaction of receptors and ligands by optical tweezers*
Dipl.-Chem. Franziska Weichelt	Prof. Dr. M. R. Buchmeiser / Prof. Dr. B. Kersting	*Synthesis und characterisation of new composite and hybrid materials based on functionalised nano- und microparticles of metal oxides and salts*
Dipl.-Phys. Franziska Wetzel	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	*Direct staging of primary mammacarcinomas by determining their cellular composition including metastatically competent cells, dormant cancer cells and cancer stem cells*
Dipl.-Phys. Micha Wiedenmann	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	*Cluster aggregation and condensation of nano-objects*
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*
Dipl.-Phys. Lars Wolff	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	*Plasticity and active remodelling of cells*
Dipl.-Phys. Hendrik Zachmann	Prof. Dr. B. Rauschenbach	*Electrical defects in ion beam assisted deposition of $Cu(In,Ga)Se_2$ thin film solar cells*
Dipl.-Phys. Jan Zippel	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	*Magnetic tunnel junctions*

Alumni 2009

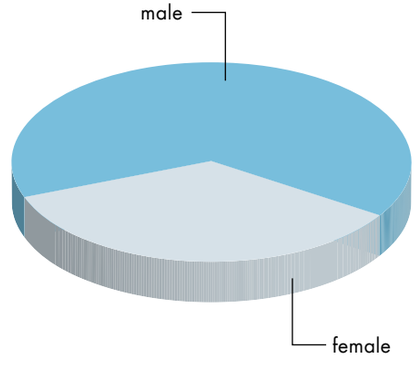
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Sebastian Bauer	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	*Synthesis of carbaboranylphosphonites as ligands for late transition metal complexes*
Dr. rer. nat. Ralf Biedermann	Prof. Dr. H. Krautscheid / Prof. Dr. T. Butz	*Synthesis and characterisation of molecular single source precursors for copper-indium-dichalcogenides*
Dr. rer. nat. Christian Czekalla	Prof. Dr. M. Grundmann / Prof. Dr. J. Haase	*Microoptical investigation of ZnO resonators*
Dr. rer. nat. Christian Patzig	Prof. Dr. B. Rauschenbach	*Glancing angle deposition of Si nanostructures*
Dr. rer. nat. Christian Raeck	Prof. Dr. S. Berger / Prof. Dr. E. Hey-Hawkins	*Investigation of phosphorylation and dephosphorylation with NMR*
Dr. rer. nat. Stefan Schnabel	Prof. Dr. W. Janke	*Adsorption and aggregation properties of short substrate binding peptides*
Dr. rer. nat. Sandro Wenzel	Prof. Dr. W. Janke	*Quantum Monte Carlo simulations of low-dimentional quantum spin systems*
Dr. rer. nat. Denise Zwanziger	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	*The labelling of peptide hormones with metal complexes for radiopharmaceutical applications in the field of tumour diagnosis and therapy*

Statistics

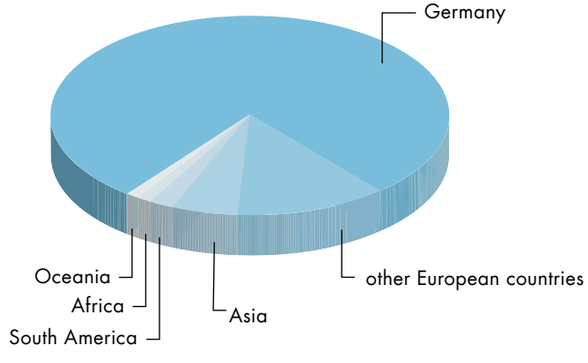
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:

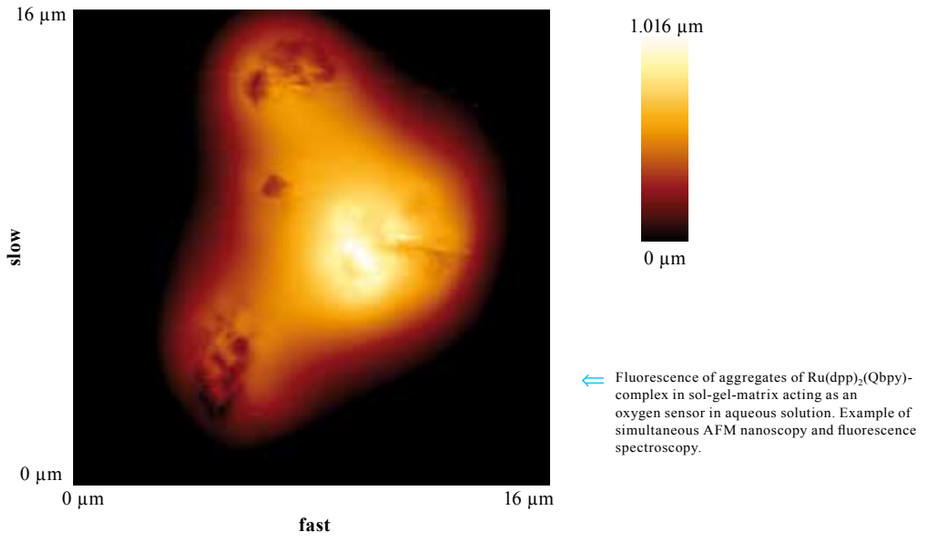


Ultrafast spectroscopy and nanoscopy

Prof. Dr. Bernd Abel

The Abel group works in the field of molecular physical chemistry and biophysical chemistry.

The main research focus at present is time-resolved dynamics of chemical and biological molecular systems or molecular assemblies in different molecular environments. The analytical tools are usually heavily based upon state-of-the-art laser or photonic technology. While the timescales and dynamics may vary between ultrafast (50 femtoseconds) and relatively slow (milliseconds up to weeks) the size of the molecular system may vary from smaller polyatomics up to large molecular nanomachines (e.g., proteins). Where possible, investigations are complemented by time-resolved nanoscale photonic imaging techniques and molecular dynamics calculations with the long-time goal of determining true "molecular movies" on an ultimate time and space scale.



⇐ Fluorescence of aggregates of $Ru(dpp)_2(Qbpy)$-complex in sol-gel-matrix acting as an oxygen sensor in aqueous solution. Example of simultaneous AFM nanoscopy and fluorescence spectroscopy.

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Chemical modification of peptides and proteins

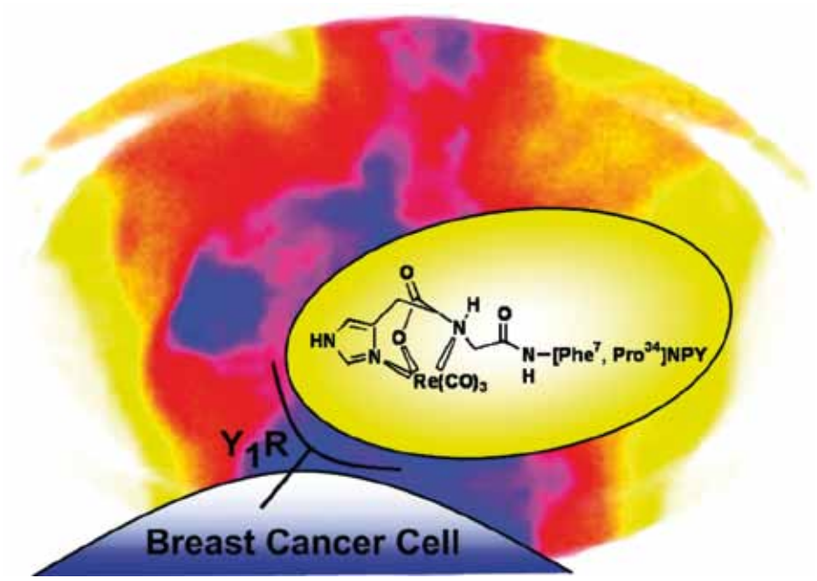
Prof. Dr. Annette G. Beck-Sickinger
Dipl.-Biochem. Lars Baumann, Dipl.-Chem. Kathrin Bellmann-Sickert, Dipl.-Biochem. Rayk Hassert, M.Sc. Chem. Cathleen Juhl, Dipl.-Biochem. Verena Ortmann, Dipl.-Chem. Daniel Rathmann, Dipl.-Biochem. Max Steinhagen, Dr. Denise Zwanziger

Aim of the project is the synthesis and testing of chemically modified peptides and proteins for different, mainly nanobiomaterial application. Peptides are synthesised by solid phase peptide synthesis. Proteins are expressed recombinantly and fused to the peptides by native chemical ligation or click chemistry.

Denise Zwanziger (Dr.) and Daniel Rathmann (Dipl.-Chem) synthesise chemically modified peptide hormones, like neuropeptide Y or Neuropeptide FF analogues for diagnostic application. Chelators are introduced into the hormones by means of selective side chain protection strategies and metals like Ga, Gd, Cu or Re are conjugated. Metall-containing peptide hormones are used to follow their uptake into cells and to localise their distribution on a subcellular level. By using ^{99m}Tc the peptides can be used for radiodiagnostics. Highlight of this year was the successful human application that clearly showed the selectivity of the approach. Denise Zwanziger finished her doctorate in November 2009.

Kathrin Bellmann-Sickert (Dipl.-Chem.), Cathleen Juhl (Dipl.-Chem.) and Lars Baumann (Dipl.-Biochem.) work on chemically modified proteins. Interleukin 8 (IL-8) and SDF-1, two chemokines, and adiponectin, an adipocytokine, are chemically modified by polyethyleneglycol, fluorescent dyes, non proteinogenic amino acids or photoactiatable protecting group to induce, follow or modulate activity. Modification with polymers and the generation of these hybrid molecules significantly improves half live under physiological conditions.

Rayk Hassert (Dipl.-Biochem.) and Max Steinhagen (Dipl.-Biochem.) work on



chemically modified peptides and proteins to improve the properties of biomaterials. Rayk develops peptides that bind to surfaces, e.g. Ti, ZnO or Au, whereas Max is engineering peptides and enzymes to modulate tailor made properties for the immobilisation of biomolecules to surfaces. Verena Ahrens (Dipl.-Biochem.) and Sylvia Els (M. Sc. Chem.) recently joined the team with projects on modified peptides.

⇒ *The First Selective Agonist of the Neuropeptide Y1-Receptor with Reduced Size*
D. Zwanziger, I. Böhme, D. Lindner, A.G. Beck-Sickinger / Journal of Peptide Science (2009) **15** 856

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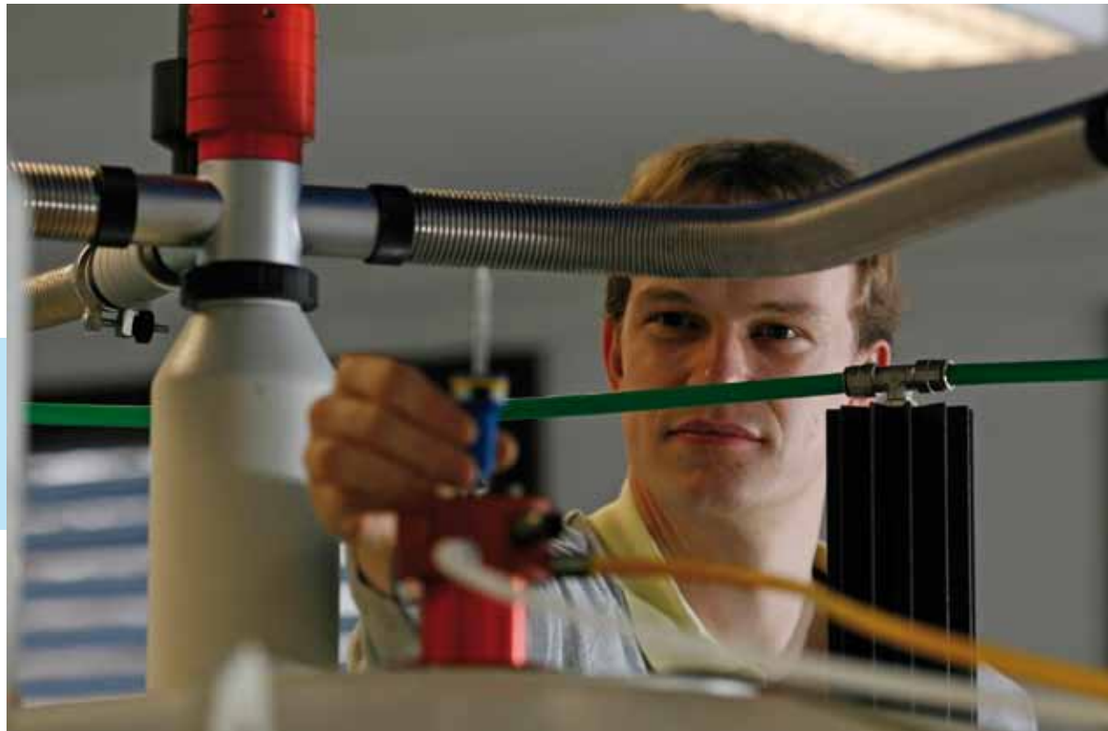
Biomolecular problems studied by NMR

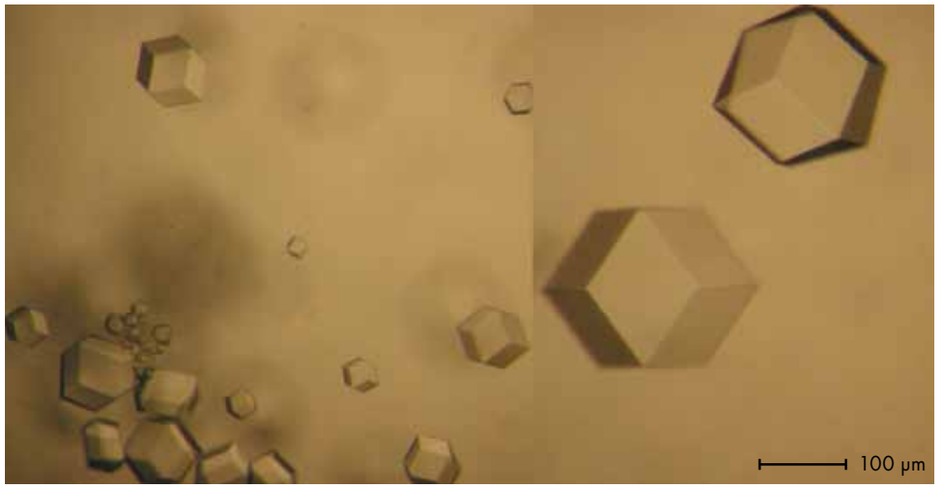
Prof. Dr. Stefan Berger
Dipl.-Chem. Nicole Jahr, Dr. Christian Raeck

Christian Raeck concluded his work on NMR detection of phosphorylation and obtained his doctoral degree in March 2009. Directly after this he obtained a job in a local start up company. Nicole Jahr has investigated the NH-exchange rates of proteins by NMR methods in order to find a common principle to explain these exchange rates from a structural point of view. Starting from human ubiquitin she has produced by PCR techniques the variants T9V, F45W, F45W and A46S. All these new ubiquitin variants have been fully characterised by recent 3D NMR methods. The NH exchange rates have been measured by different NMR techniques and were theoretically calculated in collaboration with the group of Professor H.J. Hofmann in Biochemistry. There is, however, still a lack in quantitative and detailed under-



standing for some of the newly generated values. From the variant T9V we succeeded to obtain an X-ray structure in collaboration with the group of Prof. Sträter. This result is shown in the figure.

Closely related to this work were our NMR experiments to investigate protein ligand interaction. Christoph Räuber developed saturation transfer difference NMR experiments and could extent the known procedure for the first time to ^{13}C detection. This probably offers distinct advantages, when ligand signals are too close to the water signal.



⇑ Microscope images of UbiquitinA46S

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Nano-particle modified polymer layers and monolithic separation media for the analysis of biologically relevant compounds

Prof. Dr. Michael R. Buchmeiser
since 01.12.2009 Universität Stuttgart and ITCF Denkendorf
M.Sc. Marina L. Drob, M.Sc. Chem. Mavila Sudheendran,
M.Sc. Santosh-Kumar Podiyanacharim, Dipl.-Chem. Franziska Weichelt

Franziska Weichelt synthesises and characterises functional nano-particles for the enforcement of monolithic materials for tissue engineering. The corresponding nano-composites are designed in a way that they exhibit improved mechanical properties and that the nanoparticles provide a source of Ca^{2+}, which is to be converted into Ca-hydroxylapapite by stem cell-derived osteoblasts that are grown on

the nanocomposite. Santosh K. Podiyanacharim entails the tailor made synthesis of conjugated polymers with high effective conjugation lengths. These are designed in a way that they are soluble in organic solvents and can thus be easily dispersed in coating formulations. The focus here is on antistatic/conductive coatings. Additional applications aim on printable electronics. The polymers are prepared via cyclopolymerisation applying both well-defined Schrock and Buchmeiser-Grubbs-Hoveyda initiators.

Marina L. Drob deals with the application-oriented synthesis of micro-, meso- and nanoporous monolithic materials for tissue engineering. The corresponding polymers are designed in a way that they are biocompatible and biodegradable. Synthesis is accomplished both via ring-opening metathesis polymerisation (ROMP) and electron beam-triggered free radical polymerisation. The pore sizes are tailor made and designed in a way that sufficient cell adhesion is guaranteed. Cell proliferation and ingrowth is enabled by providing a substantial amount of large interpenetrating pores in the 200 µm range.

⇒ *Factors Relevant for the Regioselective Cyclopolymerization of 1,6-Heptadiynes, N,N-Dipropargylamines, N,N-Dipropargylammonium Salts, and Dipropargyl Ethers by Ru-IV-Alkylidene-Based Metathesis Initiators*
P.S. Kumar, K. Wurst, M.R. Buchmeiser / Journal of the American Chemical Society (2009) **131** 387

⇒ *Ru-Alkylidene Metathesis Catalysts Based on 1,3-Dimesityl-4,5,6,7-tetrahydro-1,3-diazepin-2-ylidenes: Synthesis, Structure, and Activity*
P.S. Kumar, K. Wurst, M.R. Buchmeiser / Organometallics (2009) **28** 1785

⇒ *Isocyanate- and Isothiocyanate-Derived Ru-IV-Based Alkylidenes: Synthesis, Structure, and Activity*
P.S. Kumar, K. Wurst, M.R. Buchmeiser / Chemistry – An Asian Journal (2009) **4** 1275

Prof. Dr. Michael R. Buchmeiser
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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. René Feder, Dipl.-Phys. Martin Rothermel

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

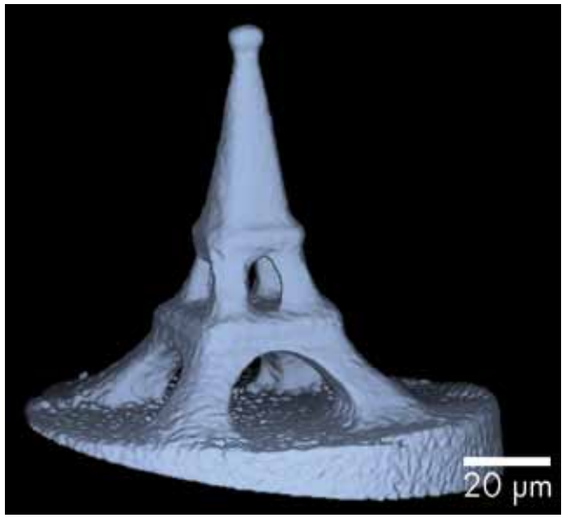
Martin Rothermel's research focuses on the refinement of the element-sensitive technique of PIXE (particle induced X-ray emission) tomography using a submicron proton beam. Due to the complex probe-sample-interactions a highly sophisticated reconstruction algorithm is needed, which is able to accurately model the

effects of particle deceleration and X-ray attenuation within the sample. A phantom sample comprising several previously known elements with unknown localisation was fabricated and subjected to experiment.

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. A limited-angle approach has been chosen for the tomography of cells on substrate in order to minimise irradiation damage and sample preparation difficulties. A newly-developed iterative reconstruction algorithm permits the reconstruction of intracellular structures.

Also, the combination of tomography with proton beam writing has proved fruitful, resulting in the creation of 3D microsculptures and workpieces.

René Feder is part of the ESF-Nachwuchsforschergruppe "funktionale multiskalige Strukturen". His research topic is the defect production by single ions traversing multigraphen. Therefore resistance, magneto-resistance and Hall-measurements are performed during and directly after the irradiation of multigraphen samples by high energy protons and α-particles. The setup will be modified to measure under vacuum conditions and allow for sample cooling.



⇐ Scanning transmission ion microtomogram of 3D architectural structure created by proton beam sculpting in PMMA

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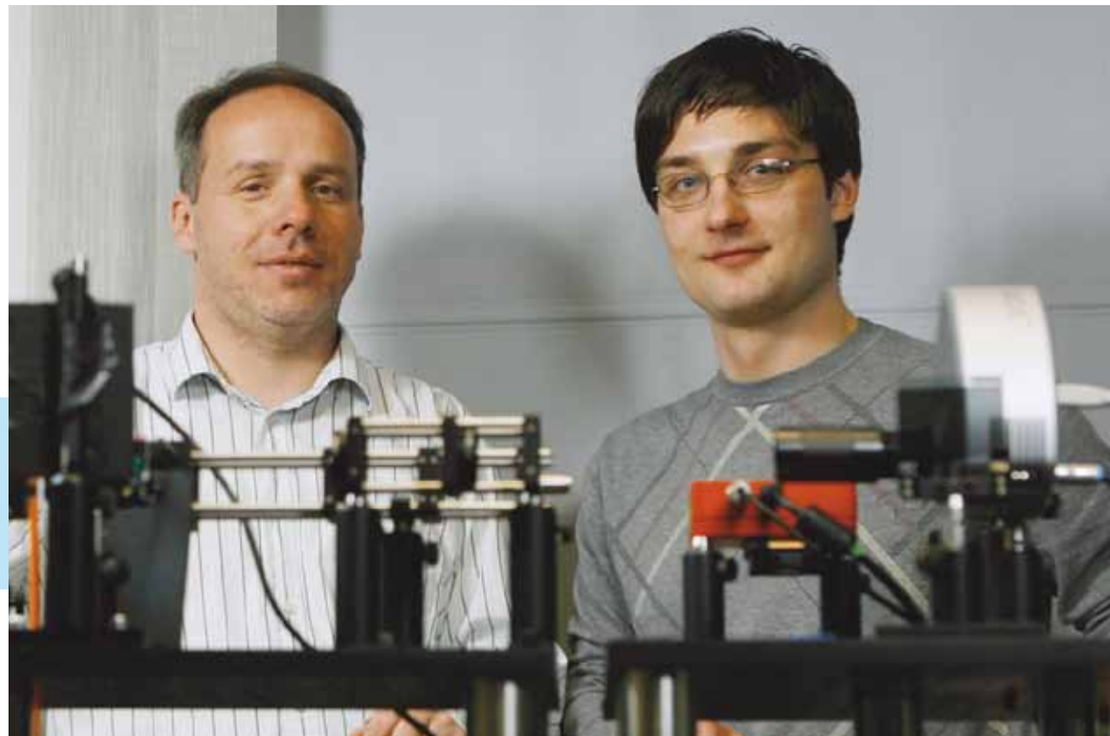
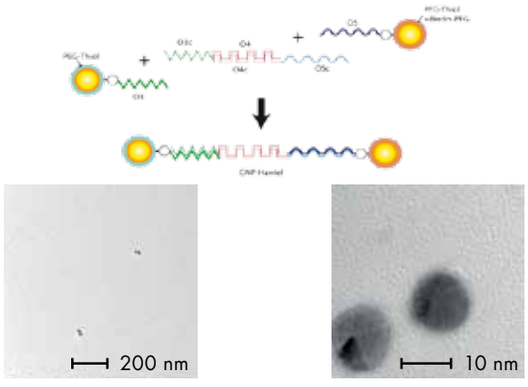
Photothermal detection of noble metal nanoparticles – Single Photon Emission from ZnO Nanowires

Prof. Dr. Frank Cichos
Dipl.-Phys. Nils Neubauer

We employ small heat releasing noble metal particles as a tool to measure heat propagation in liquids and polymers as well as to explore distance fluctuations on the nanometer scale. As compared to the widely used organic chromophores that suffer from photochemical limitations, such as photoblinking and photobleaching, our ex-





⇑ *Top*: Synthesis strategy for gold nanoparticle dimers seperated by a DNA strand. The dimers are created by binding functionalised gold nanoparticles to the sticky ends of a DNA strand.
Bottom: Electron microscopy images of the synthesised gold nanoparticle pairs, which have been separated from monomers and trimers by electrophoresis. The particles are separated by 30 nm.

perimental approach based on metal nanoparticles provides extreme photostability, sensitivity and detection speed. We are able to detect single gold nanoparticles of 2 nanometer diameter at a time resolution of 20 microseconds in our home-built photothermal microscope setup. The photothermal microscopy technique relies on a modulated optical heating of the gold nanoparticles. The resulting temperature gradient around the particles causes a local refractive index change that is monitored by a highly sensitive heterodyne detection technique.

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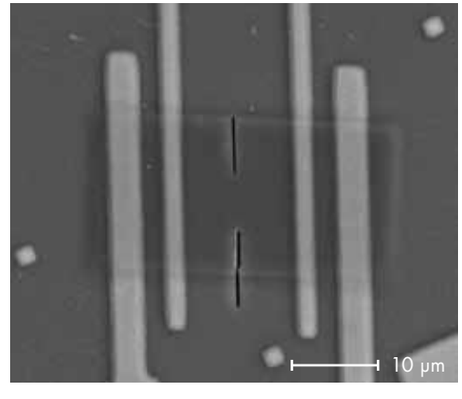
This new photothermal technique has been used to develop new detection schemes for nanoscale distance fluctuations in which the plasmon resonances of two gold nanoparticles are coupled in the optical near field. The gold nanoparticles have been linked together by a DNA strand of 30 nm length. Optical heating of the nanoparticle pair is carried out in the coupled plasmon resonance, which disappears in the limit of large particle separations. This technique of distance measurements and local heat release is currently applied to the study of DNA melting. Combined with a newly developed correlation method the photothermal technique is further extended to the detection of rotational diffusion of noble metal nanorods

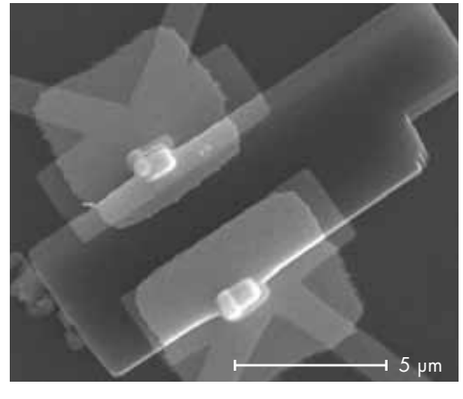
As a second new topic, we have started the investigation of single photon emission from core/shell ZnO/ZnMgO quantum well structured nanowires in collaboration with the group of Prof. M. Grundmann during the last year. Current experiments involve confocal microscopy under single and two-photon excitation.

The search for the intrinsic electronic properties of graphite

Prof. Dr. Pablo D. Esquinazi
M.Sc. Phys. Ana Isabel Ballestar Balbas, M.Sc. Phys. Srujana Dusari,
M.Eng. Material Xiaosong Jiang

The electronic properties of ideal graphite are actually not well known simply because defect-free graphite samples do not exist. In the last fifty years scientists flooded the literature with reports providing evidence for different values and behaviours of the carrier density per graphene layer, the carrier mean free path as well as the anisotropy in the electrical transport. However, it was recently demonstrated





⇑ Scanning electron microscope picture of a multigraphene sample of size ~ 20×10×0.03 µm³, covered by a rectangular 300 nm thick film of PMMA that hinders the entrance of the Ga^+-ions in the sample with exception of the region where a constriction is created, and the four contact electrodes. Measuring the temperature dependence of the electrical resistance through the constriction one observes a transition to a ballistic regime that allows to obtain the mean free path, the Fermi wavelength and the carrier density of the sample without free parameters.

⇑ Scanning electron microscope picture of a 200 nm thick graphite lamella with the *c*-axis parallel to the current and voltage line provided by the two Au-electrodes. In this way the *c*-axis resistivity, i.e. perpendicular to the graphene planes can be measured.

that the measured carrier densities are not intrinsic but influenced by lattice defects or impurities. Moreover, internal interfaces between crystalline ~50 nm thick regions, parallel to the graphene layers, strongly influence the electrical transport. A way to reduce the effect of lattice defects and internal interfaces is to measure thin graphite films of thickness less than ~50 nm and a few micrometers size. In the last year we have improved the preparation of multigraphene samples, found a way to produce micrometer small constrictions by means of a dual beam microscope without inducing defects in the sample and to prepare graphite lamellas with such an orientation that should allow us to obtain the intrinsic electrical anisotropy of ideal graphite, see figures.

⇒ *Electric carrier concentration in graphite: Dependence of electrical resistivity and magnetoresistance on defect concentration*
A. Arndt, D. Spoddig, P. Esquinazi, J. Barzola-Quiquia, S. Dusari, T. Butz / Physical Review B (2009) **80** 195402

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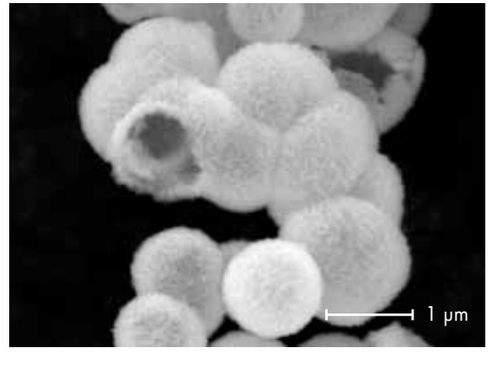
Nanoporous solids as hosts for metal nano-particles and hydrogen storage

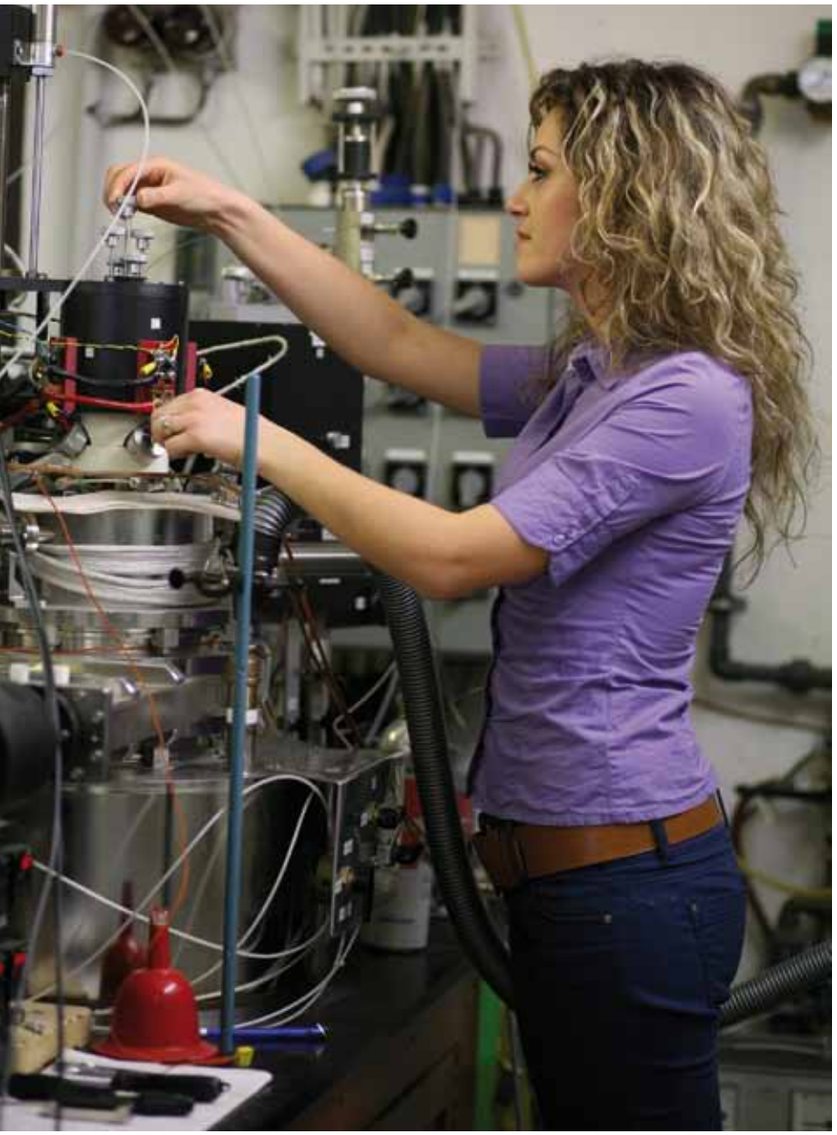
Prof. Dr. Roger Gläser
M.Sc. Chem. Eng. Neto Bastos, M.Sc. Chem. Michael Goepel, M.Sc. Erica Saraçi, M.Sc. Chem. Patrick With

The research is focused on nanoporous materials with defined porositiy on the micro-, meso- and macroscale. The chemistry of guests under nanoconfinement within the pores of these materials is the basis for innovative applications of these materials in sorption and heterogeneous catalysis. For instance, active components of metals and metal oxides are introduced as nanoparticles into the pore structures of these materials. These activities part of the BuildMoNa topical area “complex nanostructures” with contributions to the sub-fields of inorganic nanostructures and surfaces.

Besides the study of nanoporous materials as hosts for the storage of hydrogen as a fuel and energy carrier for the future economy, different materials with defined nanoporosity are studied, e.g. hollow spheres of zirconia as supports for metal catalysts (see figure). Applications for these catalysts are high-temperature conversions such as the dry reforming of the green house gases methane and carbon dioxide to the valuable synthesis gas, i.e., a micture of carbon monoxide and hydrogen.



⇐ Zirconia hollow spheres with mesoporous walls as supports for metal catalysts in high-temperature conversions



Transparent oxide electronic devices

Prof. Dr. Marius Grundmann
Dipl.-Phys. Tammo Böntgen, Dr. Christian Czekalla, M.Sc. Phys. Christof Peter Dietrich, Dipl.-Phys. Heiko Frenzel, Dipl.-Phys. Helena Hilmer, Dipl.-Phys. Alexander Lajn, Dipl.-Phys. Martin Lange, Dipl.-Phys. Michael Lorenz, Dipl.-Phys. Alexander Müller, Dipl.-Phys. Marco Stölzel, Dipl.-Phys. Chris Sturm, Dipl.-Phys. Jan Zippel

Metal-semiconductor field-effect transistors (MESFETs) are fabricated from wide band-gap oxide semiconductors. In such devices, the current flow in the channel (thin film of about 20 nm thickness on insulating substrate) between source and drain electrode is controlled by the gate voltage via the extension of a charge-carrier-depleted region, induced by the Schottky gate electrode. Our devices are fabricated on high quality sapphire substrates or cost efficient glass substrates, both being transparent. The Mg-doped zinc oxide semiconductor is grown by pulsed-laser deposition and the source/drain (gate) electrodes are deposited by (reactive) sputtering of Au (Pt, Pd, Au or Ag). The current through the channel can be controlled over 8 orders of magnitude by changing the gate voltage by less than 3 Volts.

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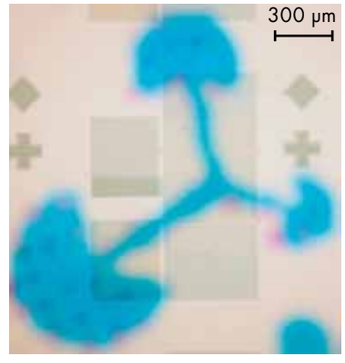
This is especially favourable in low-power mobile electronic devices. In a first step towards integrated electronic devices, inverter circuits were fabricated, showing a voltage gain of nearly 200, which is an order of magnitude superior compared with reports in literature. By using transparent and conductive aluminum-doped ZnO for the source/drain electrodes and reducing the thickness of the gate electrode to about 100 Å, the MESFETs can be fabricated fully transparent, reaching a mean transmission of 70 % in the visible spectral range. The electrical properties of such devices are among the best reported in literature.



⇐ Optical microscopic image of a fully transparent inverter circuit consisting of two MESFETs (background: laser-printed logo of BuildMoNa on an overhead transparency)

⇒ *Shallow Donors and Compensation in Homoepitaxial ZnO Thin Films*
A. Lajn, H. von Wenckstern, G. Benndorf, C.P. Dietrich, M. Brandt, G. Biehne, H. Hochmuth, M. Lorenz, M. Grundmann / Journal of Electronic Materials (2009) DOI: 10.1007/s11664-009-1017-7

⇒ *The E3 defect in $Mg_xZn_{1-x}O$*
H. von Wenckstern, K. Brachwitz, M. Schmidt, C.P. Dietrich, M. Ellguth, M. Stölzel, M. Lorenz, M. Grundmann / Journal of Electronic Materials (2009) DOI: 10.1007/s11664-009-0967-0

⇒ *Lineshape Theory of Photoluminescence from Semiconductor Alloys*
M. Grundmann, C.P. Dietrich / Journal of Applied Physics (2009) **106** 123521

⇒ *ZnO-based metal-semiconductor field-effect transistors on glass substrates*
H. Frenzel, M. Lorenz, A. Lajn, H. von Wenckstern, G. Biehne, H. Hochmuth, M. Grundmann / Applied Physics Letters (2009) **92** 153503

⇒ *Observation of strong light-matter coupling by spectroscopic ellipsometry*
H. Hilmer, C. Sturm, R. Schmidt-Grund, B. Rheinländer, M. Grundmann / Superlattices and Microstructures (2009) **47** 19

⇒ *ZnO nano-pillar resonators with coaxial Bragg reflectors*
R. Schmidt-Grund, A. Hinkel, H. Hilmer, J. J. Zúñiga-Pérez, C. Sturm, B. Rheinländer, M. Grundmann / Materials Research Society Symposium Proceedings (2009) 1178-AA10-13

⇒ *Anionic and cationic substitution in ZnO*
H. von Wenckstern, H. Schmidt, M. Brandt, A. Lajn, R. Pickenhain, M. Lorenz, M. Grundmann, D.M. Hofmann, A. Polity, B.K. Meyer, H. Saal, M. Binnewies, A. Börger, K.-D. Becker, V.A. Tikhomirov, K. Jug / Progress in Solid State Chemistry (2009) **37** 153

⇒ *ZnO-based metal-semiconductor field-effect transistors with Ag-, Pt-, Pd-, and Au-Schottky gates*
H. Frenzel, A. Lajn, H. von Wenckstern, G. Biehne, H. Hochmuth, M. Grundmann / Thin Solid Films (2009) **518** 1119

⇒ *Zinc Oxide Nanorods Based Photonic Devices: Recent Progress in Growth, Light Emitting Diodes and Lasers*
M. Willander, O. Nur, Q.X. Zhao, L.L. Yang, M. Lorenz, B.Q. Cao, J. Zúñiga-Pérez, C. Czekalla, G. Zimmermann, M. Grundmann, A. Bakin, A. Behrends, M. Al- Suleiman, A. Al-Shaer, A. Che Mofor, B. Postels, A. Waag, N. Boukos, A. Travlos, J. Guinard, D. Le Si Dang / Nanotechnology (2009) **20** 332001

⇒ *Observation of strong exciton-photon coupling at temperatures up to 410 K*
C. Sturm, H. Hilmer, R. Schmidt-Grund, M. Grundmann / New Journal of Physics (2009) **11** 073044

⇒ *Homogeneous core/shell ZnO/MgZnO quantum well heterostructures on vertical ZnO nanowires*
B.Q. Cao, J. Zúñiga-Pérez, N. Boukos, C. Czekalla, H. Hilmer, J. Lenzner, A. Travlos, M. Lorenz, M. Grundmann / Nanotechnology (2009) **20** 305701

⇒ *Properties of reactively sputtered Ag, Au, Pd, and Pt Schottky contacts on n-type ZnO*
A. Lajn, H. von Wenckstern, Z. Zhang, C. Czekalla, G. Biehne, J. Lenzner, H. Hochmuth, M. Lorenz, M. Grundmann, S. Wickert, C. Vogt, R. Denecke / Journal of Vacuum Science & Technology B (2009) **27** 1769

⇒ *Temperature Dependence of Localization Effects of Excitons in ZnO/$Cd_xZn_{1-x}O$/ZnO Double Heterostructures*
M. Lange, J. Zippel, G. Benndorf, H. Hochmuth, M. Lorenz, M. Grundmann / Journal of Vacuum Science & Technology B (2009) **27** 1741

⇒ *Electronic coupling in $Mg_xZn_{1-x}O$/ZnO double quantum wells*
J. Zippel, J. Lenzner, G. Benndorf, M. Lange, H. Hochmuth, M. Lorenz, M. Grundmann / Journal of Vacuum Science & Technology B (2009) **27** 1735

⇒ *Optical characterization of zinc oxide microlasers and microwire core-shell heterostructures*
C. Czekalla, C. Sturm, R. Schmidt-Grund, B. Cao, J. Zúñiga-Pérez, M. Lorenz, M. Grundmann / Journal of Vacuum Science & Technology B (2009) **27** 1780

⇒ *Defects in zinc-implanted ZnO thin films*
M. Schmidt, M. Ellguth, C. Czekalla, H. von Wenckstern, R. Pickenhain, M. Grundmann, G. Brauer, W. Skorupa, M. Helm, Q. Gu, Ch.Ch. Ling / Journal of Vacuum Science & Technology B (2009) **27** 1597

⇒ *Strong Exciton-Photon Coupling In ZnO based Resonators*
C. Sturm, H. Hilmer, R. Schmidt-Grund, C. Czekalla, J. Sellmann, J. Lenzner, M. Lorenz, M. Grundmann / Journal of Vacuum Science & Technology B (2009) **27** 1726

⇒ *Ferroelectric thin film field-effect transistors based on ZnO/$BaTiO_3$ heterostructures*
M. Brandt, H. Frenzel, H. Hochmuth, M. Lorenz, M. Grundmann, J. Schubert / Journal of Vacuum Science & Technology B (2009) **27** 1789

⇒ *Stable p-type ZnO:P nanowire/n-type ZnO:Ga film junctions, reproducibly grown by two-step pulsed laser deposition*
M. Lorenz, B. Cao, G. Zimmermann, G. Biehne, C. Czekalla, H. Frenzel, M. Brandt, H. von Wenckstern, M. Grundmann / Journal of Vacuum Science & Technology B (2009) **27** 1693

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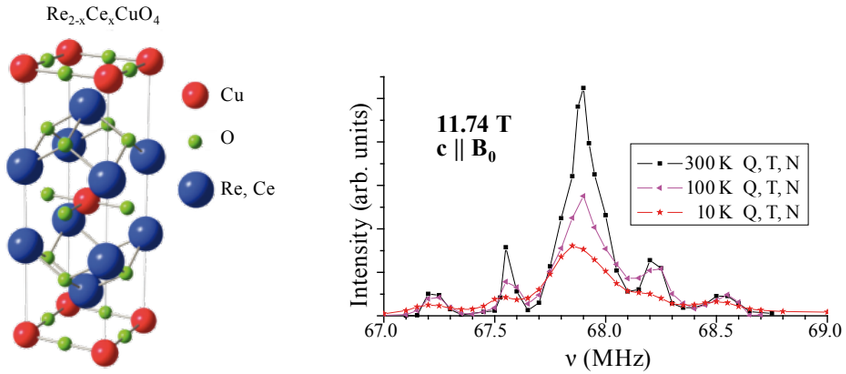
Electronic properties of modern materials investigated with magnetic resonance techniques

Prof. Dr. Jürgen Haase
M.Sc. Phys. Michael Jurkutat, Dipl.-Phys. Benno Meier

Our group focuses on the investigation of the electronic properties of modern materials such as high-temperature superconductors, ferroelectrics, and multiferroics, as well as the chemical structure of porous media and large molecules. Our tools are the many methods of Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR), however, we also have a strong focus on developing such methods. Here, our group is pioneering the application of the highest magnetic fields and the highest pressures with NMR.

Within BuildMoNa two doctoral students began their work on the development of ultra-high magnetic field techniques (B. Meier), and on the electronic properties of electron doped high-temperature superconducting cuprates (M. Jurkutat) in 2009.



The work in ultra-high magnetic fields is performed in collaboration with the High-Field Laboratory Dresden (HLD) that was able to supply long-pulse high magnetic field pulses last year. We designed the NMR apparatus and probes that work in the HLD and fit the pulsed magnets there. Performing NMR in time-dependent magnets is very demanding, but warrants the highest fields. A burning question was the determination of the precise field parameters, in particular its time-dependence. In the now available long-pulse coils that we operate with energies that are almost a factor of 200 larger than previously, we could record many NMR signals on a single field pulse and, to our surprise, this let us determine the field with a precision of a few parts per million. Why is that so important? First, this enables signal averaging during a single field pulse, and second, we can now perform NMR shift measurements with high precision by operating a double-resonance probe that measures the field in one channel and the desired signal of a sample in the second channel. Such a double-resonance setup is now being developed. As a first application we hope to be able to measure quantum oscillations through NMR experiments, soon.

There is still no theory of high-temperature superconductivity and the electron doped cuprate materials have not been investigated much with NMR, a local probe that gives bulk information. In particular the oxygen resonance was not observed as two signals obstruct each other. We have developed a new method that lets us differentiate between the two signals and we believe that this will greatly help in understanding these materials. In fact, our most recent results show that the electronic fluid leaves imprints at the planar oxygen that look very much like those for the hole-doped materials. This comes as a big surprise and points to a two-liquid scenario.

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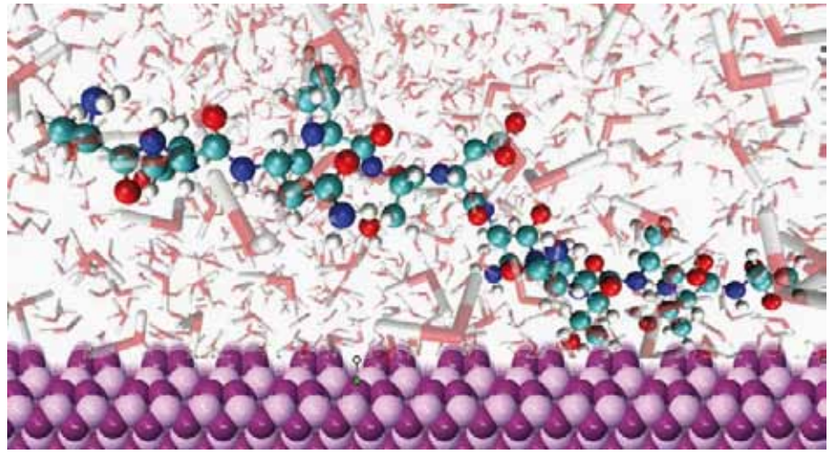
Multiscale modelling of molecular phenomena at solvation interfaces

Prof. Dr. Dr. h.c. Wolfgang Hackbusch
M.Sc. Chem. Anastacia Romanova

Our research activities lie at the interface between advanced numerical mathematics and computational molecular sciences. We are applying novel modelling techniques to different challenging problems in bio and nano sciences such as peptide/protein adhesion to semiconductor interfaces, ion effects on biopolymer stability in water and at different interfaces, supramolecular self-assembly and integration of nano-objects to biological aqueous environments.

We are developing new theoretical and numerical tools for multiscale computational treatment of solvation phenomena. In this new approach we combine several theoretical methods (integral equations theory, quantum-classical DFT, molecular mechanics and coarse-grained models) with advanced mathematical tools of the multiresolution analysis, global energy matching and multigrid to construct a universal methodological platform for modelling condensed molecular systems. In this framework, multiscale is naturally incorporated into the theoretical part of the model as well as into the computational part. The main advantages of this approach are: *(i)* its flexibility which allows one to apply it to various kinds of solvation phenomena spanning from solvation of electrons in polar liquids to self-assembled nanostructures; *(ii)* the theoretical and mathematical background of this approach allows one to employ very efficient multiscale algorithms which dramatically reduce the computational cost. We apply our methods to simulate at the atomic level the adsorption behaviour of ions and biomolecules at different liquid-solid interfaces.



⇑ Fully atomistic simulations of a synthetic oligopeptide (AQNPSDNNTATA) at the water-semiconductor interface

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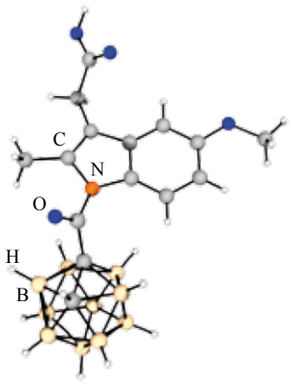
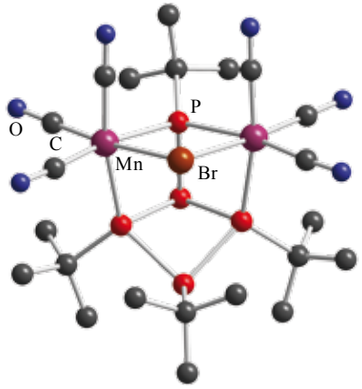
Smart carbaborane- or phosphorus-containing molecules as building blocks in medicinal chemistry, materials science, and catalysis

Prof. Dr. Evamarie Hey-Hawkins
Dr. Sebastian Bauer, M.Sc. Chem. René Frank, Dipl.-Chem. Julia Haushälter, M.Sc. Chem. Aslihan Kircali, Dipl.-Chem. Carolin Limburg, M.Sc. Chem. Martyna Madalska, M.Sc. Chem. Souvik Pandey, M.Sc. Chem. Julian Rodger Frederic Pritzwald Stegmann, Dipl.-Chem. Matthias Scholz, M.Sc. Chem. Markus Streitberger

Besides three-dimensional aromaticity, *carbaboranes* exhibit extremely high hydrophobicity. They can be easily integrated into organic and biochemical structures due to their organic reaction behaviour, and can therefore replace phenyl groups as pharmacophoric moieties in biologically active structures, e.g., aspirin and indomethacin (Matthias Scholz). Another approach is the integration of carbaborane-containing amino acids into carrier peptides (René Frank).



⇑ Indoborin – the carbaborane-analogue of indometacin



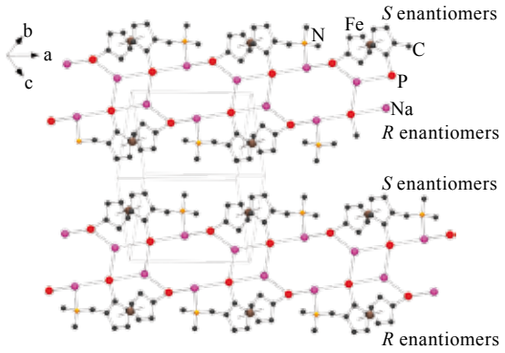
⇑ Organometallic manganese-phosphorus precursor molecule

We are developing novel synthetic approaches to *binary metal phosphides* MP_x ($x > 1$) which often exhibit interesting optical, electronic and/or magnetic properties, starting from volatile phosphorus-rich transition metal complexes as molecular precursors (Aslihan Kircali).

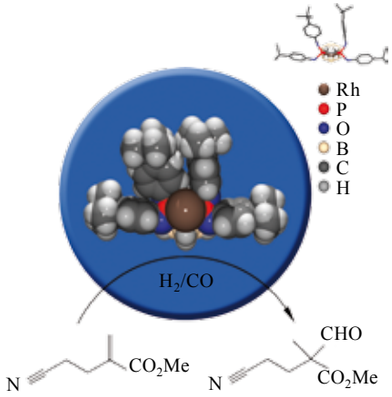
Primary (chiral) ferrocenyl phosphines are useful starting materials for metal phosphanides $M(PRR')_x$ and phosphanediides $M(PR')_y$ (R' = ferrocenyl, R = H, alkyl, aryl, etc.), which can exhibit unusual structures in solution and in the solid state (*polymers*, *clusters*), as well as unusual electronic, magnetic and optical properties (Carolin Limburg, Julian Pritzwald-Stegmann). Furthermore, catalytic dehydrogenation of the respective ferrocenyl phosphine–borane adducts yields (chiral) *inorganic polymers* with a P–B-based backbone which are expected to exhibit electrical conductivity, magnetic properties, thermal stability and possibly superconductivity as well as NLO properties (Souvik Pandey).

Chiral phosphines play an important role as ligands in *catalytically active complexes*. Carbaboranyl bis-phosphines combine the properties of the electron-poor cluster with those of a bis-phosphine and can, furthermore, be selectively functionalised in the 9-position to allow immobilisation and thus combine the advantages of homogeneous and heterogeneous catalysis (Sebastian Bauer). Similarly, chiral ferrocenyl phosphines will be immobilised on electrode surfaces (graphite, gold, etc.), and their applications as switchable catalysts (redox-active ferrocenyl unit) will be explored (Martyna Madalska).

Cyclic phosphines (*phosphine baskets and macrocycles*) are useful as ligands for catalytically active metals and as selective sensors. Variation of the coordinated metal atom or the size of the cavity should influence the selectivity in catalytic processes and sensing (Julia Haushälter, Markus Streitberger).



⇑ Disodium-1,1'-bisphosphanidoferrocene forms one-dimensional polymers consisting of an inorganic layer (four- and eight-membered Na,P rings) and an organometallic exterior (chiral 1,1'-ferrocenediyl units)



⇑ Rhodium bis-phosphine complex in catalysis

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⇒ *Asborin: The Carbaborane Analogue of Aspirin*
M. Scholz, K. Bensdorf, R. Gust, E. Hey-Hawkins / ChemMedChem (2009) **4** 746

⇒ *Synthesis and Reactivity of ortho-Carbaborane-Containing Chiral Aminohalophosphines*
S. Stadlbauer, R. Frank, I. Maulana, P. Lönnecke, B. Kirchner, E. Hey-Hawkins / Inorganic Chemistry (2009) **48** 6072

⇒ *Enantiomerically Pure Bisphosphonito Carbaborane(12)s*
S. Bauer, S. Tschirschwitz, P. Lönnecke, R. Frank, B. Kirchner, M. L. Clarke, E. Hey-Hawkins / European Journal of Inorganic Chemistry (2009) 2776

⇒ *Boron Clusters in Cancer Therapy*
S. Stadlbauer, R. Frank, J. Kunig, V. Ortmann, A. G. Beck-Sickinger, E. Hey-Hawkins / In: Metal Elements in Environment, Medicine and Biology, Vol. 9, ed. G. Garban, R. Silaghi-Dumitrescu, Cluj University Press, ISSN 1583-4202, 2009, p. 3–10

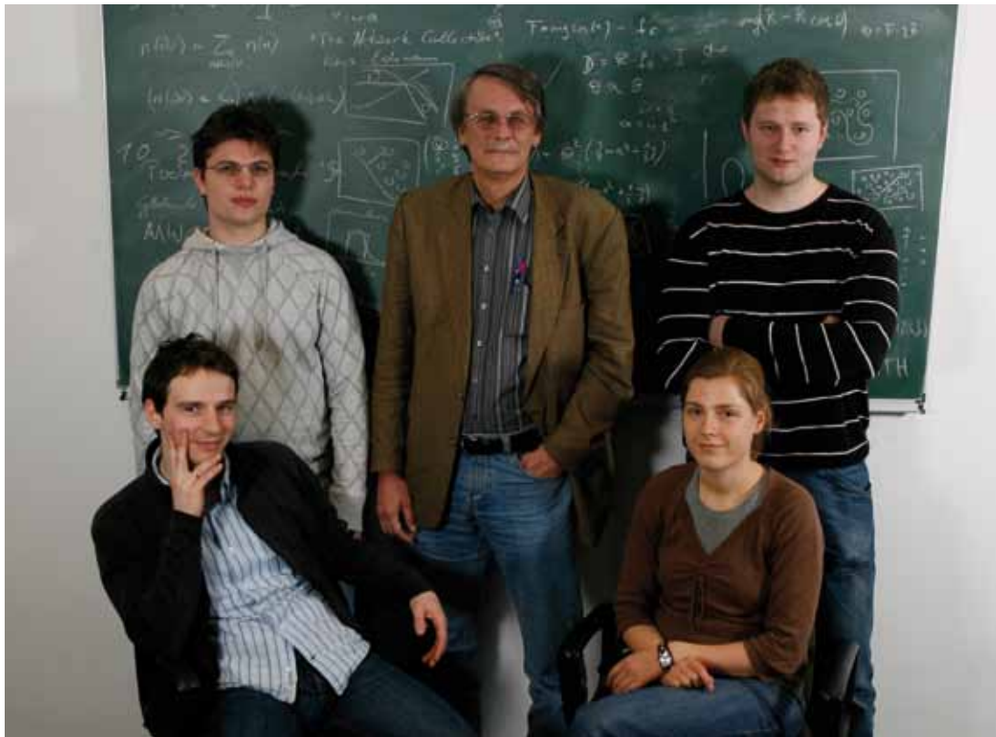
Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke
Dipl.-Phys. Monika Möddel, Dr. Stefan Schnabel, Dipl.-Phys. Sebastian Schöbl, Dr. Sandro Wenzel, Dipl.-Phys. Micha Wiedenmann

The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on five interrelated subprojects:

Monika Möddel studies the conformational mechanics of polymer adsorption transitions at attractive solid substrates. This research is conducted in cooperation with the experimental semiconductor and biochemistry groups.

Micha Wiedenmann investigates condensation phenomena in liquid/gas or solid/



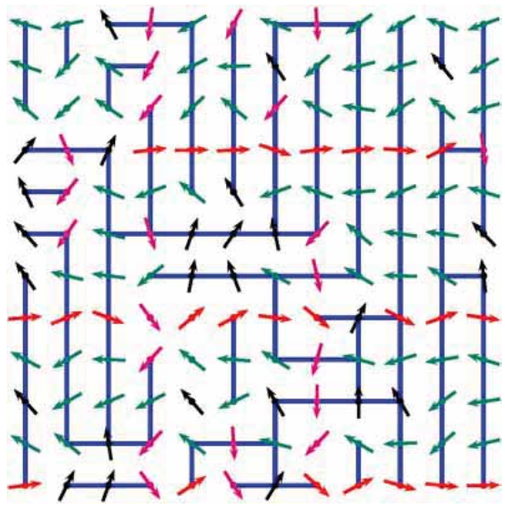
gas mixtures described by simplified lattice gas models, which are of importance for aggregation processes in general.

Sandro Wenzel performs research into the physics of quantum phase transitions in dimerised Heisenberg models and other quantum effects for patterned spin systems, for which he has identified an unconventional universality class. Further results for the quantum compass models may yield important insights into some aspects of quantum computing.

Stefan Schnabel classifies the symmetry properties of crystallisation of single polymers and studies the relation to compact hydrophobic-core formation and the collapse transition, within mesoscopic models for the folding of flexible homopolymers.

Sebastian Schöbl explores the conformational statistics of polymers in disordered environments which is important for a basic understanding of, e.g., the universal properties of the cycloskeleton investigated by several other BuildMoNa groups.

The employed methodology mainly relies on sophisticated Monte Carlo computer simulations based on stochastic series expansions or multicanonical ensembles, chain-growth algorithms with population control, and thermostated Molecular Dynamics methods, which are adapted by us to the problems at hand and constantly further improved in order to cope with the complexity of the considered problems.



⇑ Visualisation of the disordered phase of the two-dimensional compass model. For $T > T_c$ the distribution of bonds possessing less than average bond energy (thick lines) is rather random. Small arrows indicate the spin degree of freedom. For $T < T_c$ the prevalent correlations order spontaneously into one direction, i.e., the system is in a directionally ordered state.

⇒ *Comprehensive Quantum Monte Carlo Study of the Quantum Critical Points in Planar Dimerized/Quadrumerized Heisenberg Models*
S. Wenzel, W. Janke / Physical Review B (2009) **79** 014410-1-11

⇒ *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*
M. Möddel, M. Bachmann, W. Janke / The Journal of Physical Chemistry B (2009) **113** 3314

⇒ *Surface Effects in the Crystallization Process of Elastic Flexible Polymers*
S. Schnabel, T. Vogel, M. Bachmann, W. Janke / Chemical Physics Letters (2009) **476** 201

⇒ *Finite-Temperature Néel Ordering of Fluctuations in a Plaquette Orbital Model*
S. Wenzel, W. Janke / Physical Review B (2009) **80** 054403-1-6
[Fig. 2(c) selected for Physical Review B "Kaleidoscope" August 2009]

⇒ *Elastic Lennard-Jones Polymers meet Clusters – Differences and Similarities*
S. Schnabel, M. Bachmann, W. Janke / The Journal of Chemical Physics (2009) **131** 124904-1-9

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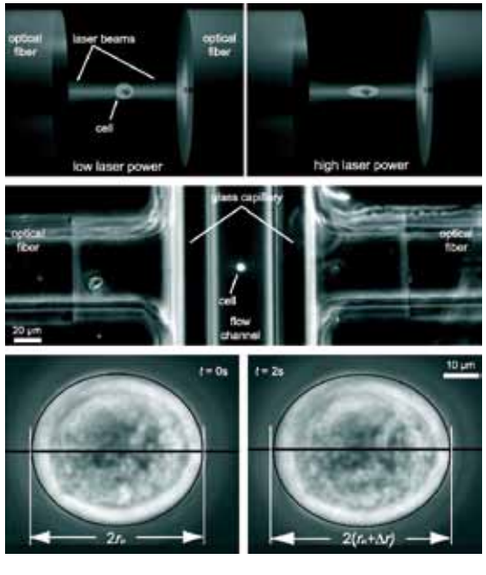
The optical stretcher – probing active and passive biomechanics of living cells

Prof. Dr. Josef Alfons Käs
M.Sc. Phys. Susanne Ebert, Dipl.-Phys. Anatol Fritsch, M.Sc. Phys. Markus Gyger, Dipl.-Phys. Florian Huber, Dipl.-Phys. Tobias Kießling, Dipl.-Math. Melanie Knorr, Dipl.-Phys. Karla Müller, M.Sc. Phys. David K. Nnetu, Dipl.-Phys. Dan Strehle, Dipl.-Phys. Franziska Wetzel

Recent studies clearly showed that the mechanical properties of living cells are crucial in understanding proliferation, migration and cell adhesion. Furthermore, it turned out that the cell's elasticity is a cellular marker to differentiate normal cells from malignantly transformed cells. How changes of the cytoskeleton influence the cell's mechanical properties is the focus of the BuildMoNa students' studies, as well as the detection of cancer and metastatic cells by probing the cells deformability.



⇐ The Optical Stretcher is a tool to probe viscoelastic properties of individual cells utilizing the pressure refracted light exerts on a surface. During a measurement cells are in suspension in a flow channel. Individual cells are trapped between two counter-propagating divergent laser beams emitted from opposing optical fibers. By increasing the laser power, the surface stress (due to the light pressure) increases and deforms the cell along the laser axis.

The Optical Stretcher technology – which was developed in the group – probes the mechanical properties of single cells by first trapping the cells between two laser beams with subsequent optical deformation with increased laser power. BuildMoNa students developed a new microfluidic chip for the Optical Stretcher that enables cell sorting after deformation. Additionally, a computer-controlled system of vacuum pumps was set up to fully automate the experimental procedure which increased the through-put of cells during a measurement by a factor of five.

Recent experiments on the mechanical properties of malignant cell lines with the Optical Stretcher clearly showed a stronger elastic response of malignant cells compared to normal cells. First clinical studies of the elasticity of primary human breast cancer cells in comparison to normal primary breast cells corroborated this result.

⇒ *The Cytoskeleton: An active Polymer-based Scaffold*
D. Smith, B. Gentry, B. Stuhrmann, F. Huber, D. Strehle, C. Brunner, D. Koch, M. Steinbeck, T. Betz, J. A. Käs / Biophysical Reviews and Letters (2009) **4** 179

⇒ *Compaction of cell shape occurs before decrease of elasticity in CHO-K1 cells treated with actin cytoskeleton disrupting drug cytochalasin D*
Ch. Schulze, K. Müller, J. A. Käs, J. C. Gerdelmann / Cell Motility and the Cytoskeleton (2009) **66** 193

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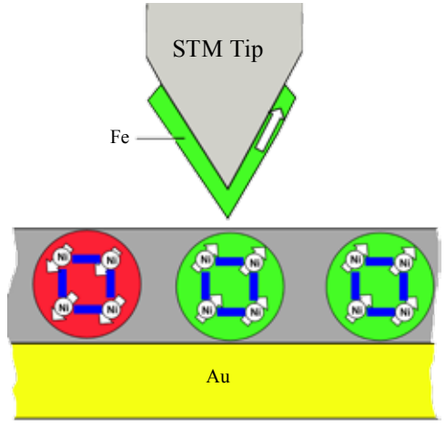
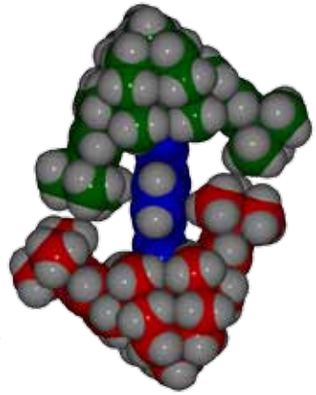
Metalated container molecules in catalysis and molecular magnetism

Prof. Dr. Berthold Kersting
M.Sc. Chem. Matthias Golecki, Dipl.-Chem. Jochen Lach, M.Sc. Chem. Ulrike Lehmann, Dipl.-Chem. Ronny Syre

We investigate various aspects of the chemistry of metalated container molecules. An attractive feature is the use of such complexes as molecular reaction chambers for promoting reactions within their interiors. The corresponding compounds are designed in such a way that they unite molecular recognition and transition metal catalysis within one molecule. Ulrike Lehmann synthesises and characterises novel capsule-like macromolecules which can be used as nano-vessels for the activation and transformation of small molecules. Ronny Syre is studying compounds of the type "catalyst in a molecule". Known catalysts such as Jacobsen's Mn-salenes are



⇐ Polarised conduction electrons in a metal-molecule-metal junction



Paramagnetic Ni^{II}_4 complex ⇒

functionalised and coordinatively attached to the open coordination sites of a metalated container molecule. The encapsulation of the catalyst has a marked influence on its selectivity and activity.

The project of Jochen Lach on the other hand is related to spintronics. He develops novel non-oxide single molecule magnets for use in information storage devices. Particular emphasis of his project is put on the targeted assembly of novel non-oxide based single-molecule magnets (SMMs) by using a modular approach. The molecules can be deposited and arranged on metallic (Au(111), Co), insulating (SiO_2), or semiconducting surfaces (Si, GaAs) by spin-coating or the self-assembled monolayer approach.

⇒ *Chemistry of Metalated Container Molecules*
B. Kersting, U. Lehmann / Advances in Inorganic Chemistry (2009) **61** 407

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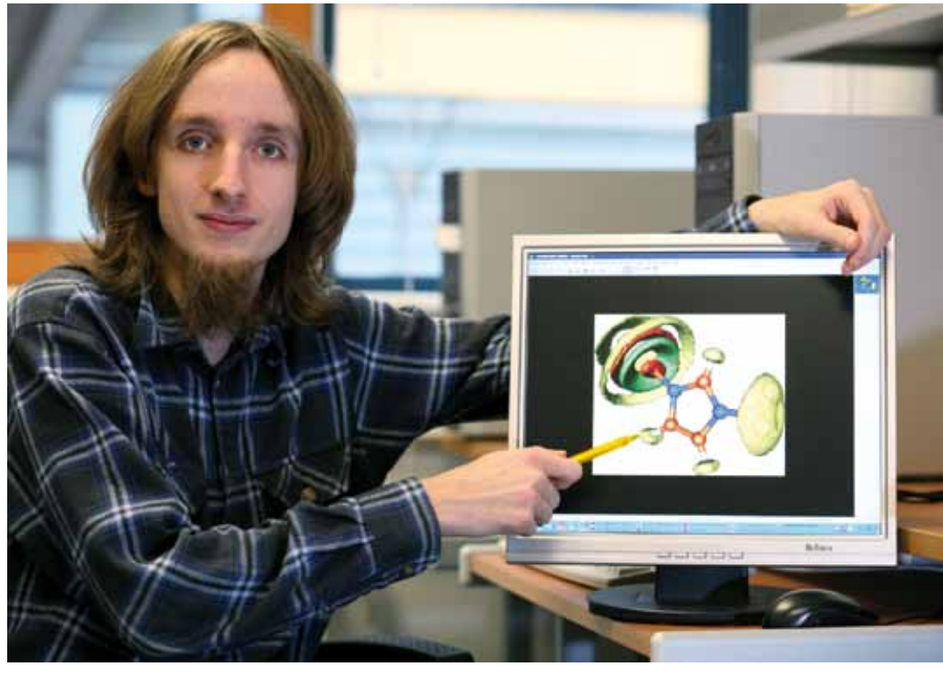
Smart molecules from theoretical calculations

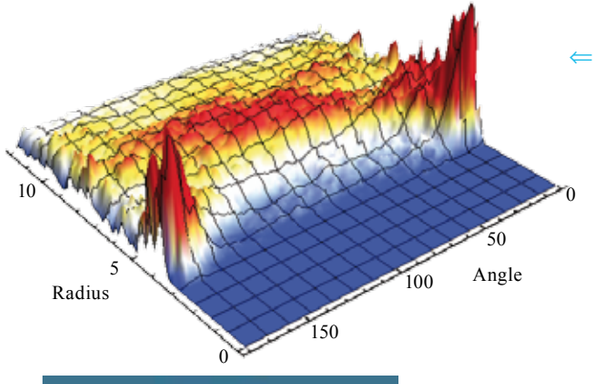
Prof. Dr. Barbara Kirchner
Dipl.-Chem. Martin Brehm

In order to analyse and visualise trajectories from molecular dynamics simulations a program package was developed. The program package allows the calculation of a variety of functions by reducing the high dimensional information of the trajectory. Mapping a distinct property onto the surface of a particular function allows the characterisation of certain new features.

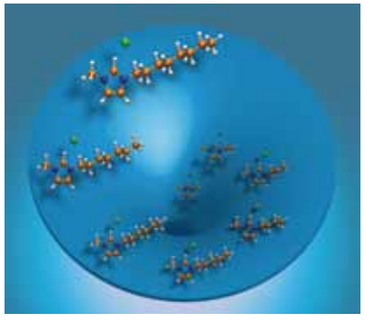
Employing ab initio molecular dynamics simulations to the ionic liquid [Emim][SCN], the structural and dynamical properties were determined. The geometric picture indicated a superior role for the most acidic hydrogen bond at the front of the imidazolium ring. Despite this structural picture, the hydrogen bond dynamics at this proton was observed to decay faster than the according dynamics at the rear protons. Neglecting the directionality provides a dynamics which reflects the geometrical analysis. Two movements are identified. First, a fast hopping of the anion above and below the ring and second a translational motion of the anion away from the cation in-plane of the ring.

Several ionic liquid ion pairs were studied in order to resolve the intermolecular interaction. These interactions – especially the nature of hydrogen bonding – showed a strong dependence on the anion but also on the size of the side chain.

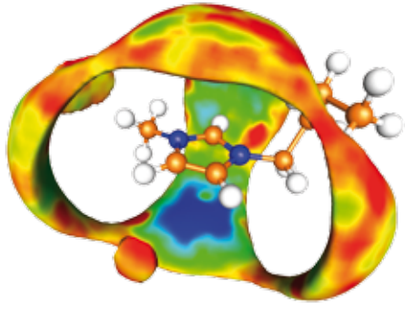




⇐ Radial angular distribution function



⇑ Different imidazolium chloride ion pairs with varying side chain



⇑ Spatial distribution function of [SCN] – around imidazolium with mapped velocities of the anions

⇒ *Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids*
J. Thar, M. Brehm, A. P. Seitsonen, B. Kirchner / Journal of Physical Chemistry B (2009) **113** 15129

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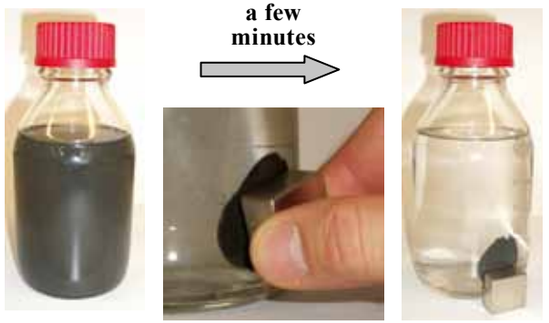
Wastewater and -air treatment with colloids and nano-catalysts

Prof. Dr. Frank-Dieter Kopinke
M.Sc. Chem. Dalia Angeles-Wedler, M.Sc. Chem. Engineer. Abhinnandan Banerjee, Dipl.-Phys. Markus Kraus, M.Sc. Chem./Environ. Prot. Ksenia J. Ramus, Dipl.-Chem. Techn. Klara Rusevova, Dipl.-Phys. Jens Schneider

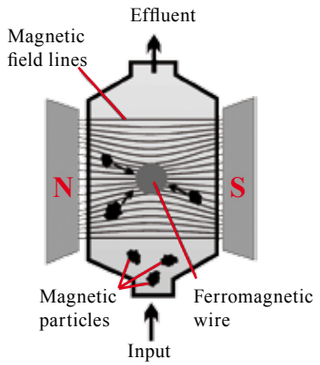
Dalia Angeles-Wedler has finished her doctoral work on "Application, Protection and Regeneration of Palladium as Hydrodechlorination Catalyst for Chlorinated Organic Pollutants" in the cumulative form after acception of her third original paper. She found procedures to protect Pd catalysts, which are highly active in the hydrodechlorination of chlorinated compounds, against fouling in contaminated wastewaters by silicone coating and to regenerate deactivated catalysts by permanganate treatment.

Markus Kraus has finished his doctoral work on "Anwendung gekoppelter Temperatur- und Konzentrationspulse für die effiziente adsorptiv-katalytische Entfernung von Schadstoffen aus kontaminierten Abluftströmen" and is going to join our group as a postdoc.

Ksenia Ramus deals with the influence of natural colloids such as humic acids on the transport of organic pollutants in water. She developed further the so-called



⇑ Magnetic separation of magnetite nano-particles suspended as catalyst in water in the laboratory scale



⇑ Scheme of magnetic separation of small particles suspended in water flows

⇑ "Burning water" in a high frequency electromagnetic field

"in tube solid phase micro-extraction (IT-SPME)" technique in a way that enables us to measure the desorption kinetics in a wide range of time resolution, from the sub-second up to the minutes range. This has never been achieved before.

Klara Rusevova started recently her work in our group on nano-catalysts for oxidation of pollutants in water. It is focused on nano-magnetite and mixed metal oxides as redox-catalysts for activation of hydrogen peroxide.

Jens Schneider investigates the phenomenon of water dissociation under the action of high-frequent electromagnetic fields ("burning water"). Beside that, he developed a "chemical thermometer" which enables us to measure "effective surface temperatures" of nano-particles in aqueous suspensions. This methodical work aims at elucidating if there is any overheating or specific activation of nano-particles in high-frequency fields, such as micro-waves, radio-waves or ultra-sound.

Abhinnandan Banerjee has measured carbon and chlorine kinetic isotope effects in the hydrodechlorination reaction catalyzed by different palladium species, among them nano-particles. After one year in our group he decided to return to India by personal reasons. We wish Abhinnandan all the best for his further scientific career.

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⇒ *Sulphide-induced Deactivation of Pd/Al_2O_3 as Hydrodechlorination Catalyst and its Oxidative Regeneration with Permanganate*
D. Angeles-Wedler, K. Mackenzie, F.-D. Kopinke / Applied Catalysis B, Environmental (2009) **90** 613

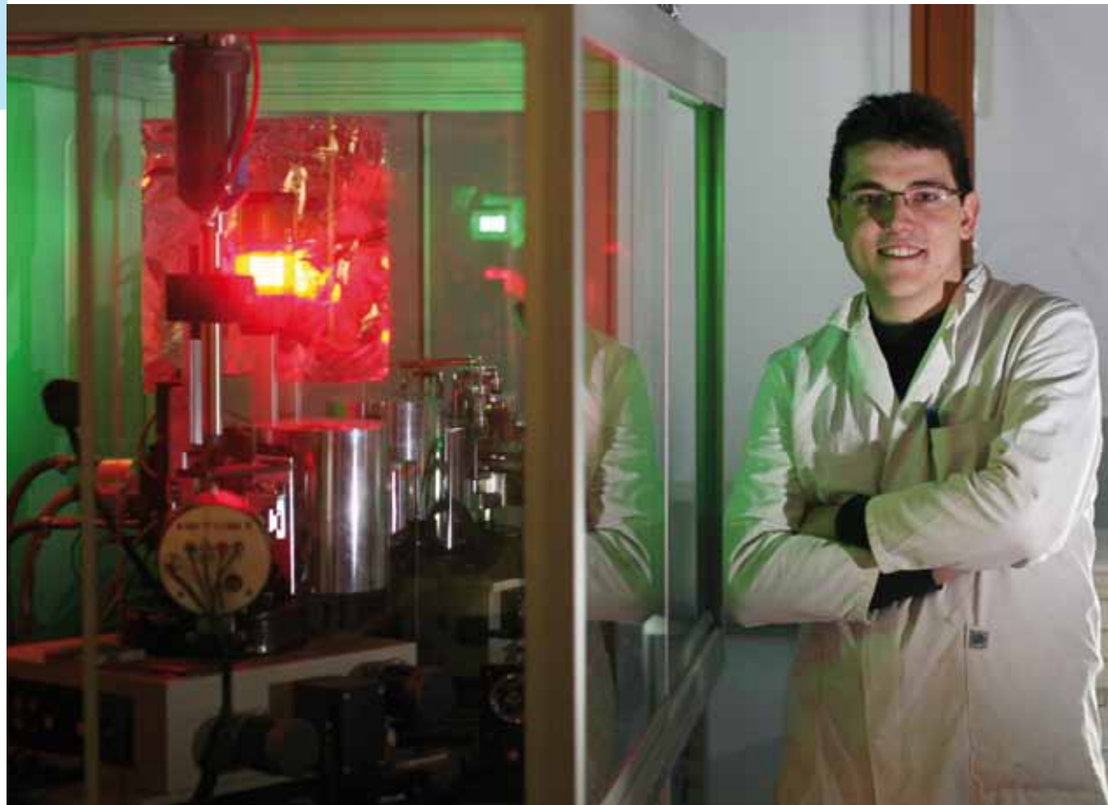
⇒ *Kombination von Adsorption, Katalyse und Radiowellen-Anwendung gegen VOC: Mit Radiowellen gegen kontaminierte Abluft*
M. Kraus, U. Roland /Entsorga (2009) **3** 25

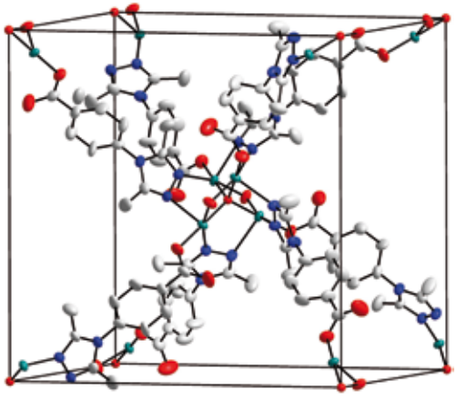
⇒ *Neues Verfahren zur Abluftreinigung*
U. Roland, M. Kraus / Besser lackieren (2009) **11** 2

Porous coordination polymers for applications in adsorption and catalysis

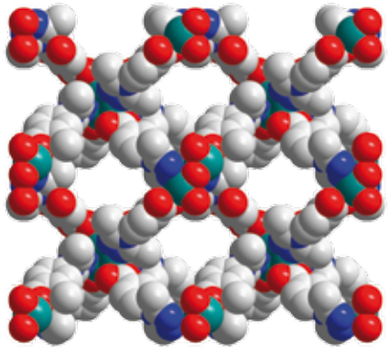
Prof. Dr. Harald Krautscheid
Dr. Ralf Biedermann, B.Sc. Chem. Jorge Luis Cholula Díaz, M.Sc. Chem. Dirk Friedrich, M.Sc. Chem. Florian Kettner, M.Sc. Chem. Daniel Lässig, M.Sc. Chem. Jörg Lincke

Microporous 3D coordination polymers, so called Metal-Organic Frameworks (MOFs), are a new class of organic-inorganic hybrid materials. Because of their wide range of pore size distributions and high inner surface areas they represent interesting materials for adsorption. Potential applications in heterogeneous catalysis are based on functional groups of the organic ligands, suitable combinations of





⇑ Unit cell of $[Cu_4(\mu_4\text{-}O)(\mu_2\text{-}OH)_2(Me_2trz\text{-}pba)_4]$ crystallising in the tetragonal space group $P\bar{4}2_1c$ with two formula units per unit cell



⇑ Space filling projection of $[Cu_4(\mu_4\text{-}O)(\mu_2\text{-}OH)_2(Me_2trz\text{-}pba)_4]$ in crystallographic *b* direction

metal ions and steric constraints in the pores.

Mainly aromatic or heterocyclic linkers with carboxylic groups, nitrogen or sulphur containing groups as substituents have been used. We have recently presented a series of ligands containing both carboxylate and triazole functions. Currently we are investigating their coordination behaviour towards transition metal ions and the properties of the resulting networks.

Using a triazolyl substituted benzoate (Me_2trz-*p*ba) as ligand, we obtained $[Cu_4(\mu_4\text{-}O)(\mu_2\text{-}OH)_2(Me_2trz\text{-}pba)_4]$ containing a $Cu_4(\mu_4\text{-}O)(\mu_2\text{-}OH)_2$ core as central structural motif. According to the space filling plot (see figure) it contains a three-dimensional pore system with windows of 450×550 pm in crystallographic *a* and *b* directions and 350×850 pm in *c* direction. The calculated solvent accessible pore volume is 57 % . Adsorption measurements show a strong dependence on the applied method of synthesis, especially the solvents used. At 3.5 MPa a CO_2 capacity of about 9.5 mmol/g corresponding to 42 weight% is observed.

⇒ *Halogeno(triazolyl)zinc complexes as molecular building blocks for metal-organic frameworks*
J. Lincke, D. Lässig, H. Krautscheid / Acta Crystallographica (2009) **C65** m488

⇒ *Highly functionalised 3,4,5-trisubstituted 1,2,4-triazoles for future use as ligands in coordination polymers*
J. Lincke, D. Lässig, H. Krautscheid / Tetrahedron Letters (2009) doi:10.1016/j.tetlet.2009.11.098

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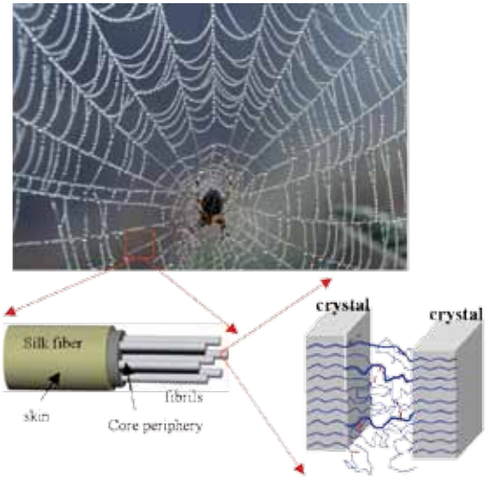
From the structure of spider silk to receptor-ligand force spectroscopy for Alzheimer's disease – molecular biophysics in basic research and application

Prof. Dr. Friedrich Kremer
Dipl.-Phys. Roxana-Giogiana Ene, M.Sc. Phys. Ciprian-Ghiorghita Iacob, M.Sc. Phys. Wilhelm Kossack, M.Sc. Phys. Ilya Semenov, Dipl.-Phys. Olaf Ueberschär, Dipl.-Phys. Carolin Wagner

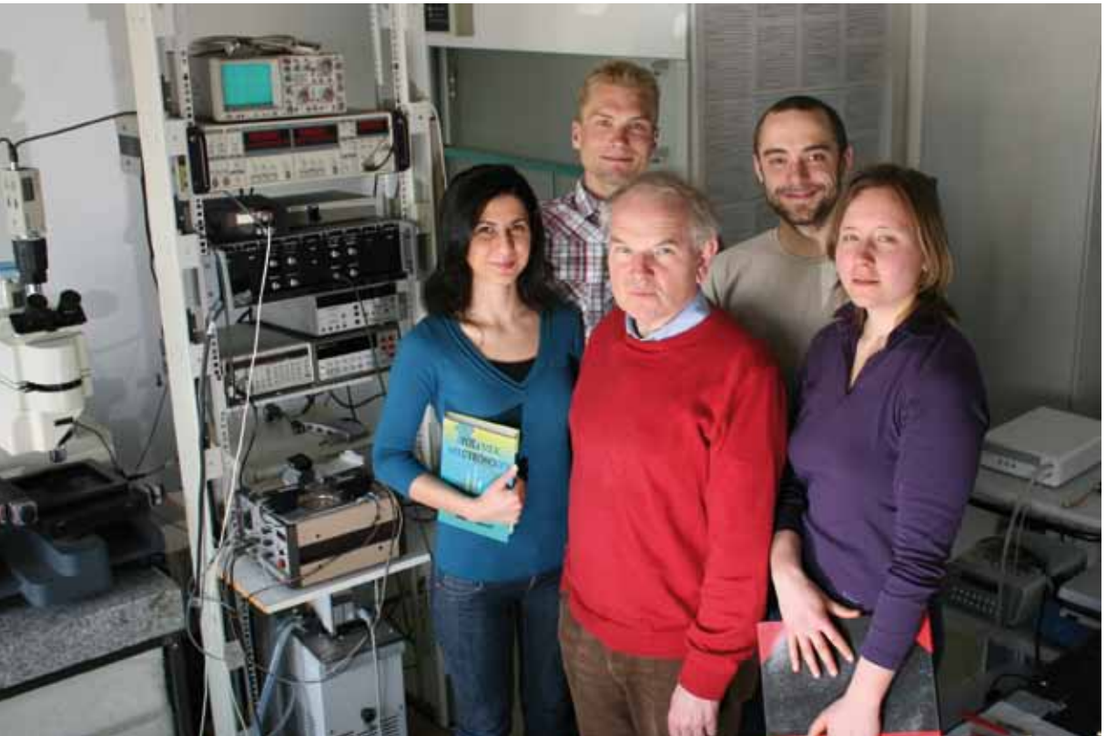
Unravelling the structure of spider silk: Combined time-resolved mechanical and polarised FTIR measurements allow us to determine the interconnection of the nanocrystal and amorphous phases in spider silk in the native and super-contracted state. Deuteration can probe the molecular moieties that are accessible by water. The chemical exchange of amide hydrogen occurs in a large fraction of amino acids including β-sheeted alanine residues, suggesting that also the crystalline regions are accessible to water.

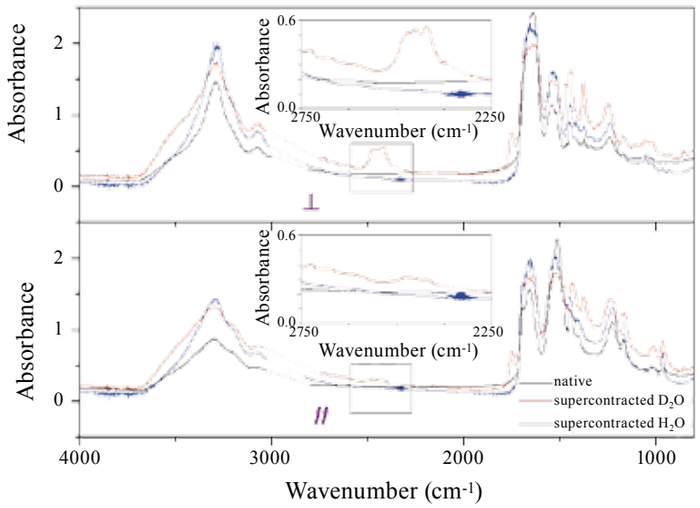


Advances in IR spectrometry: A novel spectroscopic method is developed for probing the molecular order in any IR-transparent material. By combining the variation of inclination and polarisation angle with the specificity of the IR spectral range, the dependence of the absorption coefficient provides detailed information concerning the orientational distribution of the different molecular moieties of the sample.

Stochastic thermodynamics: How can macroscopic quantities such as heat and entropy be consistently translated to the microscopic regime of single microparticles or molecules? How does macroscopic irreversibility emerge from the reversible motion on the micrometer scale? We have been investigating these key issues in the context of fluctuation theorems by means of single micrometer-sized colloids being held in an optical trap. Several theoretical predictions could already be verified in the course of this experimental endeavour.

Studying single receptor-ligand contacts: By utilizing dynamic force spectroscopy (DFS) the specific binding of the monoclonal antibody HPT-110 to a synthetic double phosphorylated tau-peptide is investigated. Amongst others, the massive accumulation of tangles which mainly consist of hyperphosphorylated tau-proteins is characteristic for Alzheimer's disease. Single-molecule DFS enables the investigation of the energy landscape of the bond and benefits from the fact that only minimal amounts of the sample are necessary.





⇒ *Similarities in the structural organization of major and minor ampullate spider silk*
P. Papadopoulos, R. Ene, I. Weidner, F. Kremer / Macromolecular Rapid Communications (2009) **30** 851

⇒ *Combined structural model of spider dragline silk*
R. Ene, P. Papadopoulos, F. Kremer / Soft Matter (2009) **5** 4568

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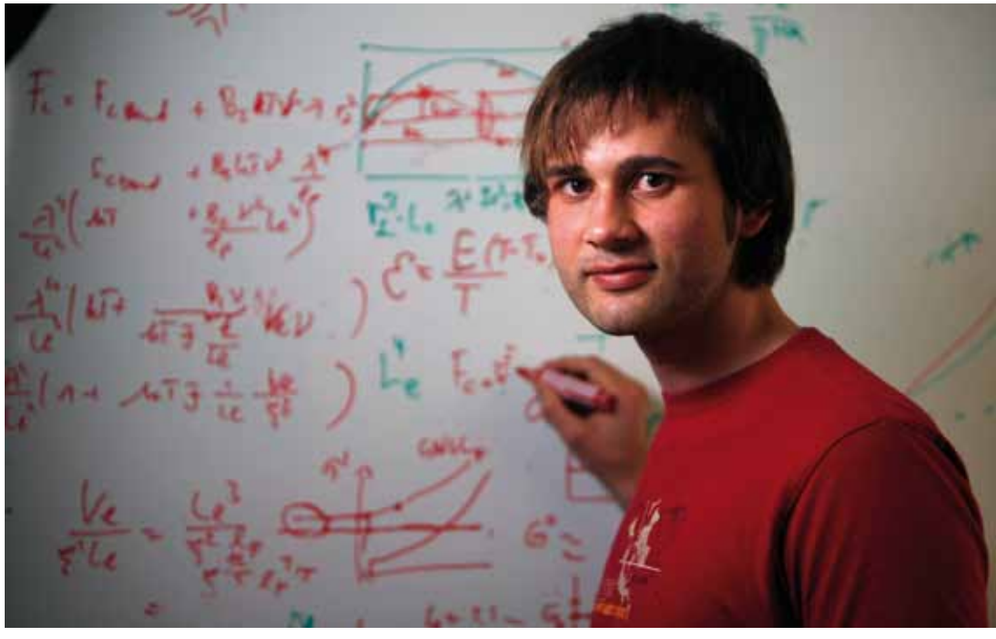
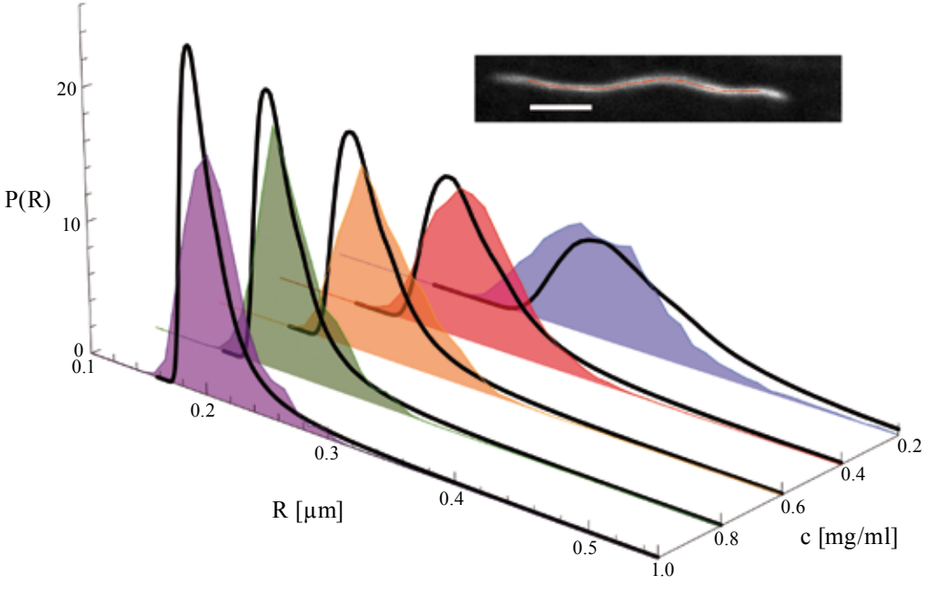
From single molecule dynamics to slow glassy relaxation of networks and living cells

Prof. Dr. Klaus Kroy
Dipl.-Phys. Jens Glaser, Dipl.-Phys. Sebastian Sturm, Dipl.-Phys. Lars Wolff



A main focus of the research in the group is the coarse-grained molecular description of solutions and networks of biopolymers, such as those responsible for the remarkable mechanical properties of cells and biological tissue. In this respect, we have studied the effect of stress propagation and relaxation in stiff and semiflexible polymers and their networks, building on the mathematical standard model of semiflexible polymers, the so-called wormlike chain. To account for the complicated interactions in polymer solutions and networks, we rely on our recently developed phenomenological extension of this model, the glassy wormlike chain (GWLC). This provides a systematic approach to the rapid non-equilibrium response of biological systems to external perturbations. Many present-day experiments probe larger time and length scales that require explicit modelling of structural rearrangements within the cell. In the inelastic GWLC, a version of the model that accounts for plastic mechanical deformations, we describe the interplay between single-polymer dynamics and bond kinetics as supposedly relevant in weakly crosslinked networks and living cells under external load. This model predicts a range of physical, or "passive" remodelling effects (as opposed to the active biological remodelling), such as viscoelastic shakedown and fluidisation, which was recently discovered to be characteristic of adherent living cells.

We also developed a systematic theory for computing the confined Brownian motion of biopolymers in solutions. As a starting point, the complicated many-body problem of an entangled polymer solution is reduced to that of a test polymer in a



⇑ A systematic theory explains the heterogeneous shape of the tube-shaped next-neighbor cages around stiff biopolymers by analyzing the tube radius distribution P(R) of cytoskeletal F-actin polymers (shaded areas) at various monomer concentrations. Solid lines represent a global fit by the analytical theory.

tube-like cage representing the constraints due to the other, uncrossable polymers. This is then further developed into what we call a segment-fluid model that captures the most salient static and dynamic heterogeneities on the molecular scale. In a collaboration with our experimental partners in Jülich we were able to demonstrate excellent agreement with measurements.

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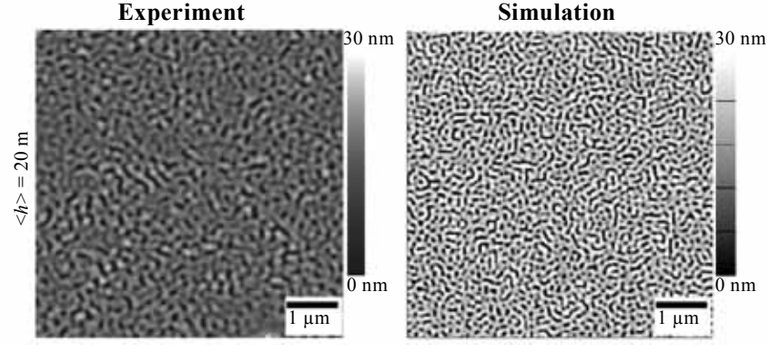
New functional materials for biomedical applications

Prof. Dr. Stefan G. Mayr

The main focus of our research lies on development of new functional materials. Conceptually this requires a detailed understanding of physical processes/properties at the nanoscale and their impact on meso- and macroscopic scales, which is generally addressed by complementary approaches of experiments and applied computer modeling. Within BuildMoNa we focus on three areas of research: *(i)* nanoscale structured materials, *(ii)* magnetic shape memory alloys and *(iii)* complex fluids and glasses.

Our interest in *(i)* nanoscale structured materials currently focuses on self-organised structure formation – primarily at surfaces – in systems which are exter-



⇑ Comparison of experiments (*left*) and computer simulations (*right*) on structure formation during vapor deposition of thin polycarbonate films on GaAs

nally driven e.g. by materials deposition, ion bombardment or electrolytic etching, biocompatible materials coating as well as multicomponent nanoclusters for biomedical application, e.g. drug delivery. *(ii)* Magnetic shape memory alloys are a novel class of materials which can yield length extensions up to 10 % upon application of an external magnetic field. Using molecular beam epitaxy (MBE) we are currently working on optimisation and miniaturisation as functional thin films towards integrated actuators. Our research on *(iii)* complex fluids and glasses primarily focuses on mechanical properties and the underlying atomistic foundations in disordered matter.

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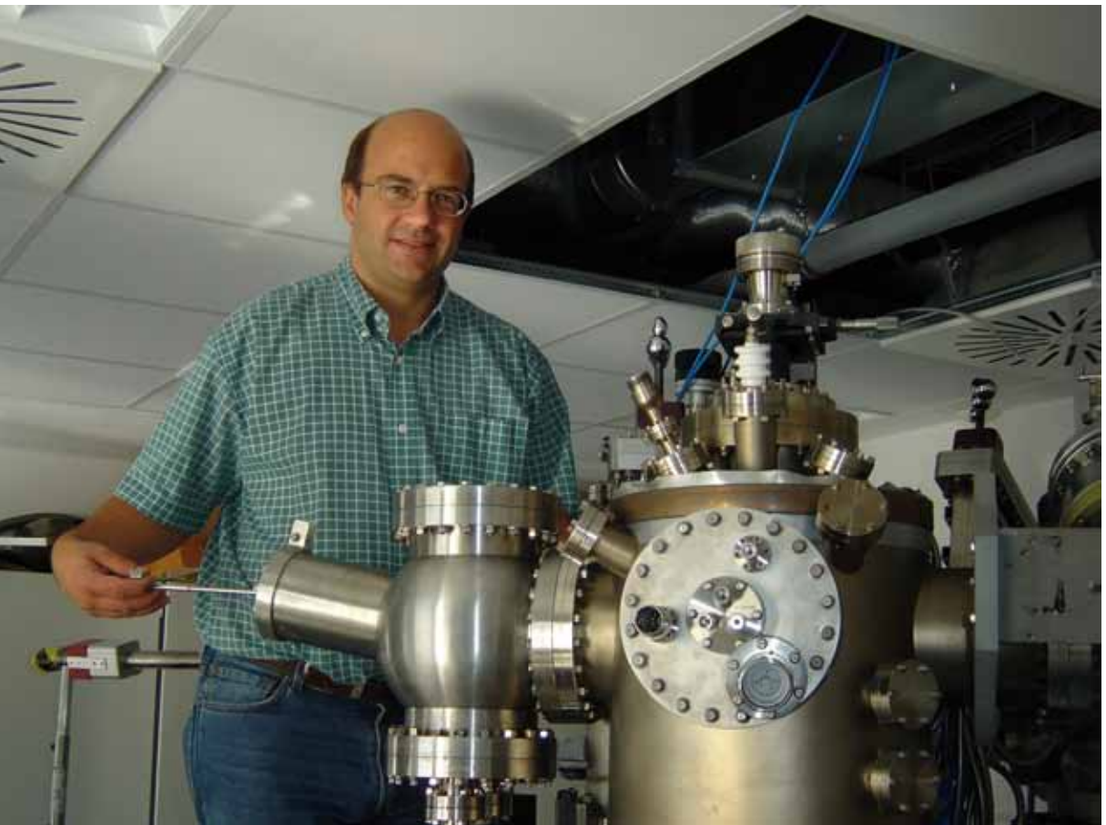


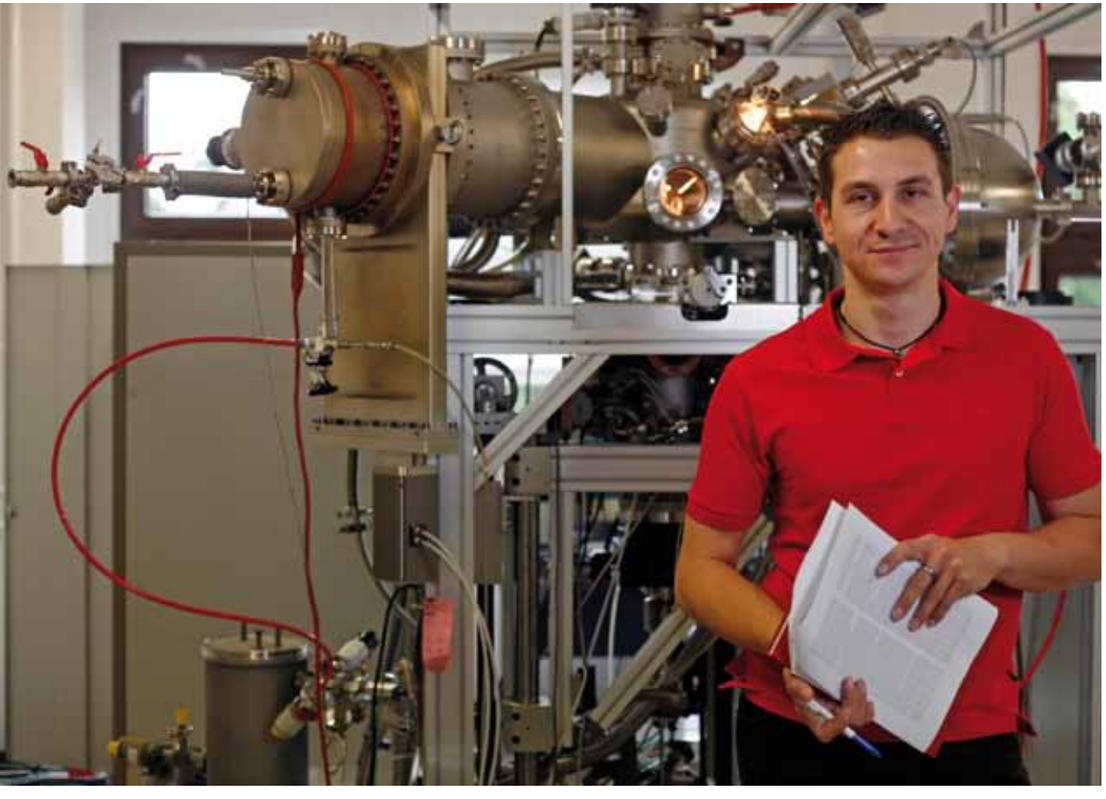
Neutral impact collision ion scattering spectroscopy for the investigation of liquid surfaces

Prof. Dr. Harald Morgner
M.Sc. Chem. Tobias Hammer

NICISS (Neutral Impact Collision Ion Scattering Spectroscopy) is used to study the molecular surface structure of ionic liquids. Ionic liquids are investigated with emphasis on the question of how the aliphatic chain length of the cation is accomodated at the surface. The standard technique of NICISS is able to yield the concentration depth profiles of all elements present in the sample. The angular resolved version of the technique which we have developed can even characterise the three dimesional structure of the surface.

The technique NICISS is developed further to allow access to volatile liquids, in particular to water at ambient temperature. The construction of the improved apparatus is underway. Preliminary experiments with water exist, but are restricted to aqueous solutions with high salt concentrations and low temperatures. This project aims at the application of the technique to systems of biological relevance and to atmospheric chemistry.

A new development is the theoretical description of inhomogeneous systems within a thermodynamical framework. Inhomogeneous distributions of matter are encountered almost everywhere in the world of small (nano) dimensions: interfaces, nanoparticles, as well as fluids in porous material.



Nano-structures by low-energy ion beam and laser techniques

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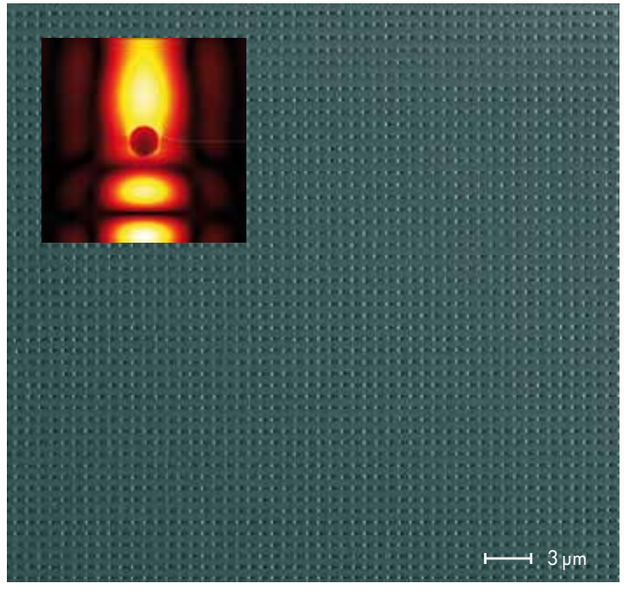
M. Eng. Mat. Marina I. Cornejo, M.Sc. Phys. Chinmay Khare, Dipl.-Phys. Johanna Lutz, Dipl.-Phys. Marisa Mäder, Dipl.-Phys. Lena Neumann, Dr. Christian Patzig, M.Sc. Chem. Eng. Erik Thelander, Dipl.-Phys. Hendrik Zachmann

The fundamental processes at the formation of nano-structures by hyperthermal ion beam and laser assisted deposition and structuring are in the focus of the interest. The influence of the ion and laser irradiation on the nucleation density, the formation of nano-structures, as well as on the structural properties of the growing ultrathin film as a consequence of the near surface energy and momentum input and ballistic adatom rearrangement by atomic collisions are to be studied. Silicon and germanium nano-structures are grown with the so-called glancing angle deposition



⇐ A large area Au nanodot-matix on sapphire prepared by diffraction mask projection laser ablation. The inset shows a 1×1 mm² overview of the total electric field distribution near a single Au sphere of radius 75 nm, semisubmersed in sapphire. H-polarised darkfield illumination of 532 nm excites the sphere from the sapphire side just above the critical angle for total internal reflection. In the upper domain a focal region is formed (IOM Leipzig in cooperation with MPI für Festkörperforschung Stuttgart).

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technique, a sophisticated vacuum deposition process with precise control of the angle between target and substrate as well as substrate rotation. This technology allows the formation of a manifold of differently shaped nano-structures. A diffraction mask projection laser ablation technique is developed of generating well-ordered nanodot matrices bound to several substrates, which have a potential use for plasmonic applications.

⇒ *Surface-enhanced fluorescence from metallic nano-sculptured thin films with application to biosensing in water*
I. Abdulhalim, A. Karabchevsky, C. Patzig, B. Rauschenbach, B. Fuhrmann, E. Eltzov, R. S. Marks, J. Xu, F. Zhang, A. Lakhtakia / Applied Physics Letters (2009) **94** 063106

⇒ *Ion beam induced anisotropic deformation of Si nanosprings*
R. Nagar, C. Patzig, B. Rauschenbach, V. Sathe, D. Kanjilal, B.R. Metha, J.P. Singh / Journal of Physics D: Applied Physics (2009) **42** 145404

⇒ *Deposition of nanostructures with arbitrary periods: new patterning concept for glancing angle deposition*
C. Patzig, J. Zajadacz, K. Zimmer, R. Fechner, C. Khare, B. Rauschenbach / Applied Physics Letters (2009) **95** 103107

⇒ *Surface Plasmon resonance from metallic columnar thin films*
A. Shalabney, A. Lakhtakia, I. Abdulhalim, A. Lahav, C. Patzig, I. Hazek, A. Karabchevsky, B. Rauschenbach, F. Zhang, J. Xu / Photonics and Nanostructures – Fundamentals and Applications (2009) **7** 176

⇒ *Ultra-thin titanium nitride film epitaxy with hydrothermal titanium ions*
J.W. Gerlach, T. Höche, L. Neumann, B. Rauschenbach / Proceed. 9th IEEE International Conference on Nanotechnology, Genua (2009) Paper No. 406

⇒ *Swift heavy ion irradiation induced effects in Si/SiO_x multi-layered films and nanostructures*
J.W. Gerlach, C. Patzig, W. Assmann, A. Bergmaier, Th. Höche, J. Zajadacz, R. Fechner, B. Rauschenbach, / in "Ion Beams and Nano-Engineering" edited by D. Ila, P.K. Chu, N. Kishimoto, J.K.N. Lindner, J. Baglin (Mater. Res. Soc. Symp. Proc. Volume **1181**, Warrendale, PA, 2009), 1181-DD04-01

⇒ *Si nanocolumns on nanosphere lithography templated substrates: effect of sphere size and substrate temperature*
C. Patzig, B. Fuhrmann, H.S. Leipner and B. Rauschenbach / Journal of Nanoscience and Nanotechnology (2009) **9** 1985

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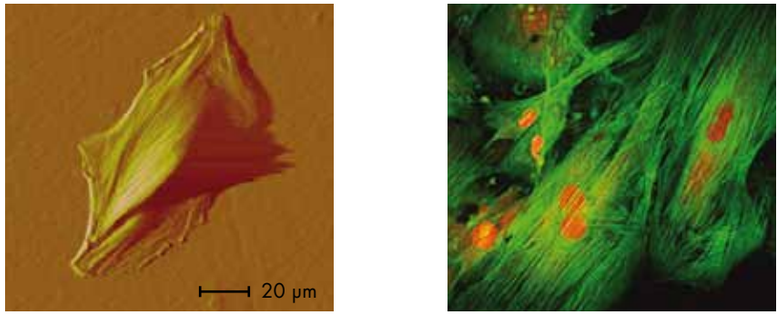
NanoBioengineering – novel nano- and micro-technological aspects of multi-electrode arrays in life sciences

Prof. Dr. Andrea A. Robitzki
Dipl.-Biochem. Marco Glaß, Dipl.-Biochem. Sina Haas,
Dipl.-Biochem. Dana Krinke, Dipl.-Biochem. Anja Steude

Anja Steude developed an electrochemical immuno-based biosensor which constitutes a tool for various diagnostic applications. This work aims at the development and fabrication of a novel multielectrode array (MEA) for immuno-assisted whole cell detection systems. The presented MEA is compatible with the 96-well format containing nine wells initially, but allows upscaling for high-throughput screening application. Each well features a gold working electrode permitting surface modification with thiol chemistry, a platinum auxiliary electrode, and an Ag/AgCl reference electrode for voltammetric and impedimetric analyses.

Dana Krinke's topic was the establishment of a cardiomyocyte ischemia model on a chip for screening of drugs directed to the molecular target Rac1. The focus of the research was *(i)* target identification, *(ii)* development of novel anti-target drugs, and *(iii)* real time screening on chips. We demonstrated for the first time an in vitro cardiac ischemic model simulating a cardiac infarct on a chip. The functionality of the novel microarray-assay was demonstrated by real-time monitoring of the selective Rac1 inhibitor NCS23766.



⇑ Viable rat smooth muscle cells are documented via atomic force microscopy (*left*); immunohistochemically stained actin filaments (stress fibers, green; nuclei, Sytox orange) of rat smooth muscle cells are shown using confocal laser scanning microscopy (*right*).

Sina Haas showed a novel impedimetric-based biosensor for label-free detection of vascular smooth muscle cell activation and contractility for real time monitoring of atherosclerotic injury.

Marco Glass could identify several potential neuronal markers concerning screenings of neuronal guiding cues and their receptors in human neuronal cells for a novel BioForce-array.

⇒ *A microelectrode-based sensor for label-free in vitro detection of ischemic effects on cardiomyocytes*
D. Krinke, H.-G. Jahnke, O. Pänke, A. A. Robitzki / Biosensors and Bioelectronics (2009) **24** 2798

⇒ *Develoment of a novel 3D-culture model for a label-free impedance based screening system*
D. Krinke, H.-G. Jahnke, T. G. A. Mack, F. Striggow, A. A. Robitzki / Journal of Neurochemistry (2009) **110** 45

⇒ *Label-free detection of ischemic effects on the cardiomyocytes by impedance spectroscopy*
D. Krinke, H.-G. Jahnke, O. Pänke, A. A. Robitzki / International Federation for Medical and Biomedical Engineering (2009) ISBN 978-3-642-03897-6 ISSN 1680-0737 **25/VII** 157

⇒ *Contractile tension and beating rates of self-exciting monolayers and 3D-tissue constructs of neonatal rat cardiomyocytes*
P. Lindner, J. Trzewik, M. Rüffer, G. M. Artmann, I. Digel, R. Kurz, A. Rothermel, A. A. Robitzki, A. Temiz-Artmann, A. / Medical Biological Engineering and Computation (2009) 1599.2, DOI: 10.1007/s11517-009-0552-y-48

⇒ Reverse Transcription PCR Screening of different neuronal guiding cues and their receptors in human staurosporine differentiated SH-SY5Y cells
M. Glaß, H.-G. Jahnke, A. A. Robitzki / International Federation for Medical and Biomedical Engineering (2009) ISBN 978-3-642-03897-6, ISSN 1680-0737, **25/X** 98

⇒ *Development and Fabrication of Multielectrode Arrays for Immuno-Assisted Whole Cell Detection Systems*
A. Steude, O.Pänke, S. Schmidt, A. A. Robitzki / International Federation for Medical and Biomedical Engineering (2009) ISBN 978-3-642-03897-6, ISSN 1680-0737 **25/VIII** 153

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Experiences

BuildMoNa's second year – a PI's view

Prof. Dr. Jürgen Haase

BuildMoNa has changed things in the natural sciences in Leipzig. You hear students talk about other work over in chemistry or biology, about how stimulating or how difficult the doctoral training was the other day. They know each other, share experience, and have fun together. It also is good to see the international crowd grow. I think that the students feel and like the way they are being taken care of. They are a part of a bigger group that seems to have critical mass, which I think is important. On the other hand, I feel that BuildMoNa has a positive impact to students funded by other programmes. Yes, the number of small children around and in our department has grown tremendously, it seems. Maybe they are just more visible now.

As a professor I am happy to receive funding for doctoral students. The funds for consumables and travel are good to have. It is also important that the students feel they are in charge of funds. The doctoral candidates can focus on their work. Administrative overhead such as signing of time sheets for the ESF funded positions is eased by the school's office. Our students work long and strange hours, share night shifts on instruments, look after their children, and, do not get a tremendous amount of money.

Also at the professorial level BuildMoNa has changed the environment. I am much more aware of what other people are doing, new connections have emerged through joint research topics and teaching. Of course, it takes more time to foster interdisciplinary growth, but it has become visible already. This is also true for the teaching efforts. It is difficult to teach, for example, physics methods and theories to chemists and biologists (the same is true, of course, the other way around). In fact, I am not quite sure that we understand the process well enough, as comprehension is partly "non-interdisciplinary". Should we have modules that are "truly interdisciplinary" and modules that are broad, but based in the disciplines?

I was heavily engaged in conceiving BuildMoNa, but when it started, I had to serve as Dean, which made me spend too much time on other things. I might not have seen enough of BuildMoNa growing, and I was spared the problems arising from getting it started. Nevertheless, it is impossible to think of life without BuildMoNa anymore – in particular since it has been quite beneficial for the doctoral students around here, the PIs, our university, and state of Saxony.

Prof. Dr. Jürgen Haase

BuildMoNa's second year – a DC's view

Dipl.-Phys. Martin Rothermel

In the course of the first line funding of the German Excellence Initiative more than 40 Graduate Schools have been established, among them the Leipzig School of Natural Sciences – BuildMoNa.

Having in mind the good reputation of German academic degrees all over the world, it is clear that critical thoughts arose concerning the adaption of foreign models in higher education. This also includes the Bologna reform. The regimentation of higher education restricts the freedom of students in general. But at the same time it opens up a new discussion among professors and academic administration about a state of the art doctoral education. Of course, not all related guidelines could be implemented immediately; there are lots of bureaucratic obstacles and open questions. To face this, we have an unhesitant Steering Committee which deals with all the challenging administrative input and an active BuildMoNa Office giving fast and uncomplicated help. The adaption of existing doctoral training structures of the Research Academy Leipzig permits to offer an interdisciplinary programme of key qualifications.

In the BuildMoNa programme we read:

"The Graduate School's main objective is 'Building with Molecules and Nano-objects (BuildMoNa)'. The central themes will connect interdisciplinary, fundamental Research, the use and development of suitable, novel Methods, and interdisciplinary graduate Training."

Let's have a look, how the basis, the doctoral candidates, is involved in this programme.

Every year, the doctoral candidates can choose between scientific modules, soft skills workshops, the symposium and, the doctoral workshop to gain the requested credit points. Regarding the scientific modules I want to note the deplorable circumstance that only few doctoral candidates attend modules outside of their discipline. Deplorable, because an organised interdisciplinary doctoral training is a chance to get new insights. On the other hand, I comprehend the doctoral candidates who avoid these modules. Most not-in-subject doctoral candidates have a lack of background knowledge in a foreign research discipline. In my opinion making up contexts – even with 45 h self-studies – is difficult, but is often demanded in the examinations. This sometimes bad experience in getting in touch with a new discipline counteracts the aim of BuildMoNa. Furthermore, the standards differ largely among the involved professors, especially with respect to this not-in-subject cases.

Besides giving thought-provoking impulses on self-perception, self-expression and further social competencies, the workshops and symposia contribute to an interdisciplinary discourse and networking activities among the doctoral candidates, revealing unknown possibilities of collaborations.

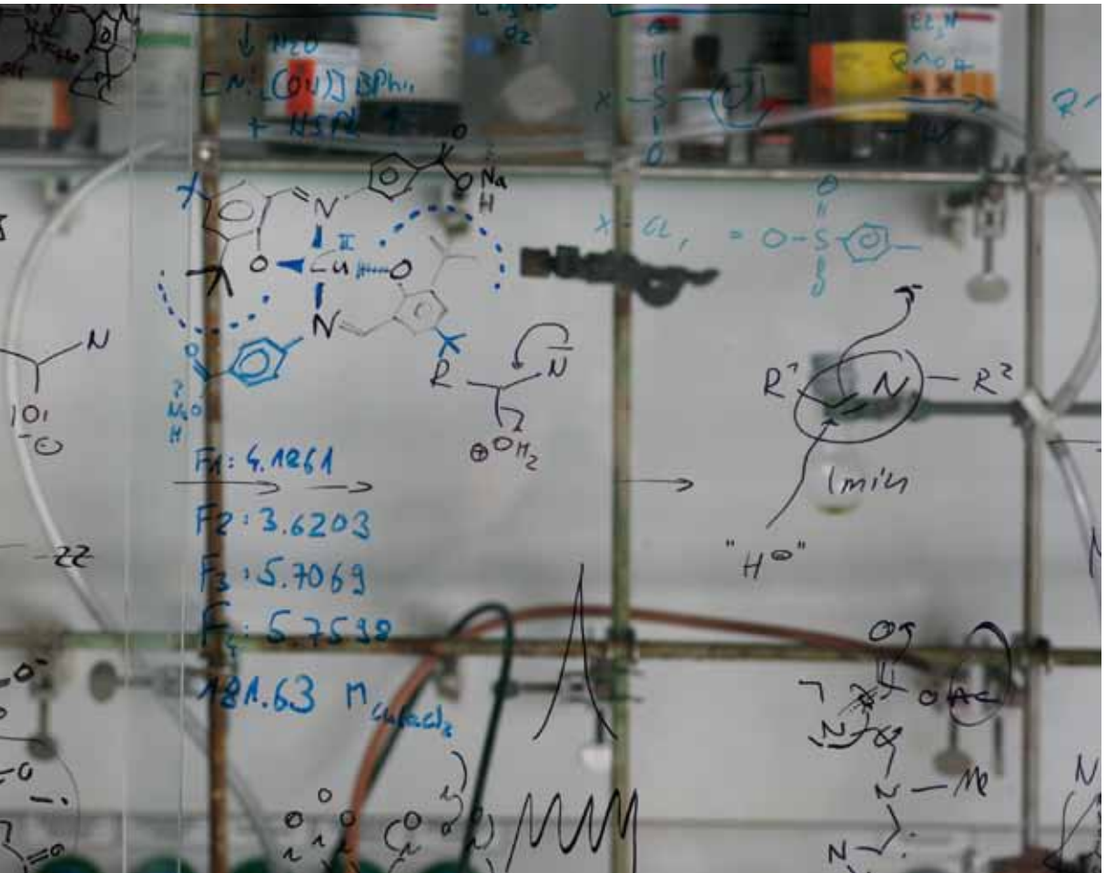
To adjust the Graduate School to the doctoral candidates' prospect, their opinion is required. So, I ask all doctoral candidates to communicate their questions and wishes!

Dipl.-Phys. Martin Rothermel

Training

The research training programme consists of the research work and a well-structured training programme in accordance with the RAL guidelines. The training programme 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 graduate studies, provided that 20 credit points (10 graded, 10 non-graded) have been acquired.

Nine Scientific and Methods Modules as well as five Transferable Skills Workshops were offered during BuildMona's first year, which are described on the following pages.



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

Hybrid systems (2008-M09)

11 / 12 February 2009,
written exam, 2 credit points, yearly recurrence with modification, 30 participants

Understanding the principles in preparation and application of hybrid systems, including immobilisation of biomolecules and prerequisites for materials to attach biomolecules, as well as possible future application in biomedicine, biotechnology, and informatics.

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

Lecturers:
Prof. Dr. A.G. Beck-Sickinger, UL, Germany; Dr. I. Neundorf, UL, Germany; Dr. K. Holland-Nell, Carlsberg-Institute Copenhagen; Prof. D. Scharnweber, TU Dresden, Germany; Prof. Dr. D. Huster, UL, Germany; Dr. M. Hacker, UL, Germany

Contents:
⇒ Protein expression by specific methods that allow modification and introduction of non proteinogenic amino acids, intein and impact system, modification of tRNA and genetic code expansion, selective chemical modification of proteins, pegylation of proteins, biocompatibility of materials, problems of toxicity and biodegradation
⇒ Material aspects, including generation of polymers, surface modification, nanoscaffolds, preparation of building blocks, chemical modification of surfaces
⇒ Preparation and analysis of hybrid compounds, ligation strategies, immobilisation, application of hybrid materials in biomedical science, for biosensors, and for functional materials

Methods:
⇒ Techniques to obtain modified proteins
⇒ Side chain protection strategies in peptide synthesis
⇒ Cell-based assays to study toxicity
⇒ Biostability and immflammation, Analytics including solid-state NMR

Nano-manipulations (2009-M01)

28 / 29 May 2009,
oral exam, 2 credit points, yearly recurrence with modification, 27 participants

Building with molecules and nano-objects requires the manipulation of these entities on a nanoscale. Such manipulations have to be local and therefore require the use of localised force fields that act on single particles, cells or even single molecules. The lecture series gave an introduction into modern techniques and the physical principles behind.

Responsible Scientist:
Prof. Dr. F. Cichos

Lecturers:
Prof. Dr. F. Cichos, UL, Germany; Prof. Dr. F. Kremer, UL, Germany; Prof. Dr. J. Käs, UL, Germany; Dipl.-Phys. C. Wagner, UL, Germany; Ph.D. M. Elmahdy, UL, Germany; Dipl.-Phys. F. Weinert, LMU, Germany; A. Cohen, Havard; Dr. R. Seidel, Biotechnology Center TU Dresden, Germany; M.Sc. M. Bertz, TUM, Germany; Dr. F. Rehfeld, Universität Göttingen, Germany

Contents:
⇒ Electromagnetic forces: electric fields and dielectric materials, electrophoresis for molecules, proteins, and cells, magnetic forces
⇒ Optical forces: gradient, scattering, and optical surface forces, Maxwell surface
⇒ Tensor, momentum transfer, transferring angular momentum, holographic tweezers, Mie- vs. Raleigh-regime
⇒ Scanning force approaches: Van der Waals forces, inter- and intra-molecular interactions, detection with quadrant diodes
⇒ Thermophoretic forces, thermo-viscous pumping, opto-thermal module trapping
⇒ Soft lithography

Methods:
⇒ Optical traps: optical tweezers, optical stretcher, optical cell guidance, optical spanners and rotators, optical sorting and deposition, laser dissection
⇒ Magnetic tweezers
⇒ Scanning force microscopy and spectroscopy
⇒ Electrokinetic trapping
⇒ Thermophoretic forces

From molecules to materials: Nanostructured materials by rational design – from organic to inorganic functionality (2009-M02)

3 / 4 June 2009,
written exam, 2 credit points, yearly recurrence with modification, 25 participants

This module linked molecular sciences with materials science. It explained how materials with optimised catalytic activity and adjustable magnetic, electronic, or optical properties are obtained from molecules. It provided a basis for understanding properties and applications of these materials.

Responsible Scientists:
Prof. Dr. M. R. Buchmeiser, Prof. Dr. R. Gläser

Lecturers:
Prof. Dr. M. R. Buchmeiser, IOM, Germany; Prof. Dr. R. Gläser, UL, Germany; Prof. Dr. H. Krautscheid, UL, Germany; Prof. Dr. F. Schüth, MPI für Kohleforschung, Germany; Prof. Dr. M.-O. Coppens, DelfChemTech, NL

Contents:
⇒ "Hard" (synthetic molecules and crystalline nano-structures) and/or "soft" (polymers) building blocks
⇒ Novel materials: polymers, hybrid materials, supra-molecular arrangements
⇒ Modifications to improve material quality
⇒ Metal-organic frameworks (MOFs)
⇒ Thin films
⇒ Nano-structures
⇒ Properties of these materials: mass transfer, porosity, pore size distribution, specific surface areas, functionality, thermal properties, thermodynamics
⇒ Application of these materials: catalysis, gas separation or gas storage, sensors, electronics

Methods:
⇒ Templated synthesis
⇒ Immobilisation techniques
⇒ Polymer synthesis
⇒ Generation of porosity by micro- and macro-phase separation
⇒ Heterogeneous molecular catalysis

Theory (2009-M03)

30 June / 1 July 2009,
written exam, 2 credit points, yearly recurrence with modification, 15 participants

Introduction into the most important quantum chemical methods for the study of the behaviour of matter and the properties of molecules. Interpretation of the results of quantum chemical calculations. Application of quantum chemical methods to chemical problems.

Responsible Scientist:
Prof. Dr. B. Kirchner

Lecturers:
Prof. Dr. B. Kirchner, UL, Germany; Dr. W. Reckien, UL, Germany

Contents:
⇒ Introduction in theory: Hartree Fock method and density functional theory
⇒ Potential energy surfaces, computational thermochemistry and theoretical spectroscopy
⇒ Practical course: Introduction in computational chemistry: handling of modern quantum chemical methods to chemical problems

Methods:
⇒ Hartree-Fock and density functional theory (DFT)

From biomolecules to cells (2009-M04)

12 / 13 November 2009,
written exam, 2 credit points, yearly recurrence with modification, 30 participants

The module helped to understand the biophysics of cells to manipulate them and use them as bioreactors. This includes the combination of cells with bioelectronics and nano-biotechnological applications and understanding how the cellular machinery changes when intracellular proteins are changed.

Responsible Scientists:
Prof. Dr. A. G. Beck-Sickinger, Prof. Dr. J. Käs

Lecturers:
Prof. Dr. A.-G. Beck-Sickinger, UL, Germany; Prof. Dr. J. Käs, UL, Germany

Contents:
⇒ Cell compartments with their different functions: cytoskeleton, cell membrane compartments, selected cell types (cardiac and neural cells/tissues, stem cells)
⇒ Biophysical techniques to characterise cells, manipulation of cell growth and orientation with physical and chemical tools, application of cell manipulation in biosensor technology
⇒ Tumor biology
⇒ Eukaryotic expression of proteins in cell culture, 2D and 3D tissue culture, comparison of primary versus altered cells

Methods:
⇒ Techniques to characterise cells: microscopic techniques, staining and bioelectronical recording vs. optical analysis
⇒ Transfection studies to create artificial cells with different activities
⇒ Impedance spectrometry to characterise modified cells

Smart molecules (2009-M05)

25 / 26 November 2009,
written exam, 2 credit points, yearly recurrence with modification, 17 participants

This module aimed at linking molecular sciences, homogeneous, heterogeneous and bio-catalysis.

Responsible Scientist:
Prof. Dr. J. Haase

Lecturers:
Prof. Dr. J. Haase, UL, Germany; Dr. M. Bertmer, UL, Germany; Prof. Dr. A. Pöppl, UL, Germany; Prof. Dr. M. Hartmann, Uni Erlangen-Nürnberg, Germany; Prof. Dr. Y.Y. Tong, Georgetown University, Washington D.C., USA

Contents:
⇒ Specific synthesis, modification and understanding of the changes in the (electronic) structure of molecules that are precursors for materials with optimised catalytic activity and adjustable magnetic, electronic, and optical properties
⇒ Small molecules: organometallic and transition metal complexes, building blocks for metal-organic frame works (MOFs), immobilisation of catalysts (on solid or in liquid supports), electronic structure of active units
⇒ Designing and synthesising smart molecules that contain biological and chemical segments, strategies to introduce metals into biomolecules by selectively introduced chelators, monitoring structural changes
⇒ Clusters and polynuclear compounds: links between mononuclear complexes and the corresponding solid-state phase, homo- and heterometallic systems, metallated container molecules, supramolecular chemistry
⇒ Supramolecular chemistry, self-assembly (concepts, strategies)

Methods:
⇒ Synthesis of new building blocks, characterisation of their electronic properties by molecular spectroscopy (IR, NMR, UV-Vis, etc.), structural changes due to interconnection

Magnetic resonance – Physical concepts and chemical applications (2009-M06)

08 / 09 September 2009,
written exam, 2 credit points, yearly recurrence with modification, 34 participants

Magnetic resonance, in particular NMR, is one of the very few local probes of bulk matter with applications in almost all natural sciences. Leipzig has a great tradition in applying and developing magnetic resonance in various areas. The powerful spectroscopic insight from magnetic resonance requires, however, a special knowledge of its methods, techniques, and hardware. Therefore, basic courses in magnetic resonance will be provided that lay the foundation for its application. Due to the exceptional breadth of applications, advanced courses will focus on current research needs.

Responsible Scientists:
Prof. Dr. S. Berger, Prof. Dr. J. Haase

Contents:
⇒ Basic principles of NMR and EPR
⇒ NMR of liquids and of solids as a basic analytical tool
⇒ Advanced methods: in biological systems, quantum solids, surfaces
⇒ Hardware development for special applications: thin films, high fields and frequencies

Methods:
⇒ High-resolution methods for liquids
⇒ Nuclear double-, triple-resonance, higher dimensional NMR methods
⇒ Pulsed fields, EPR, ENDOR

Complex nano-structures – Nanoparticles and catalysis (2009-M07)

17 / 18 September 2009,
oral exam, 2 credit points, yearly recurrence with modification, 22 participants

Deepen the understanding of generation and handling of nanoparticles and catalysts with nanostructures.

Responsible Scientists:
Prof. Dr. R. Gläser, Prof. Dr. F.-D. Kopinke

Lecturers:
Prof. Dr. R. Gläser, UL, Germany; Prof. Dr. F.-D. Kopinke, UFZ, Germany; Prof. Dr. U. Heiz, TU Munich, Germany; Prof. Dr. H. Harms, UFZ, Germany; Dr. K. Schirmer, EAWAG Zürich, Switzerland; Dr. A. Georgi, UFZ, Germany; Dr. K. Mackenzie, UFZ, Germany; Prof. Dr. C. H. Christensen, Haldor Topsøe, Lyngby, Denmark; Dr. Stöcker, Sumitomo Chemical Europe; Prof. Dr. K. Tryantafillidis, Aristotle University of Thessaloniki, Greece

Contents:
⇒ Nanostructures and nanoparticles are two basic and emerging concepts in modern heterogeneous catalysis. Nanoclusters on microporous carriers are known for a long time and widely applied in various catalytic processes, whereas catalysis with suspended nanoparticles is a relatively new, upcomming approach. Its specific advantages and challenges were discussed with a focus on applications, e.g., in water treatment processes.

Methods:
⇒ Techniques for measurement of chemical reaction kinetics
⇒ Characterisation of nanostructures and free nanoparticles

Synthesis – Synthesis, properties and applications of supramolecular systems and nanoobjects (2009-M08)

29 / 30 October 2009,
written exam, 2 credit points, yearly recurrence with modification, 25 participants

Deepen the understanding of the field of supramolecular chemistry and its evolution into nanoscale. Deepen the understanding of the synthesis of selected supramolecular systems and nano-objects. Understand the properties and applications of these systems.

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

Lecturers:
Prof. Dr. E. Hey-Hawkins, UL, Germany; Prof. Dr. B. Kersting, UL, Germany; Prof. Dr. J. W. Steed, Durham University, UK; Prof. Dr. O. Reinaud, Université René Descartes, Paris, France; Prof. Dr. P. A. Gale, University of Southampton, UK; Prof. Dr. K. N. Raymond, University of California, USA; Prof. Dr. U. Kynast, FH Münster, Germany

Contents:
⇒ Introduction: Principles and concepts in supramolecular chemistry, non-covalent interactions, host-guest chemistry, self-assembly (examples, applications)
⇒ Design and application of supramolecular gels; crystallisation and self-assembly
⇒ Calixarenes: Synthesis, fundamentals and applications
⇒ Anion complexation and membrane transport
⇒ Coordination cages and nanocages
⇒ Rare earth luminescence from 2D nanostructures

Methods:
⇒ Introducing the synthestic tools for host molecules and materials, especially the methods to prepare and characterise complex and multifunctional host-guest molecules and self-assembled nanostructures, templates and related growths schemes, preparation and characterisation of nanomaterials
⇒ Synthesis of building blocks, characterisation of their structures and properties by molecular spectroscopy (IR, NMR, UV-Vis, etc.) and X-ray crystallography

Multifunctional scaffolds (2009-M10)

09 / 10 July 2009,
written exam, 2 credit points, yearly recurrence with modification, 29 participants

The basic background in soft matter physics and the state of the art knowledge in active and passive biopolymer networks (with a focus on molecular motors) was taught to enable the students to use highly dynamic polymer scaffolds as an organizing matrix for smart nanoelements and active proteins. A particular focus was to build mechano-sensing, force-generating, moving, polymeric machines.

Responsible Scientist:
Prof. Dr. J. Käs

Guest Lecturers:
Prof. Dr. J. Käs, UL, Germany; Prof. Dr. W. Frey, University of Texas, USA

Contents:
⇒ Different architectures of semiflexible polymer networks
⇒ Polymer physics of semiflexible polymer chains (individual filaments, entangled and cross linked solutions)
⇒ Liquid crystal physics of lipid membranes (self-assembly, phase diagrams, vesicles, Langmuir monolayers, supported bilayers, thermal ratchets and molecular motors, thermal ratchets and polymerisation, self-organisation in active polymer networks, active and passive filaments bundles contractile structures)

Methods:
⇒ Rheology and microrheology techniques
⇒ Single molecule imaging
⇒ Digital polarisation microscopy
⇒ Confocal/multiphoton microscopy
⇒ Dielectric spectroscopy
⇒ Single particle tracking
⇒ Soft lithography and micro-fluidics
⇒ Biochemistry, recombinant DNA

Transferable skills workshops

Conflict management for doctoral candidates – From a clash to a culture of conflict

Peter Witchalls, Golin Wissenschaftsmanagement,
29 June 2009, 16 participants

Conflicts are unavoidable in the normal course of the working life, in academia as well as outside. Whether it is about subject specific differences, competition amongst colleagues or disagreements with the supervisor or boss – there are plenty of potentially explosive situations.

But it does not have to come to a detonation which damages the atmosphere in the long run! It is not difficult to deal with conflicts in a constructive manner and to solve them before they grow into a substantial problem. If conflict is neither ignored nor allowed to escalate into a personal power struggle and the own as well as the others' motives are reflected upon, one can act consciously instead of only reacting emotionally. This way there is a chance of finding a solution with which all parties are satisfied.

This workshop conveyed fundamental knowledge about dealing with conflict and trains the powers of observations as well as negotiation skills. The participants learned to better judge the impact of their behaviour and to develop strategies for solving conflicts.

Networking for academics – Creating perspectives through contacts

Dr. Simon Golin, Golin Wissenschaftsmanagement,
23 July 2009, 18 participants

The possibilities to make quick and target focused contact with experts, colleagues, potential employers and staff members, funders and business partners have increased in number and significance. In the light of growing complexity in the knowledge society and better electronic contact possibilities, the 'know-who' is gaining in importance next to the 'know-how'.

In the academic sector, as elsewhere, personal contacts enhance the chances of finding supporters and funders for one's own project, of receiving conference

invitations, of being involved in publications, and of being told about interesting positions.

Networking requires initiative and continued investment. It is helpful, in this context, to be able to rely on proven strategies to make the right contacts, to communicate in a target focused way and to find the balance between giving and taking. The workshop transmitted these proven networking techniques.

Team work & leadership competencies in academia and beyond: Youngster – team player – key player

Dr. Simon Golin, Golin Wissenschaftsmanagement,
1 October 2009, 15 participants

When doctoral candidates make the transition into the labour market they are often expected to take on leadership responsibilities. Not only careers outside the higher education sector but also such in academia involve leadership roles – e.g. in the supervision of students or junior colleagues or the 'lateral guidance' of colleagues. A better understanding of leadership mechanisms is also useful in situations where one is being led, for example as a doctoral candidate by a supervisor. 'Bottom up' leadership techniques can contribute to the success of cooperation in this context.

With sound knowledge of leadership, team dynamics can be optimised and situations of conflict better managed. New recruits can therefore grow with their leadership role and constructively work with their colleagues.

In this workshop participants were introduced to the most important leadership styles and techniques and acquired knowledge of the methodical approach to leadership tasks.

Career planning for PhD students: Application standards – personal strategies

Dr. Simon Golin, Golin Wissenschaftsmanagement,
5 November 2009, 15 participants

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

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

Advanced presentation skills

Prof. Dr. R. Gläser, UL,
5 / 8 / 9 October 2009 within the BuildMoNa workshop for doctoral candidates,
14 participants

How to give successful oral presentations in the natural and related sciences? The present workshop (held in English language throughout) aims at an improvement of the presentation skills of graduate students. Besides a short review of the basic foundations of successful oral presentations, the workshop will cover 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 will jointly prepare and practice their yearly progress report presentation in front of their colleagues and advisors. The presentation at the report meeting will be monitored by video and thoroughly analyzed in group and plenary discussions with the colleagues on the second workshop day. With the goal to reach an advanced level, the attendees should have basic experience in giving oral presentations, e.g., from the workshop "Erfolgreich Präsentieren", and should have a fair knowledge of the English language.

Colloquia

Invited Speaker	*Institution*	Title	Date	*Place*
Prof. Dr. Sascha Hilgenfeldt	*Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, USA*	Cellular matter: The fly eye and other interfaces	13 January 2009	*Faculty of Physics and Earth Sciences*
Prof. Dr. Alok Srivastava	*Chemistry Department, Panjab University, Chandigarh, India*	Synthesis, characterisation and application of swift heavy ion modified insulating/conducting polymers	23 January 2009	*Faculty of Physics and Earth Sciences*
Prof. Dr. Peter A. Grünberg	*Forschungszentrum Jülich*	Magnetische Schichtsysteme: Schalten der Magnetisierung durch spinpolarisierte Ströme	7 April 2009	*Faculty of Physics and Earth Sciences*
Prof. Dr. Philip Dyer	*Department of Chemistry, Durham University, UK*	Aminophosphines: Intriguing building-blocks for making multi-functional molecules and materials	22 April 2009	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Dieter Fenske	*Institute of Nanotechnology, KIT, University of Karlsruhe*	Molekulare Cluster als Brücke zwischen Molekülstrukturen und den Strukturen ionischer Festkörper	24 April 2009	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Phil Andrews	*School of Chemistry, Monash University, Australia*	Exploring the structural diversity and biological activity of metal-organic bismuth compounds	27 May 2009	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Narayan S. Hosmane	*Department of Chemistry and Biochemistry, Northern Illinois University, USA*	Nanostructured cages and dendrimers: From materials to cancer therapy	10 June 2009	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Eric Masson	*Department of Chemistry and Biochemistry, Ohio University, USA*	Nanoscopic tweezers and self-sorting rotaxanes: An excursion into the world of molecular machines	17 June 2009	*Faculty of Chemistry and Mineralogy*
Prof. Dr. Katharina Fromm	*Department of Chemistry, University of Fribourg, Switzerland*	Agent silver: With a license to kill	8 July 2009	*Faculty of Chemistry and Mineralogy*
Dr. Paul W. Krieber	*Laboratory of Cellular and Molecular Biology, National Cancer Institute Washington D.C., USA*	Vesicular trafficking is required for chemoattractant delivery at the trailing edge of rapidly migrating cells	17 July 2009	*Faculty of Physics and Earth Sciences*
Prof. Dr. Tobias Kippenberg	*Max Planck Institute of Quantum Optics, Garching*	Cavity optomechanics: Putting quantum into mechanics	27 October 2009	*Faculty of Physics and Earth Sciences*

Events

2nd Scientific symposium

The second scientific symposium of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-Objects (BuildMoNa)" was held on the 2nd and 3rd of April 2009 at the Faculty of Chemistry and Mineralogy. Interdisciplinary topics from the current research on the development and investigation of new materials were presented. Renowned guest speakers from science and industry gave talks on current topics of BuildMoNa. During the poster session, as one part of the symposium, doctoral candidates were able to present their scientific topics and discuss these with the international guests, thereby receiving plenty of input for their oncoming work at the Graduate School BuildMoNa.
International and industrial guests were:

⇒ Prof. Dr. Bruce Weisman (Rice University Houston, USA)
⇒ Prof. David P. Landau (University of Georgia, Athens, USA)
⇒ Prof. Dr. S.G. Mayr (Universität Göttingen, Germany)
⇒ Dr. Karin Schütze (CellTool GmbH, Germany)
⇒ Prof. Dr. Jean Louis Barrat (Université Claude Bernard-Lyon I, France)
⇒ Prof. Dr. Bernhard Kräutler (Universität Innsbruck, Austria)
⇒ Prof. Dr. Michaela Schulz-Siegmund (Universität Leipzig, Germany)

⇑ Participants of the 2nd Scientific symposium

2nd Workshop for doctoral candidates

30 doctoral candidates presented their first scientific results with short talks at the 2nd BuildMoNa Workshop on 8 and 9 October 2009. About 90 BuildMoNa participants followed the lectures in the Europasaal, the conference venue of the Hotel Schloss Schweinsburg. 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., by self-organisation, were also included.

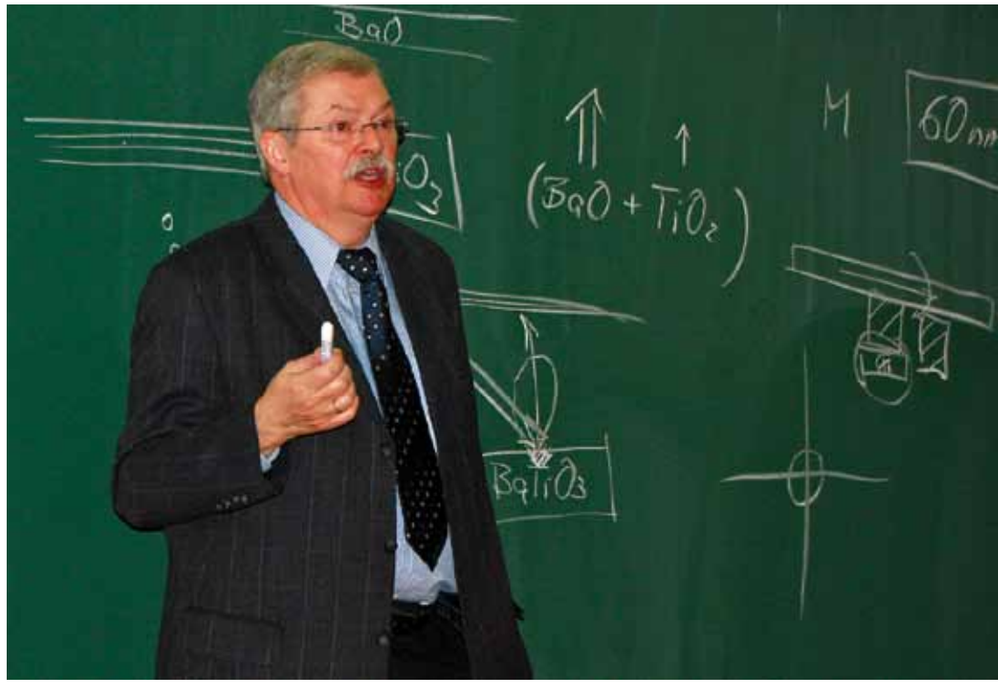
For the 14 participants of the Transferable Skills Workshop “Advanced Presentation Techniques” by Prof. Dr. Roger Gläser this was the opportunity to directly apply their newly acquired knowledge in that area. Their talks were filmed and critically discussed afterwards. Prof. Dr. Bernd Abel, Universität Leipzig, complemented the scientific programme with the talk “Shedding light on (bio)molecular transformations near interfaces”. At the end of the workshop a jury selected the best three presentations given by the doctoral candidates: The first prize was awarded to Alexander Lajn, the second to René Frank and the third to Sebastian Sturm.

⇑ Participants of the 2nd Workshop for doctoral candidates

⇐ Winners of the presentation awards at the 2nd Workshop: Alexander Lajn (l.), René Frank (2. l.) and Sebastian Sturm (r.) with Prof. Dr. Evamarie Hey-Hawkins, speaker of BuildMoNa

2nd Annual reception

On 9 December 2009 BuildMoNa celebrated its second anniversary. Professor Dietrich Hesse (Max Planck Institute of Microstructure Physics, Halle) gave a lecture called “Nanostructured ferroelectric and multiferroic epitaxial perovskite heterostructures”. At this event, the BuildMoNa Awards were given to doctoral researchers to recognise their outstanding scientific achievements. Denise Zwanziger (Institute of Biochemistry) received the first prize for her dissertation, in which she identified a new cancer marker. Her results contributed to the publication “Breast cancer diagnosis by neuropeptide Y analogs: from synthesis to clinical application”, that was published as a “very important paper” (VIP) in the peer-reviewed scientific journal Angewandte Chemie. Jens Glaser (Institute for Theoretical Physics) received the second prize for his research achievements and the subsequent publication “Tube width fluctuations in F-actin solutions” (submitted to Physical Review Letters), in which he introduces a new perspective in polymer dynamics. The theoretical work of Stefan Schnabel (Institute for Theoretical Physics), investigating low-temperature behaviour of polymers by means of Monte Carlo computer simulations, was recognised by awarding him the third prize.



⇑ Prof. Dr. Dietrich Hesse during his lecture at the annual reception

⇓ The winners of the BuildMoNa Awards 2009 with the speakers of the Graduate School; from left to right:
Prof. Dr. Evamarie Hey-Hawkins, Dr. Denise Zwanziger, Jens Glaser, Prof. Dr. Marius Grundmann

Integration of foreign doctoral candidates

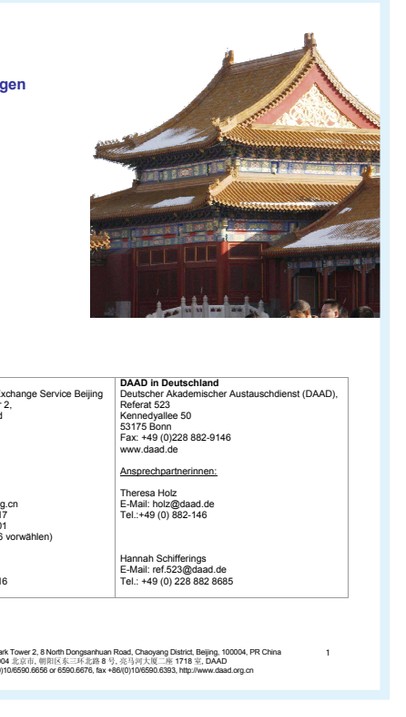
German classes for foreign doctoral candidates

To integrate foreign doctoral candidates German language courses for beginners and advanced persons are offered at the Graduate School. These not only facilitate the transmission of language skills, but also particularly help building a platform for the establishment of social and scientific contacts and moreover support the exchange of questions about the residence in Germany.

Promotion activities

PhD Workshop China

From 11 to 13 December 2009, Professor Bernd Abel and Professor Pablo Esquinazi of the Graduate School BuildMoNa took part in a PhD Workshop in Peking, organised by the DAAD (German Academic Exchange Service). The fair's guests included highly qualified and motivated students who are interested in pursuing doctoral research abroad as well as representatives of Chinese universities. The Graduate School was represented by a lecture as well as at the DAAD stand. The aim was to attract excellent Chinese postgraduates that are likely to receive a grant from the China Scholarship Council (CSC).



Childcare

Flexible childcare services at BuildMoNa

On the basis of the experiences of the collaborative research centre SFB 610 at the Universität Leipzig, a flexible childcare concept for the "offsprings" of doctorate parents is realised at the Graduate School BuildMoNa. Thus, childcare is guaranteed at daytimes, which are not covered by usual childcare institutions, such as municipal children education institutions or child minders of the RAL. This service enables the doctorate 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 was employed as child minder and teacher.

⇒ www.buildmona.de

www.buildmona.de