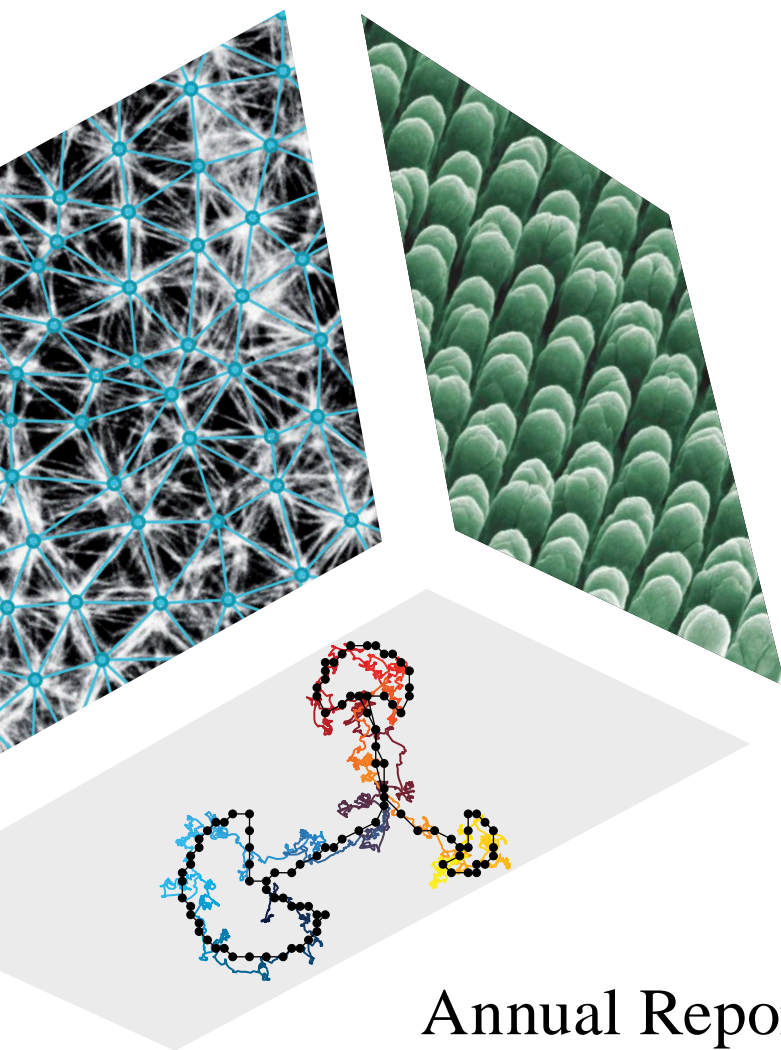


BuildMoNa

Graduate School
Building with Molecules and Nano-objects



Annual Report 2011

Cover image:

- ⇒ *Left:* Actin network
- ⇒ *Right:* Multilayered Si/Ge nano-columns for thermoelectric devices produced by glancing angle deposition
- ⇒ *Bottom:* Sample trajectory of a thermophoretically steered Janus particle in water; the black points describe the target path for the particle propulsion; the coloured curve is the particle trajectory



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Universität Leipzig, Johannisallee 29, 04103 Leipzig, Germany
Tel.: +49 341 97-36015, Fax.: +49 341 97-36017
buildmona@uni-leipzig.de, www.buildmona.de
- ⇒ Authors: Prof. Dr. B. Abel, Prof. Dr. A.G. Beck-Sickinger, Prof. Dr. S. Berger, Prof. Dr. T. Butz, Prof. Dr. F. Cichos, Prof. Dr. P.D. Esquinazi, Prof. Dr. R. Gläser, Prof. Dr. M. Grundmann, Prof. Dr. J. Haase, Prof. Dr. Dr. h.c. W. Hackbusch, Prof. Dr. H. Harms, Prof. Dr. E. Hey-Hawkins, Prof. Dr. D. Huster, Prof. Dr. W. Janke, Prof. Dr. J.A. Käs, Prof. Dr. B. Kersting, Prof. Dr. B. Kirchner, Prof. Dr. F.-D. Kopinke, Prof. Dr. H. Krautscheid, Prof. Dr. F. Kremer, Prof. Dr. K. Kroy, Dr. D. Lippa, Prof. Dr. S.G. Mayr, Prof. Dr. H. Morgner, Prof. Dr. F. Otto, Prof. Dr. T. Pompe, Prof. Dr. Dr. h.c. B. Rauschenbach, Prof. Dr. A.A. Robitzki, Prof. Dr. B. Rosenow
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Table of contents

4 Preface

6 Organisation and management

8 Doctoral candidates

15 Alumni 2011

16 Mini-projects

17 Statistics

18 Research Topics

- 18 ⇒ Nanoscale photonic imaging and molecular movies on ultimate time and space scales
- 21 ⇒ Chemical modification of peptides and proteins
- 24 ⇒ Polyisocyanides as reagent to observe residual dipolar couplings in NMR
- 27 ⇒ The focused ion beam at LIPSION – a versatile research tool for 2D and 3D analysis, imaging and materials modification
- 29 ⇒ Thermophoretic trapping and steering of Janus particles
- 31 ⇒ Electronics properties of sub micrometre graphite samples
- 34 ⇒ Building complex nanostructures for applied catalysis
- 36 ⇒ Oxide-based novel electronic and photonic building blocks
- 40 ⇒ Electronic and chemical structure of modern materials investigated with magnetic resonance
- 42 ⇒ Multiscale modelling of solvent effects in biomolecular systems
- 44 ⇒ Smart phosphorus- or carbaborane-containing molecules as building blocks in catalysis, materials science and medicinal chemistry
- 48 ⇒ Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake
- 50 ⇒ Monte Carlo and molecular dynamics simulations of structure formation processes
- 53 ⇒ From nanometre polymers to microscopic cells
- 56 ⇒ Coordination compounds in supramolecular chemistry and materials chemistry
- 59 ⇒ Development of novel approaches for the investigation of complex systems
- 62 ⇒ Nano-catalysts for water treatment – nano-catalysis in water
- 65 ⇒ Metal-organic frameworks – porous materials for gas storage and separation
- 68 ⇒ From glassy dynamics to colloidal drag effects
- 71 ⇒ Anomalous Brownian motion of bio-polymers and hot nanoparticles
- 73 ⇒ Surface- and materials physics for bio/medical applications
- 76 ⇒ Neutral impact collision ion scattering spectroscopy for the investigation of liquid surfaces

- 78 ⇒ Modelling ligand friction in cell adhesion using peptide mimetics
- 80 ⇒ Synthesis of thin films and nanostructures far from the thermodynamic equilibrium
- 83 ⇒ NanoBioengineering
- 85 ⇒ Coherent transport in quantum condensates

88 Experiences

- 88 ⇒ BuildMoNa's fourth year – a principal investigator's view
- 90 ⇒ BuildMoNa's fourth year – a doctoral candidate's view

92 Training

Scientific and methods modules

- 94 ⇒ Hybrid systems (2010-M09)
- 95 ⇒ Nano-manipulations: From self-propelled particles to molecular motors (2011-M01)
- 95 ⇒ From molecules to materials: Solid state inclusion compounds (2011-M02)
- 96 ⇒ Theory: Structure and mechanics of foams and cellular matter (2011-M03)
- 97 ⇒ From biomolecules to cells (2011-M04)
- 98 ⇒ Smart molecules: Ionic liquids (2011-M05)
- 99 ⇒ Magnetic resonance: Fundamentals and applications (2011-M06)
- 100 ⇒ Complex nanostructures: Nanoparticles and catalysis (2011-M07)
- 101 ⇒ Synthesis: Preparative methods in chemistry (2011-M08)
- 102 ⇒ Multifunctional scaffolds: From model systems to living cells (2011-M10)

Scientific minisymposium

- 103 ⇒ Hot nanoparticles and nanostructures

Transferable skills workshops

- 105 ⇒ Scientific writing and publishing research, part II
- 105 ⇒ Conflict management for doctoral candidates – From a clash to a culture of conflict
- 106 ⇒ Scientific writing and publishing research, part I
- 106 ⇒ Mastering the selection process: Developing job application strategies
- 107 ⇒ Advanced presentation skills

108 Colloquia

110 Events

- 110 ⇒ 4th Scientific symposium
- 112 ⇒ 4th Workshop for doctoral candidates
- 114 ⇒ 4th Annual reception

116 Childcare

117 Funding of doctoral candidates

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

Preface Prof. Dr. Evamarie Hey-Hawkins

The challenge and promise of nanoscience is that traditionally diverse disciplines are transforming themselves to merge into a new type of integrated multi-science, as demanded by their common subject of interest. This rapid development urgently calls for a new generation of researchers, trained not only to survive in this post-disciplinary environment, but also to grasp and harness its innovative potential creatively.



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

Since the establishment of the graduate school, the number of doctoral candidates has continuously grown. At the end of 2011, 116 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 31 young scientists have already finished their doctoral studies. Today, 21 doctoral candidates were awarded a BuildMoNa scholarship, and 56 doctoral candidates are financed by means of third-party funds. Additionally, 26 doctoral candidates are funded by ESF doctoral positions, 13 doctoral candidates as well as two post docs are promoted within two ESF young researchers groups affiliated to the graduate school.

In addition, associated principal investigators who further strengthen the academic profile of the graduate school have been accepted: Prof. Dr. Hauke Harms,

Helmholtz Centre for Environmental Research, Prof. Dr. Daniel Huster, Institute of Medical Physics and Biophysics, Prof. Dr. Felix Otto, MPI for Mathematics in the Sciences, Prof. Dr. Tilo Pompe, Institute of Biochemistry, and Prof. Dr. Bernd Rosenow, Institute for Theoretical Physics.

The graduate school provides a well-structured training programme including multi-disciplinary scientific training and a transferable skills programme in cooperation with the Research Academy Leipzig. The major part of the scientific training consists of ten scientific and methods modules that are organised according to the overall research concept of the graduate school. Additionally, the minisymposium “Hot Nanoparticles and Nanostructures” was organised by Prof. Dr. Frank Cichos, Prof. Dr. Klaus Kroy and Prof. Dr. Bernd Rauschenbach. The minisymposium focused on the physics of laser-heated nanoparticles and nanostructures but also touched various aspects of physical chemistry and technological and medical applications. It gathered leading experts from a rapidly emerging and highly interdisciplinary field at the intersection of nanophotonics and nanoscale nonequilibrium stochastic thermodynamics.

Science-related events organised by BuildMoNa included the 4th BuildMoNa Symposium and the 4th BuildMoNa Workshop for doctoral candidates. These events especially provide a platform for interdisciplinary exchange and discussion within the graduate school.

On 7 December the ceremonial event for the fourth anniversary of BuildMoNa took place. The lecture of Prof. Dr. Dr. h.c. mult. Helmut Schwarz, President of the Alexander von Humboldt Foundation, Technische Universität Berlin, dealt with “Chemistry with methane: Concepts rather than recipes”. On this occasion, the annual BuildMoNa Awards were presented to three doctoral candidates for outstanding scientific publications resulting from their doctoral research.

Following an internal evaluation in January 2011, the renewal proposal for continuation of the graduate school until 2017 has been submitted to the German Research Foundation on 1 September 2011. The final decision will be announced on 15 June 2012.


Prof. Dr. Evamarie Hey-Hawkins

Organisation and management

RESEARCH ACADEMY LEIPZIG ADVISORY BOARD

Prof. Dr. Manfred Salmhofer
Universität Heidelberg

Prof. Dr. Axel Mecklinger
Universität des Saarlandes

Prof. Dr. Michael Geyer
University of Chicago



RESEARCH ACADEMY LEIPZIG



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

BuildMoNa OFFICE

Scientific Managers

Dr. Doritt Lupp
Dr. Alexander Weber
Dipl.-Phys. Andrea Kramer

Multilingual Secretaries

Dorit Thieme
Birgit Wendisch



STEERING COMMITTEE

Speaker of the Graduate School

Prof. Dr. Evamarie Hey-Hawkins

Deputy

Prof. Dr. Marius Grundmann

Representative of Doctoral Candidates

Dipl.-Phys. Martin Lange

Deputy

M.Sc. Chem. Wilma Neumann

Representatives of Principal Investigators

Prof. Dr. Josef A. Käs
Prof. Dr. Harald Krautscheid
Prof. Dr. Annette G. Beck-Sickinger
Prof. Dr. Frank-Dieter Kopinke
Prof. Dr. Dr. h.c. Bernd Rauschenbach
Prof. Dr. Dr. h.c. Wolfgang Hackbusch



SPOKESPERSONS OF THE DOCTORAL CANDIDATES

Faculty of Biosciences, Pharmacy and Psychology

M.Sc. Biochem. Sven Hofmann

Faculty of Chemistry and Mineralogy

M.Sc. Chem. Wilma Neumann
M.Sc. Chem. Tobias Möller

Faculty of Physics and Earth Sciences

Dipl.-Phys. Martin Lange
Dipl.-Phys. Fabian Klüpfel

Leibniz Institute of Surface Modification

M.Sc. Chem. Eng.
Erik Thelander

Helmholtz Centre for Environmental Research

Dipl.-Phys. Jens Schneider

Max Planck Institute for Mathematics in the Sciences

M.Sc. Chem. Anastacia Romanova

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

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

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

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

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

The BuildMoNa Office consists of 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.-Biochem. Verena Ahrens	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	<i>Modified peptides for biotechnology</i>
Dipl.-Phys. Tobias Andrea	Prof. Dr. T. Butz / Prof. Dr. J. Käs	<i>3D-visualisation of intracellular drug delivery systems by ion micro-tomography and 3D-inverse tomography sculpting</i>
Dipl.-Phys. Ariyan Arabi-Hashemi	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	<i>Ion beam assisted deposition of intelligent and adaptive surfaces</i>
M.Sc. Phys. Ana Isabel Ballestar Balbas	Prof. Dr. P. Esquinazi / Prof. Dr. T. Butz	<i>Intrinsic anisotropy of multigraphene and transport properties of graphite interfaces</i>
Dipl.-Biochem. Lars Baumann	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. A. Robitzki	<i>Structure-activity relation of chemokines</i>
M.Sc. Phys. Francis Bern	Prof. Dr. P. Esquinazi / Prof. Dr. B. Kersting	<i>Coupling phenomena in multilayered oxide nanostructures</i>
M.Sc. Chem. Solveig Boehnke	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	<i>Carborane derivatives in tumour therapy and diagnosis</i>
M.Sc. Phys. Michael Bonholzer	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	<i>Magneto-tunnel junctions with oxidic contacts</i>
Dipl.-Phys. Tammo Böntgen	Prof. Dr. M. Grundmann / Prof. Dr. F.-D. Kopinke	<i>Optical investigation of BaTiO₃-heterostructures with ellipsometry and Raman-scattering</i>
Dipl.-Phys. Kerstin Brachwitz	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	<i>Materials of ferroic order and their interaction</i>
Dipl.-Phys. Marco Braun	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	<i>Gold nanoparticle based thermophoretic nanofluids</i>
M.Sc. Chem. Martin Brehm	Prof. Dr. B. Kirchner / Prof. Dr. R. Gläser	<i>Development of a program package for efficient simulation of complex chemical systems</i>
Dipl.-Phys. Jörg Buchwald	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	<i>Mechanical properties of surfaces at nanoscale</i>
Dipl.-Phys. Jakob Tómas Bullerjahn	Prof. Dr. K. Kroy / Prof. Dr. B. Abel	<i>How a polymer breaks a bond</i>
Dipl.-Phys. Felix Daume	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	<i>Electrical properties and long-term stability of Cu(In,Ga)Se₂ solar cells on polyimide substrate</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
B.Sc. Chem. Jorge Luis Cholula Díaz	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmann	<i>Properties of novel precursor based materials</i>
M.Sc. Chem. Murali Dama	Prof. Dr. S. Berger / Prof. Dr. J. Haase	<i>Organo gels as an alignment media for RDC measurements</i>
Dipl.-Phys. Christof Peter Dietrich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	<i>Growth and characterisation of ZnO-based microstructures</i>
M.Sc. Chem. Marina Loredana Drob	Prof. Dr. B. Rauschenbach / Prof. Dr. M.R. Buchmeiser	<i>Biopolymeric materials for regenerative medicine</i>
M.Sc. Phys. Srujana Dusari	Prof. Dr. P. Esquinazi / Prof. Dr. H. Morgner	<i>Measurements of the mean free path and spin diffusion length in multigraphene</i>
M.Sc. Chem. Sylvia Els	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	<i>Gastrointestinal peptides related to obesity</i>
M.Sc. Chem. René Frank	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	<i>Carboranyl amino acids for applications in BNCT</i>
Dipl.-Phys. Helena Franke	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	<i>Growth and characterisation of UV-microcavities</i>
Dipl.-Phys. Niklas Fricke	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	<i>Polymer conformations in disordered environments</i>
M.Sc. Chem. Dirk Friedrich	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmann	<i>Synthesis, characterisation and deposition of CIGS precursors</i>
Dipl.-Phys. Anatol Fritsch	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	<i>Growth of soft breast tumour cells in micro- and nanostructured hard environments</i>
M.Sc. Phys. Nataliya Georgieva	Prof. Dr. J. Haase / Prof. Dr. B. Rosenow	<i>Magnetic resonance of topological insulators</i>
M.Sc. Chem. Anika Gladytz	Prof. Dr. B. Abel / Prof. Dr. A.G. Beck-Sickinger	<i>Nanospectroscopy near chemical and biological interfaces</i>
M.Sc. Chem. Thomas Gladytz	Prof. Dr. B. Abel / Prof. Dr. E. Hey-Hawkins	<i>Tracing chirality, reactivity and structures in space and time of smart molecules and materials near interfaces by XUVI soft X-Ray photoelectron emission and absorption spectroscopy</i>
Dipl.-Phys. Anja Graumann	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	<i>Magneto-mechanical characterisation and training of single crystalline FePd films for the purpose of designing a thin film membrane pump</i>
Dipl.-Phys. Martin-Patrick Göse	Prof. Dr. D. Huster / Prof. Dr. T. Pompe	<i>Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Matthias Golecki	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	<i>Encapsulation of catalytically active metal complexes</i>
M.Sc. Chem. Anne Grundmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	<i>Synthesis and reactivity of transition metal phosphinidene complexes</i>
M.Sc. Chem. Sina Gruschinski	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	<i>Transition metal complexes with spin-crossover properties</i>
M.Sc. Phys. Markus Gyger	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	<i>Active and passive biomechanical measurements for characterisation and stimulation of biological cells</i>
Dipl.-Biochem. Sina Haas	Prof. Dr. A. Robitzki / Prof. Dr. J. Käs	<i>Development of a bioforce microarray sensor for measuring cellular biomechanical forces of ischemic cell layers</i>
Dipl.-Phys. Chris Händel	Prof. Dr. J. Käs / Prof. Dr. B. Abel	<i>Chemical oscillations in cell membranes</i>
Dipl.-Phys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	<i>Principles of mechanosensitivity and durotaxis in mammalian cells</i>
M.Sc. Chem. Marcel Handke	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	<i>Networks based on 4d and 5d-metal ions as possible catalysts</i>
Dipl.-Biochem. Rayk Hassert	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. M. Grundmann	<i>Peptides for specific adhesion to hard matters</i>
Dipl.-Chem. Julia Haushälter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	<i>Phosphine-baskets – ligands for selective catalysis</i>
M.Sc. Chem. Thomas Heinze	Prof. Dr. R. Gläser / Prof. Dr. B. Kirchner	<i>Noble metal nanoparticles on ordered porous supports for the in-situ synthesis and conversion of H₂O₂ in supercritical carbon dioxide</i>
Dipl.-Phys. Marcel Hennes	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	<i>Synthesis and characterisation of magnetic core-shell nanoparticles</i>
M.Sc. Biochem. Sven Hofmann	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	<i>Chemical modification of peptides</i>
Dipl.-Phys. Florian Huber	Prof. Dr. J. Käs / Prof. Dr. M. Grundmann	<i>Artificial cell motility</i>
M.Sc. Phys. Ciprian-Ghiorgita Iacob	Prof. Dr. F. Kremer / Prof. Dr. R. Gläser	<i>Molecular dynamics of organic materials confined in nano-pores</i>
Dipl.-Phys. Alexander Janot	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	<i>Quantum condensates-coherence, fluctuations and disorder</i>
M.Sc. Phys. Michael Jurkutat	Prof. Dr. J. Haase / Prof. Dr. W. Janke	<i>Investigation of the electronic properties of high-temperature superconductors by means of NMR</i>
M.Sc. Phys. Chinmay Khare	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	<i>Glancing angle deposition</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Tobias Kießling	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	<i>Molecular marker free isolation of pluripotent haematopoietic stem cells and metastatic cancer cells from blood</i>
Dipl.-Phys. Fabian Klüpfel	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	<i>Transparent active multi-electrode arrays for the measurement of nerve cell signals</i>
Dipl.-Math. Melanie Knorr	Prof. Dr. J. Käs	<i>Role of stochasticity in a moving thin polymer film</i>
Dipl.-Phys. Jonas Kohlrautz	Prof. Dr. J. Haase / Prof. Dr. P. Esquinazi	<i>Magnetic resonance under extreme conditions</i>
Dipl.-Phys. Wilhelm Kossack	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	<i>IR-spectroscopy for the analysis of structure and dynamic of polymers</i>
Dipl.-Phys. Christian Kranert	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	<i>Electron-photon-interaction in micro- and nanowires</i>
M.Sc. Chem. Anika Kreienbrink	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	<i>Synthesis and reactions of carba-borane-substituted 1,2-diphosphetanes and other phosphorus-rich heterocycles</i>
M.Sc. Appl. Chem. Anusree Viswanath Kuttatheyl	Prof. Dr. J. Haase / Prof. Dr. H. Krautscheid	<i>Structure determination and host-guest interactions in porous metal-organic frameworks studied by solid-state NMR</i>
Dipl.-Chem. Jochen Lach	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	<i>Thin films of redox-active high-spin molecules</i>
Dipl.-Phys. Alexander Lajn	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	<i>Fabrication and characterisation of transparent field-effect transistors</i>
Dipl.-Phys. Martin Lange	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	<i>Growth and characterisation of quantum wire heterostructures</i>
Dipl.-Phys. Marc Lämmel	Prof. Dr. K. Kroy / Prof. Dr. W. Janke	<i>Stiff biopolymer solutions and networks</i>
M.Sc. Chem. Jörg Lincke	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	<i>Coordination polymers with nitrogen-rich ligands</i>
Dipl.-Phys. Michael Lorenz	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	<i>Investigations on the stability of zinc oxide based metal-semiconductor field-effect-transistors</i>
M.Sc. Phys. Chem. Yanhong Ma	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	<i>Magnetic shape memory alloys for miniaturised actuators</i>
M.Sc. Chem. Martyna Madalska	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	<i>Immobilised switchable phosphine-based catalysts</i>
M.Sc. Chem. Veronika Mäde	Prof. Dr. A.G. Beck-Sickinger / Prof. Dr. E. Hey-Hawkins	<i>Modified pancreatic polypeptide for treatment of obesity</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Phys. Martin Marenz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	<i>Development of a coarse-graining procedure for polymer adsorption</i>
M.Sc. Chem. Michael Marx	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	<i>Modifying metal nanoparticles by oxidative extraction into supercritical solution</i>
Dipl.-Phys. Benno Meier	Prof. Dr. J. Haase / Prof. Dr. S. Berger	<i>Ultra-high field magnetic resonance of modern materials</i>
Dipl.-Phys. Monika Möddel	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	<i>Modelling and computer simulations of adsorption specificity of synthetic peptides</i>
M.Sc. Chem. Tobias Möller	Prof. Dr. E. Hey-Hawkins / Prof. Dr. S. Berger	<i>Synthesis of P-chiral phosphorus compounds derived from low-valent phosphorus species</i>
Dipl.-Phys. Andreas Müller	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	<i>Peptide friction in cell adhesion</i>
Dipl.-Phys. Nils Neubauer	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	<i>Photothermal fluctuation spectroscopy on gold nanoparticle dimers</i>
Dipl.-Phys. Lena Neumann	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	<i>Hyperthermal ion assisted atomic assembly</i>
M.Sc. Chem. Paul Neumann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	<i>Switchable dendritic ferrocenyl phosphines</i>
M.Sc. Chem. Wilma Neumann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	<i>Overcoming cisplatin resistance of tumour cells with cytotoxic cyclo-oxygenase inhibitor conjugates</i>
M.Sc. Phys. K. David Nnetu	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	<i>The use of biomechanics to reduce metastatic aggressiveness</i>
M.Sc. Chem. Mareen Pagel	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	<i>Chemical modification of surfaces for novel biomaterials</i>
M.Sc. Chem. Souvik Pandey	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	<i>P-based polymers: synthesis and applications in materials science</i>
Dipl.-Phys. Steve Pawlizak	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	<i>Interplay between compartmentalisation of cells and tumour spreading</i>
M.Sc. Chem. Eva Perl	Prof. Dr. B. Kirchner / Prof. Dr. B. Abel	<i>Development of methods and application to complex systems from first principles</i>
M.Sc. Chem. Julian Rodger Frederic Pritzwald-Stegmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	<i>Phosphorus-based organometallic/inorganic hybrid materials</i>
Dipl.-Phys. Stefan Puttnins	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	<i>The influence of inhomogeneities in Cu(In,Ga)Se₂ thin film solar cells</i>
M.Sc. Chem. / M.Sc. Environmental protection Ksenia Jolanta Ramus	Prof. Dr. F.-D. Kopinke / Prof. Dr. R. Gläser	<i>Thermodynamic activity versus total concentration of xenobiotics as predictors of bioavailability</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Chem. Daniel Rathmann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	<i>Structure activity relationships of RF-amide peptide receptors with chemical modified peptides</i>
M.Sc. Chem. Dennis Richter	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	<i>Heterogeneous photocatalysis: water splitting with visible-light irradiation</i>
Dipl.-Chem. Stefan Richter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	<i>New selective cytostatics</i>
M.Sc. Phys. Susanne Röncke	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	<i>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</i>
M.Sc. Chem. Anastacia Romanova	Prof. Dr. W. Hackbusch / Prof. Dr. M. Grundmann	<i>Molecular simulations of ion effects on structural and thermodynamical properties of biopolymers</i>
Dipl.-Phys. Martin Rothermel	Prof. Dr. T. Butz / Prof. Dr. M. Grundmann	<i>Spatially resolved characterisation of the composition, structural disorders and electronic properties of inorganic nanostructures</i>
M.Sc. Chem. Klara Rusevova	Prof. Dr. F.-D. Kopinke / Prof. Dr. R. Gläser	<i>Iron-based nanoparticles catalysts for oxidation of pollutants in water</i>
Dipl.-Phys. Friedrich-Leonhard Schein	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	<i>Dynamic properties of ZnO-based integrated circuits</i>
Dipl.-Phys. Florian Schmidt	Prof. Dr. M. Grundmann / Prof. Dr. R. Gläser	<i>Characterisation of defects in hetero- and nanostructures</i>
Dipl.-Phys. Jörg Schnauß	Prof. Dr. J. Käs / Prof. Dr. A.G. Beck-Sickinger	<i>Biomimetic actin networks</i>
Dipl.-Phys. Jens Schneider	Prof. Dr. F.-D. Kopinke / Prof. Dr. M. Grundmann	<i>Studies of dissociation processes of water exposed to high-frequency electromagnetic fields</i>
Dipl.-Phys. Sebastian Schöbl	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	<i>Modelling and computer simulations of molecular pattern recognition</i>
Dipl.-Phys. Carsten Schuldt	Prof. Dr. J. Käs / Prof. Dr. B. Abel	<i>Cellular force generation on the single molecule level</i>
M.Sc. Phys. Ilya Semenov	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	<i>Dynamics of DNA under tension and in confinement</i>
Dipl.-Phys. Tim Stangner	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	<i>Investigation of receptor/ligand interactions on the level of single contacts using high-resolution optical tweezers</i>
Dipl.-Biochem. Max Steinhagen	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	<i>Enzyme analytics</i>

Title and Name	First / Second Supervisor	Working title of doctoral thesis
Dipl.-Biochem. Anja Steude	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	<i>Development and fabrication of novel peptide based biosensors for neuronal diagnostic tools</i>
Dipl.-Phys. Marko Stölzel	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	<i>Time-resolved spectroscopy on ZnO based micro- and nanowire hetero-structures and -cavities</i>
Dipl.-Phys. Dan Strehle	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	<i>Mechanical and dynamic properties of actin bundles</i>
M.Sc. Chem. Markus Streitberger	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	<i>Building catalytically active bi-metallic nano-frames with flexible bisphosphine ligands</i>
Dipl.-Phys. Sebastian Sturm	Prof. Dr. K. Kroy / Prof. Dr. F. Kremer	<i>Nonequilibrium dynamics of forced and confined semiflexible polymers</i>
Dipl.-Chem. Ronny Syre	Prof. Dr. B. Kersting / Prof. Dr. M. R. Buchmeiser	<i>Photo-induced electron transfer in multimeric capsule complexes</i>
M.Sc. Chem. Eng. Erik Thelander	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	<i>Synthesis of nanostructures using laser ablation</i>
M.Sc. Phys. Martin Treffkorn	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	<i>Theoretical analysis of nanostructures for topological quantum computing</i>
Dipl.-Phys. Martin Treß	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	<i>Molecular dynamics in nanometre-thick polymer layers studied by means of broadband dielectric spectroscopy</i>
Dipl.-Phys. Olaf Ueberschär	Prof. Dr. F. Kremer / Prof. Dr. W. Janke	<i>Investigating stochastic thermodynamics by means of optical tweezers</i>
Dipl.-Phys. Carolin Wagner	Prof. Dr. F. Kremer	<i>Investigation of the interaction of receptors and ligands by optical tweezers</i>
Dipl.-Phys. Franziska Wetzel	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	<i>Direct staging of primary mammary carcinomas by determining their cellular composition including metastatically competent cells, dormant cancer cells and cancer stem cells</i>
Dipl.-Phys. Micha Wiedenmann	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	<i>Cluster aggregation and condensation of nano-objects</i>
M.Sc. Chem. Patrick With	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	<i>Preparation, physico-chemical characterisation and testing of supported metal (oxide) catalysts</i>
M.Sc. Phys. Johannes Zierenberg	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	<i>Aggregation of polymers in crowded confinement with correlated disorder</i>
Dipl.-Phys. Jan Zippel	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	<i>Magnetic tunnel junctions</i>

Alumni 2011

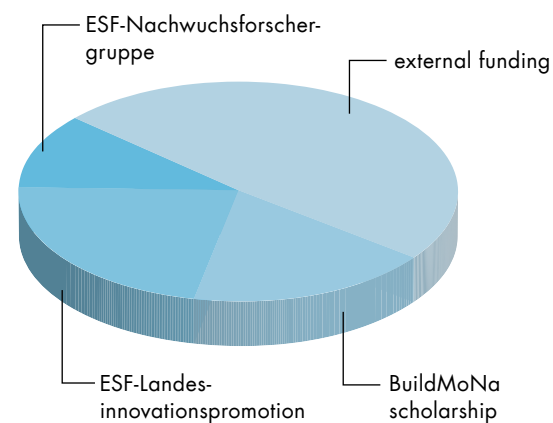
Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Kathrin Bellmann-Sickert	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	<i>Improvement of the bioavailability of neuropeptides and chemokines</i>
Dr. rer. nat. Roxana-Giorgiana Ene	Prof. Dr. F. Kremer / Prof. Dr. E. Hey-Hawkins	<i>Structural levels of organisation in spider silk as studied by time-resolved polarised rheo-FTIR spectroscopy</i>
Dr. rer. nat. Jens Glaser	Prof. Dr. K. Kroy / Prof. Dr. S. Müller	<i>Theory of semiflexible polymers</i>
Dr. rer. nat. Tobias Hammer	Prof. Dr. H. Morgner / Prof. Dr. A.G. Beck-Sickinger	<i>Investigation of aqueous solutions with Ion-Scattering-Spectroscopy</i>
Dr. rer. nat. Cathleen Juhl	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. R. Robitzki	<i>Investigation of the function of adiponektin receptors by peptide segmentation</i>
Dr. rer. nat. Aslihan Kircali	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	<i>Phosphorus-rich complexes as precursors for binary or ternary metal phosphides M_xP_y or $M_xM'_yP_z$</i>
Dr. rer. nat. Dana Krinke	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	<i>Development of an impedance-based HTS screening on novel neuronal 2D and 3D cell culture models for testing drugs against neurodegenerative diseases</i>
Dr. rer. nat. Daniel Lässig	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	<i>Synthesis and characterisation of porous coordination polymers with N-donor-ligands</i>
Dr. rer. nat. Ulrike Lehmann	Prof. Dr. B. Kersting / Prof. Dr. E. Hey-Hawkins	<i>Hydrogenation of CO₂ by supported container molecules</i>
Dr. rer. nat. Alexander Müller	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	<i>Investigation of carrier dynamics in ZnO films and microcavities</i>
Dr. rer. nat. Matthias Scholz	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	<i>Imitation and modification of bio-active lead structures via integration of clusters</i>
Dr. rer. nat. Chris Sturm	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	<i>Investigation of the cw optical properties of ZnO cavities</i>
Dr. rer. nat. Lars Wolff	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	<i>Plasticity and active remodelling of cells</i>
Dr. rer. nat. Hendrik Zachmann	Prof. Dr. B. Rauschenbach	<i>Electrical defects in ion beam assisted deposition of Cu(In,Ga)Se₂ thin film solar cells</i>

Mini-projects

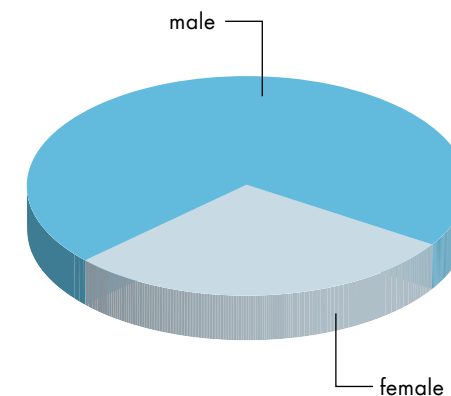
Student name	Doctoral candidate (supervisor)	Topic of mini-project
Daniel Fuhrmann	M.Sc. Chem. Dirk Friedrich	<i>Phosphine and amine stabilised ethylenedichalconides as CIGSSe-precursor</i>
Toni Grell	M.Sc. Chem. René Frank	<i>Novel reaction pattern of 7,8-dicarba dodecahydro-nido-undecaborate(-I)</i>
Sarah Heinicke	M.Sc. Chem. Anika Kreienbrink	<i>Phosphorus-rich heterocycles as precursors for organophosphorus-based polymers and as highly rigid ligands</i>
Schirin Hanf	M.Sc. Chem. Martyna Madalska	<i>Switchable ferrocenyl phosphines</i>
Merten Kobalz	M.Sc. Chem. Jörg Lincke	<i>Synthesis and characterisation of Metal Organic Frameworks</i>
Anna Reinhardt	Dipl.-Phys. Michael Lorenz	<i>Measurement and evaluation of the electrical characteristics of zinc oxide based thin-film transistors with tungsten oxide gate electrodes</i>

Statistics

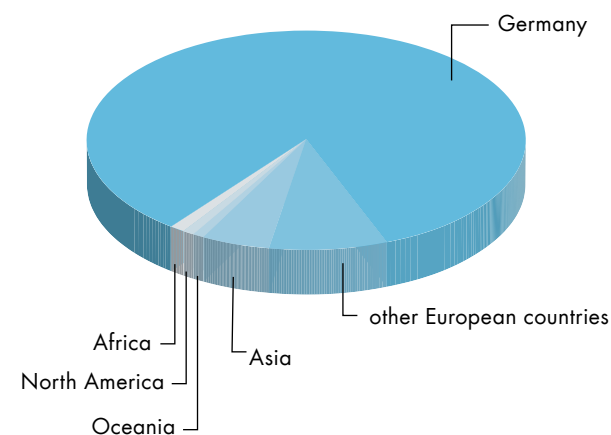
FUNDING OF THE DOCTORAL CANDIDATES' SCHOLARSHIPS:



GENDER RATIO OF DOCTORAL CANDIDATES:



ORIGIN OF DOCTORAL CANDIDATES:



Nanoscale photonic imaging and molecular movies on ultimate time and space scales

Prof. Dr. Bernd Abel

M.Sc. Chem. Anika Gladytz, M.Sc. Chem. Thomas Gladytz

The Abel group is engaged in research in the field of modern physical chemistry, biophysical chemistry, optics, and spectroscopic imaging. Our activities have the purpose of obtaining fundamental knowledge of matter (from smaller molecules up to polymers), to develop new molecular and analytical probes, and finally to use the knowledge to develop advanced analytical devices for industry and industrial applications.

Within BuildMoNa we develop and employ nanoscale photonic and AFM-imaging (fluorescence and Raman) of molecules and molecular aggregates to monitor



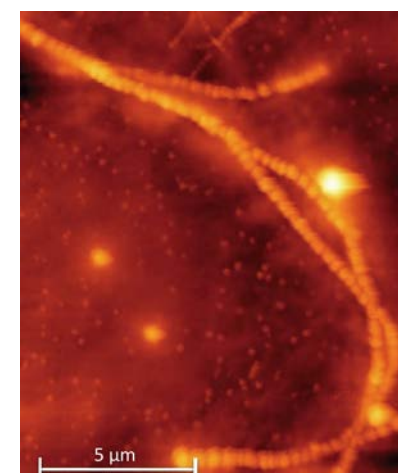
nanostructures of aggregated proteins near interfaces.

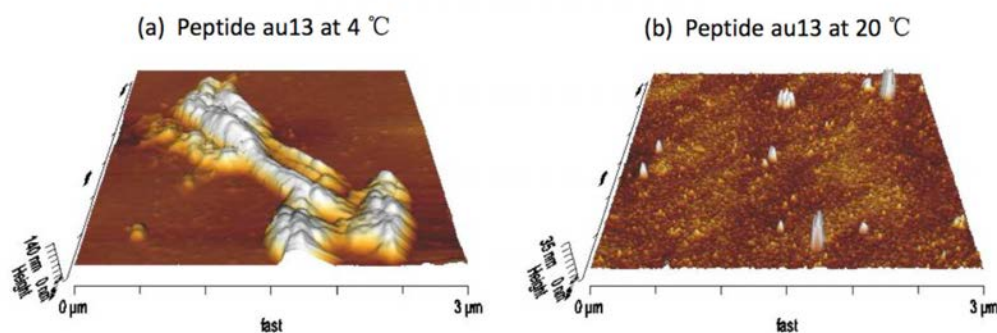
The first area where this is important is the field of biocompatibility of interfaces of implants and electronic devices. Peptide based multifunctional molecules serve as an anchor for cells near inorganic or metal interfaces.

The second area of research is amyloid protein/peptide aggregation near interfaces. The process, as well as its mechanisms are investigated via AFM- and spectroscopic probes in combination and laser induced liquid phase mass spectrometry.

Another research focus of the Abel group at BuildMoNa at present is time-resolved dynamics of chemical and biological molecular systems or molecular assemblies in different molecular environments. The analytical tools usually employ nanosecond pulsed or even ultrafast lasers. While the timescales and dynamics may vary over order of magnitudes the size of the molecular system range from smaller polyatomics up to large molecular nano-machines. Ultimately, investigations are complemented by time-resolved nano-scale photonic imaging techniques and molecular dynamics calculations with the long-time goal of determining true “molecular movies” on ultimate time and space scales.

The AFM image shows an amyloid fibre (from the sequence of the human ISLET poly-peptide), an aggregate formed by peptides (NNFGAIL). Many proteins and peptides form these kind of fibers under certain conditions. Several neural diseases are related to the formation of such fibrous aggregates in the body of a living being. The physical chemistry of the aggregations process is one of the central research topics of the Abel group.





↑ AFM image of short modified peptides (au13, 10 μM) near a silicon surface as a function of temperature
a) 4 °C and b) 20 °C

Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger

Dipl.-Biochem. Verena Ahrens, Dipl.-Biochem. Lars Baumann, Dr. Katrin Bellmann-Sickert, M.Sc. Chem. Sylvia Els, Dipl.-Biochem. Rayk Hassert, M.Sc. Biochem. Sven Hofmann, Dr. Cathleen Juhl, M.Sc. Chem. Veronika Mäde, M.Sc. Chem. Mareen Pagel, Dipl.-Chem. Daniel Rathmann, Dipl.-Biochem. Max Steinhagen

In different approaches we aim to produce different peptides and proteins that are chemically modified for application in the field of tumour targeting, nanobiomaterials and nanomedicine. Peptides are synthesised by solid phase peptide synthesis. Proteins are expressed recombinantly and fused to the peptides by native chemical ligation or click chemistry. Sylvia Els (M.Sc. Chem.), Veronika Mäde (M.Sc. Chem.) and Daniel Rathmann (Dipl.-Chem.) synthesise chemically modified peptide hormones that are modified by non natural amino acids, lipid or polyethylene glycol moieties to improve stability in biological system. They address ghrelin, pan-



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



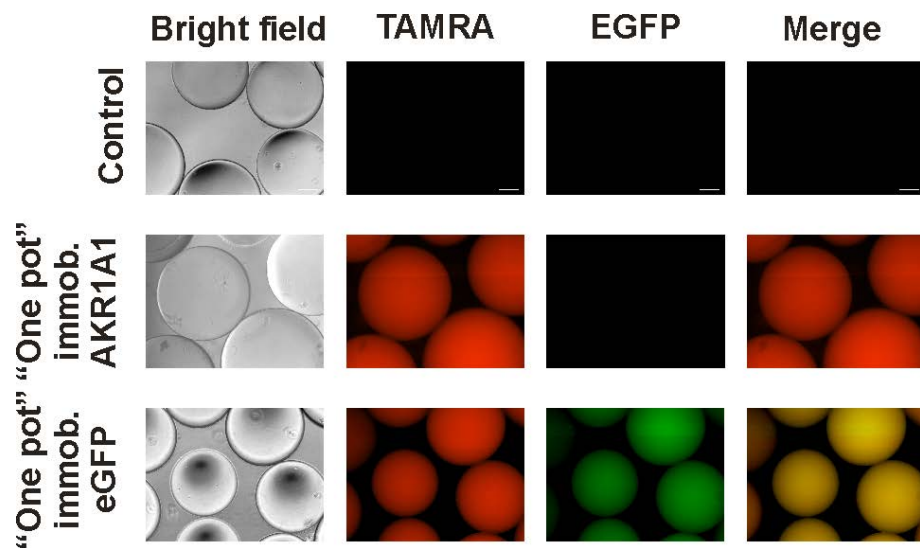
creatic polypeptide and neuropeptide FF, respectively.

Sven Hoffmann (M.Sc. Biochem.) and Verena Ahrens (Dipl.-Biochem.) work on the development of novel anti-tumour peptides by conjugation with carbaboranes or cytotoxic compounds. The peptides are used as shuttle systems to allow tumour specific uptake as the respective peptide receptors are overexpressed on tumour cells and internalise after agonist binding. One of the highlight 2011 was the proof of principle by Ahrens et al. for carboborane containing neuropeptide Y analogues.

In the field of chemical modification of proteins Dr. Cathleen Juhl, Dr. Kathrin Bellmann-Sickert and Lars Baumann (Dipl.-Biochem.) were successful. They work on adiponectin and stromal derived factor 1 alpha, two cytokines that play a role in the regulation of regeneration diseases and metabolism. Kathrin Bellmann-Sickert finished her doctorate in February 2011, Cathleen Juhl in December.

Mareen Pagel (M.Sc. Chem.), Rayk Hassert (Dipl.-Biochem.) and Max Steinhagen (Dipl.-Biochem.) work on chemically modified peptides and proteins to improve the properties of biomaterials. Rayk Hassert developed high affinity peptides for different surfaces, whereas Max Steinhagen developed a one pot method to directly immobilise proteins on surfaces. Mareen Pagel now investigated a further biocompatible ligation method, the inverse Diels-Alder reaction, and successfully applied this to the derivatisation of inorganic surfaces.

- ⇒ *Palmitoylated SDF1 α Shows Increased Resistance Against Proteolytic Degradation in Liver Homogenates*
K. Bellmann-Sickert, A.G. Beck-Sickinger / ChemMedChem. (2011) **6** 193
- ⇒ *Incorporation of ortho-Carbaboranyl-N ϵ -modified L-Lysine into Neuropeptide Y Receptor Y₁- and Y₂-Selective Analogues*
V.M. Ahrens, R. Frank, S. Stadlbauer, A.G. Beck-Sickinger, E. Hey-Hawkins / J. Med. Chem. (2011) **54** 2368
- ⇒ *Long-acting Lipidated Analog of Human Pancreatic Polypeptide is Slowly Released into Circulation*
K. Bellmann-Sickert, C. Eling, A.N. Madsen, P.B. Little, K. Lundgren, L.-O. Gerlach, R. Bergmann, B. Holst, T.W. Schwartz, A.G. Beck-Sickinger / J. Med. Chem. (2011) **54** 2658
- ⇒ *Unique Interaction Pattern for a Functionally Biased Ghrelin Receptor Agonist*
B. Sivertsen, M. Lang, T.M. Frimurer, A. Bach, S. Els, M.S. Engelstoft, T.W. Schwartz, A.G. Beck-Sickinger, B. Holst / J. Biol. Chem. (2011) **286** 20845
- ⇒ *Structure/Activity Studies of RF Amide Peptides Reveal a Subtype Selective Activation of the NPFF1 and the NPFF2 Receptor*
M. Findeisen, D. Rathmann, A.G. Beck-Sickinger / ChemMedChem (2011) **6** 1081
- ⇒ *Adiponectin Receptor 1 Interacts with both Subunits of Protein Kinase CK2*
C. Juhl, K. Mörl, A.G. Beck-Sickinger / Mol. Cell. Biochem. (2011) **15** 185
- ⇒ *A "One Pot" Combination of Expressed Protein Ligation and Cu(I)-Catalyzed Azide/Alkyne Cycloaddition to Immobilize Proteins*
M. Steinhagen, K. Holland-Nell, M.P. Meldal, A.G. Beck-Sickinger / ChemBioChem. (2011) **12** 2426
- ⇒ *Assessment of a Fully Active Class A G Protein-Coupled Receptor Isolated from in vitro Folding*
M. Bosse, L. Thomas, R. Hassert, A.G. Beck-Sickinger / Biochemistry (2011) **50** 9817



↑ Specific one-pot immobilisation of proteins (enzyme aldoketoreductase AKR1A1 and green fluorescent protein GFP) via TAMRA-labelled linker on beads as described by M. Steinhagen et al. / ChemBioChem. (2011) **12** 2426 (TAMRA: tetramethylrhodamine-dye)

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

Polyisocyanides as reagent to observe residual dipolar couplings in NMR

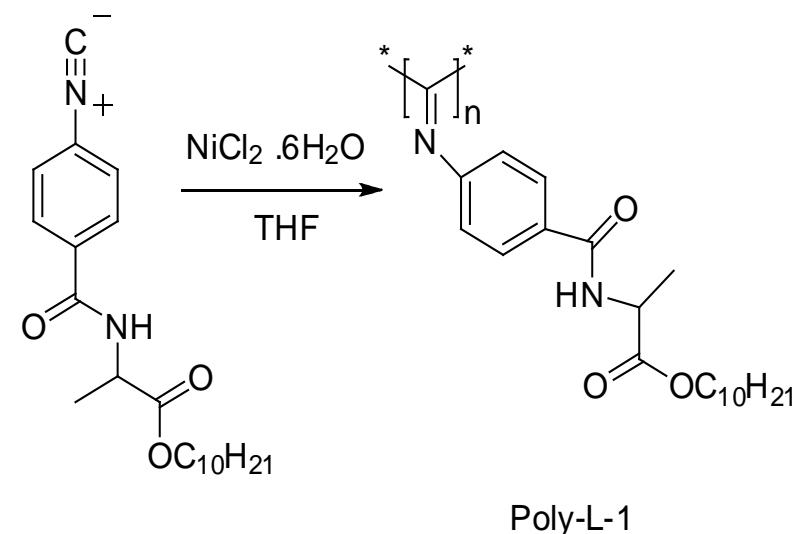
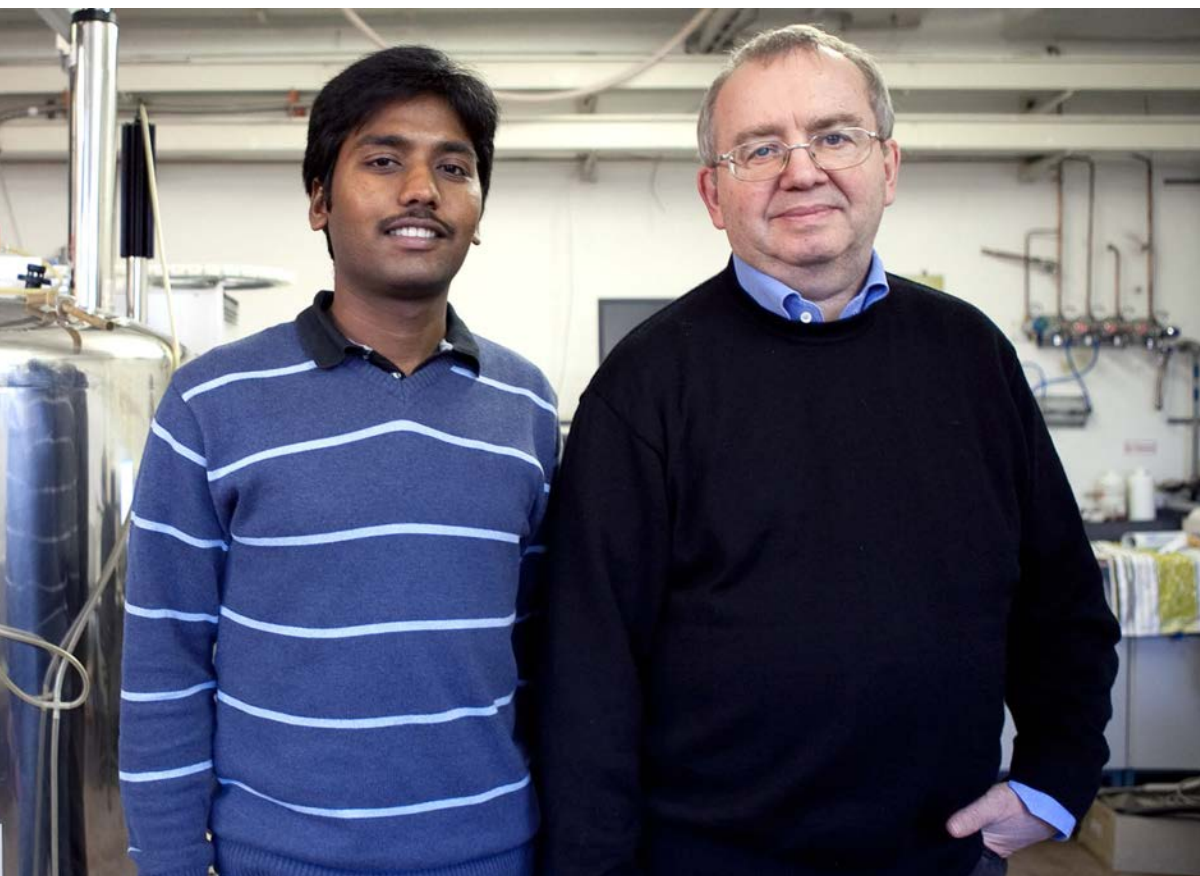
Prof. Dr. Stefan Berger
M.Sc. Chem. Murali Dama

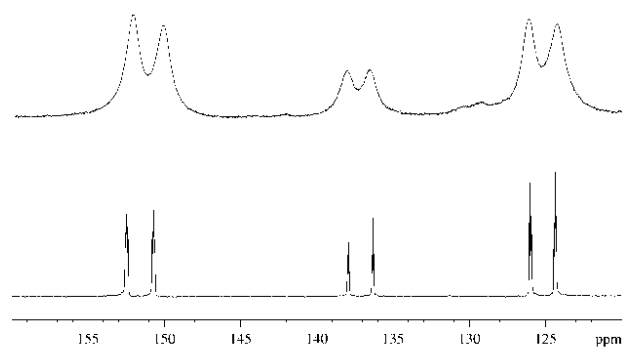
Murali Dama has investigated the alignment possibilities of organic molecules in the strong magnetic field of an NMR spectrometer. If molecules adopt to a very small degree a certain orientation with respect to the magnetic field, residual dipolar couplings can be measured. Residual dipolar couplings (RDC's) are an important parameter in organic structure determination. These RDC's are useful in configuration, conformation and constitutional analysis of molecules and support or even replace NOE information due to their r^{-3} dependence. For this alignment one needs an anisotropic medium, which orients itself and hence the dissolved analyte. So far, mainly one system, namely liquid crystals such as poly- γ -benzyl-L glutamate was known to work for organic compounds, but this system shows considerable drawbacks, e.g. very strong line broadening of the NMR spectra.

The first approach of Murali Dama was to synthesise low molecular weight organogelators (LMOG) with several aromatic rings attached. The hope was that due to the anisotropy of the aromatic rings these systems should orient themselves slightly in the NMR spectrometer. Due to their gel properties this orientation should be stable and transferrable to organic molecules. However, after two years of synthesis of many of such LMOG's we had to realise that these would not fulfil our wishes.

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

Closely related to this is a thesis work performed by Lisett Valentin who has prepared for the first time chiral polystyrene sticks which are also aligning organic molecules and provide now a second new alignment system to study the effects of chirality.





↑ Gated decoupled ^{13}C NMR spectra of pyridine in CD_2Cl_2 (bottom) and $\text{CD}_2\text{Cl}_2/\text{Poly-L-1}$ (top)

⇒ *Hairpin Conformation of an 11-mer Peptide*

C.G. Mai, N. Jahr, D. Singer, S. Berger / *Bioorganic & Medicinal Chemistry* (2011) **19** 3497

⇒ *NH Exchange in Point Mutants of Human Ubiquitin*

N. Jahr, E. Fiedler, R. Günther, H.-J. Hofmann, S. Berger / *International Journal Biological Macromolecules* (2011) **49** 154

Prof. Dr. Stefan Berger
Institute of Analytical Chemistry
<http://www.uni-leipzig.de/~nmr/ANALYTIK/>
E-mail: stberger@rz.uni-leipzig.de
Phone: +49 341 97-36101
Fax: +49 341 97-36115

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

Prof. Dr. Tilman Butz

Dipl.-Phys. Tobias Andrea, Dipl.-Phys. Martin Rothermel

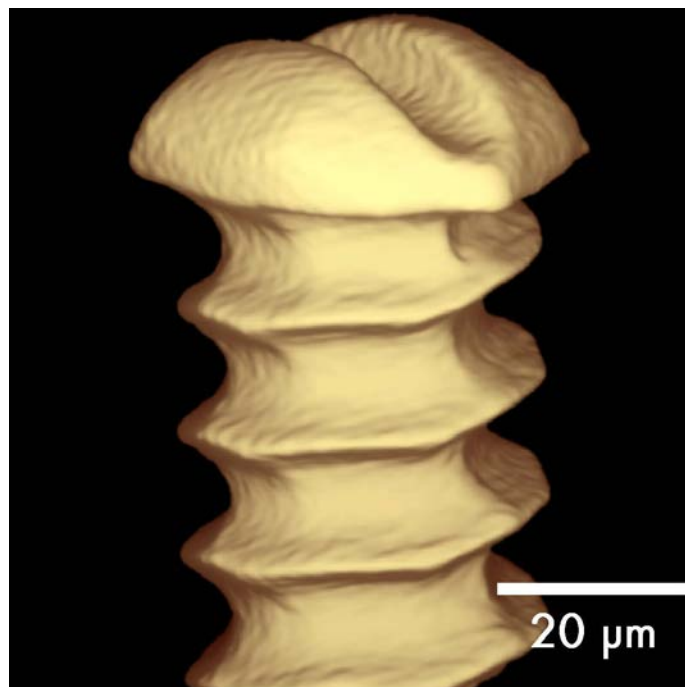
The LIPSION high energy nanoprobe enables BuildMoNa doctoral candidates to pursue a number of research projects.

The element-sensitive technique of PIXE (particle induced X-ray emission) tomography with submicron resolution has the potential to be widely used for a number of applications. However, long measurement and reconstruction times restrain potential users from making demand of this technique. Martin Rothermel's research



thus focuses on enhancing ion beam characteristics and reconstruction software performance. Due to the complex probe-sample-interactions a highly sophisticated reconstruction algorithm is needed, which is able to accurately model the effects of particle deceleration and X-ray attenuation within the sample.

Tobias Andrea is investigating the potential of ion beam tomography for the three-dimensional characterisation and elemental mapping of single cells and for the creation of 3D micro- and nanostructures. A 3D reconstruction of cells containing silica microparticles was obtained using limited-angle tomography which combined STIM (scanning transmission ion microscopy) and PIXE. Also, the technique of proton beam sculpting has been developed in which insights from tomography are applied in the field of proton beam writing. With this method several microsculptures have been created by patterned proton irradiation from multiple angles.



← Scanning transmission ion micro-tomogram of PMMA screw created by proton beam writing from 3 directions

⇒ *Creation of 3D Microsculptures in PMMA by Multiple Angle Proton Irradiation*

T. Andrea, M. Rothermel, T. Koal, T. Butz / Nuclear Instruments and Methods in Physics Research B (2011) 269 2431

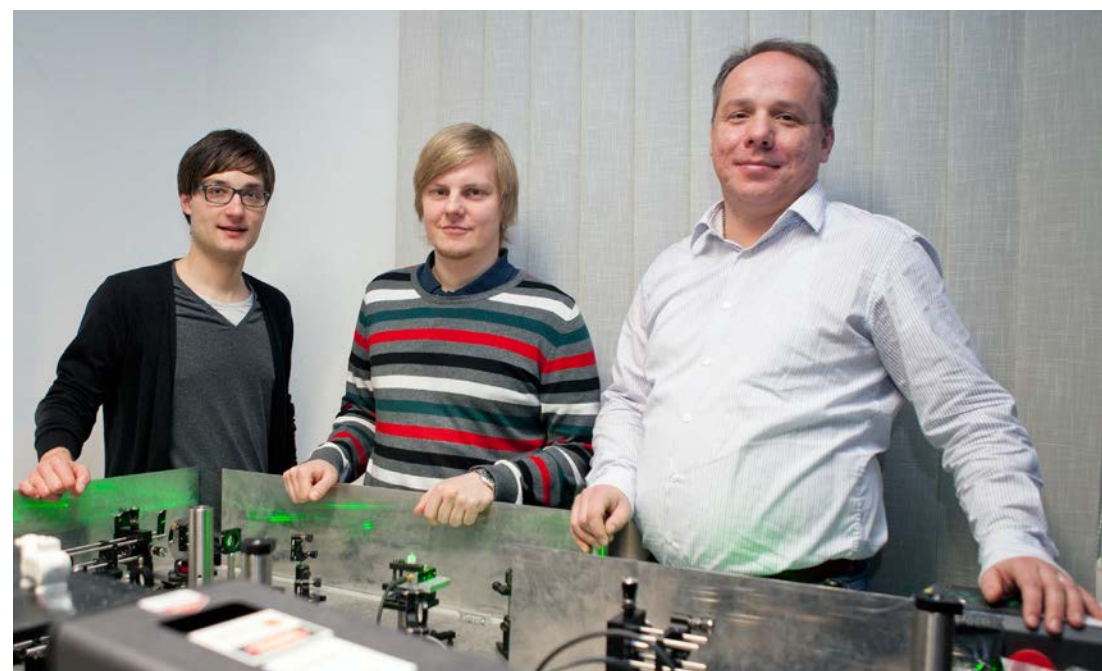
Prof. Dr. Tilman Butz
Institute for Experimental Physics II
<http://www.uni-leipzig.de/~nfp/>
E-mail: butz@physik.uni-leipzig.de
Phone: +49 341 97-32701
Fax: +49 341 97-32748

Thermophoretic trapping and steering of Janus particles

Prof. Dr. Frank Cichos

Dipl.-Phys. Marco Braun, Dipl.-Phys. Nils Neubauer

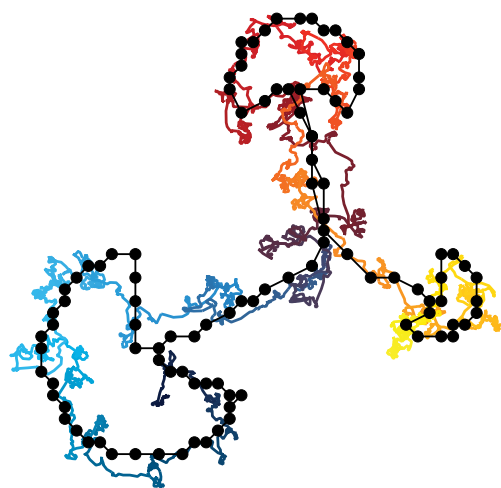
The manipulation of nano-objects in liquids on length scales of micro- and nanometres requires strategies which are different from swimming in the macroscopic world. The nanoworld is dominated by Brownian motion and viscous friction. As Brownian motion is itself a consequence of the continuous interconversion of solvent thermal energy into particle kinetic energy and back, manipulation of particles may be achieved by varying local solvent temperature and local viscous friction. Such local temperature and viscosity changes can be induced by metal nano-structures. Gold nanostructures, for example, exhibit strong coupling to visible light due to a collective excitation of conduction band electrons – plasmons – which decay quickly nonradiatively into heat. Thus highly local temperature gradients can be generated which are precisely controlled by light. We employ such gold nanostructures to establish a switchable self-propulsion of microparticles by light. Microparticles of a size of 1 μm are coated partially by a thin gold layer to prepare so-called Janus particles. The optical heating of the gold layer causes a temperature gradient across the surface of the particle. This tangential temperature gradient induces a



directed thermophoretic motion of the particle. The directed motion of the particle, however, randomises in direction within a few 100 ms due to the rotational Brownian motion of the particle

The long range particle motion is diffusive again, but with an enhanced diffusion coefficient as compared to a particle which is not propelled. To introduce a controlled particle motion on even larger length and time scales than rotational Brownian motion allows, we have introduced during the last year a feedback mechanism, which stochastically heats the particle according to its orientation and position. This feedback mechanism becomes possible by a real-time determination of the position and the 3-dimensional orientation of the particle.

Whenever the particle is oriented towards a certain target position, the propulsion mechanism is switched on by heating the gold layer optically. The mechanism is therefore not trying to beat the rotational Brownian motion but uses it instead to induce this directed motion. Thus a unique control of the particle position is possible. Due to the size dependence of particle translational diffusion and rotational diffusion coefficients, this mechanism is expected to provide even better control for smaller particles contrary to all existing trapping mechanisms i.e. with optical tweezers. More complex motion as well as collective multiple particle trapping and steering will lead to new insight into the interaction of heated microparticles.



← Sample trajectory of a thermophoretically steered Janus particle in water; the black points describe the target path for the particle propulsion; the coloured curve is the particle trajectory

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

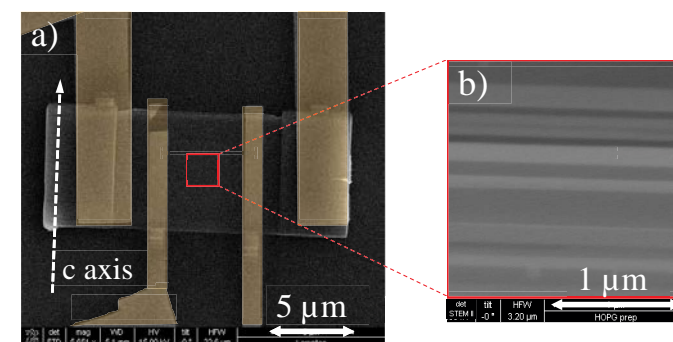
Electronics properties of sub micrometre graphite samples

Prof. Dr. Pablo D. Esquinazi

M.Sc. Phys. Ana Isabel Ballestar Balbas, M.Sc. Phys. Francis Bern,
M.Sc. Phys. Srujana Dusari

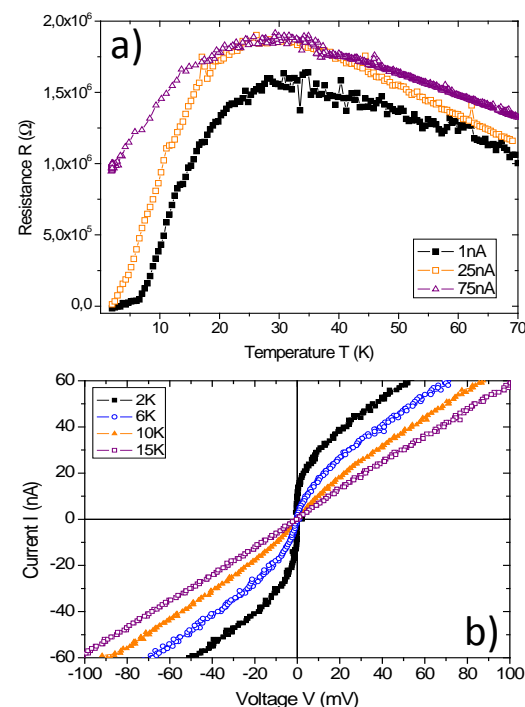
Graphene is being widely investigated due its extraordinary properties such as long electron mean free path, high carrier mobility, long spin-diffusion length and specific band structure. However, the properties of samples that consist of many of these graphene layers [i.e. multigraphene (MG)] remain unclear. The results obtained in our group show that the transport properties of the MG systems cannot be explained in terms of intrinsic properties only but the role of defects, impurities and especially interfaces plays an important role. Our work was focused in two different kinds of experiments:

Direct investigation of role of interfaces in MG samples: Transmission electron microscope images reveal the existence of interfaces between different perfectly stacked graphene layer. In order to investigate their transport properties, samples of thickness between 300 to 800 nm (in the graphene plane) and width of about 7 μm have been prepared from Highly Oriented Pyrolytic Graphite (HOPG). Four points electrical measurements show zero resistance state at low temperatures and low enough input current as well as non-linear Josephson-like current-voltage characteristics curves.



↑ Scanning electron microscope image of a sample with four electrical contacts; as indicated in the picture (dashed arrow), the c axis runs parallel to the substrate and the graphene planes are perpendicular to it

↑ Transmission electron microscope image of a sample where the different colours indicate misalignment between different perfectly stacked graphene layers regions

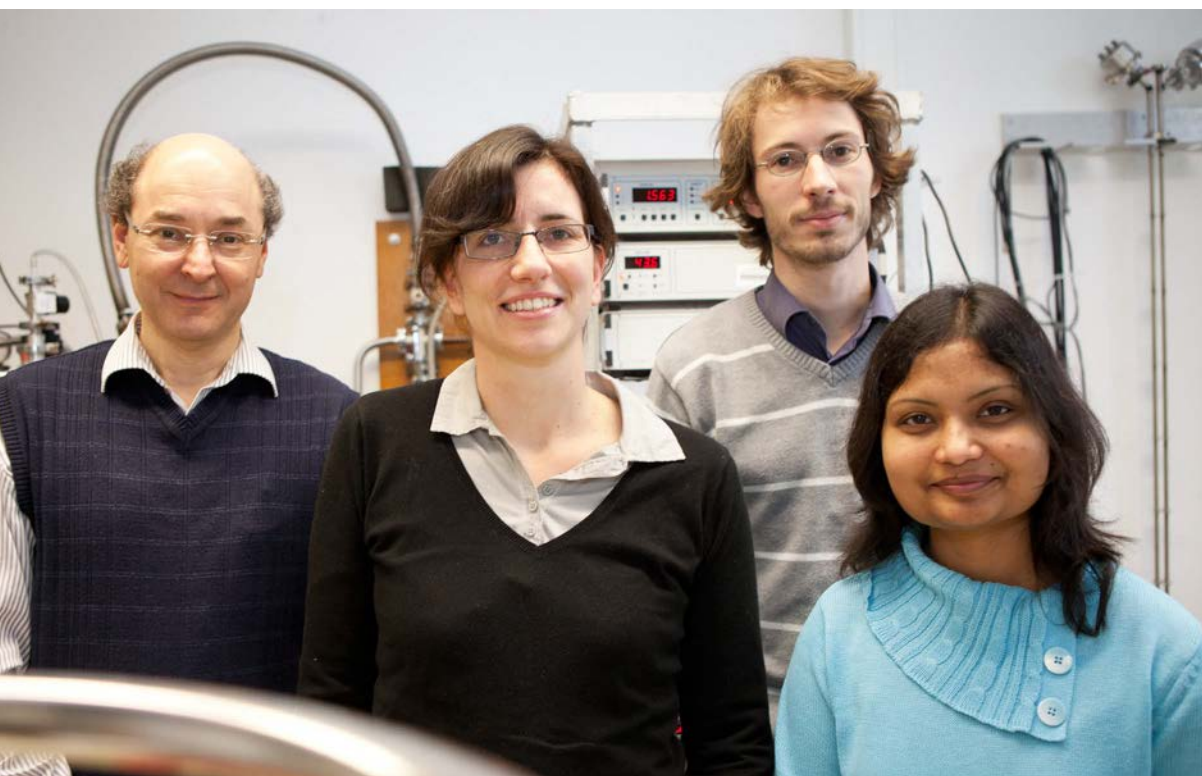


Temperature dependence of the resistance of the sample; note that for an input current of 1 nA zero resistance value is measured below ~ 8 K

Current-Voltage characteristics curve measured for the same sample as above; the typical Josephson behavior is found for temperatures below 15 K

Multigraphene samples with several contacts over their area were prepared to investigate their electronic properties and in particular the ballistic transport. The results obtained show that the usual diffusive Ohm law does not apply in this system and the contribution due to the ballistic transport has to be taken into account. Supporting previous results, micrometre mean free path and Fermi wavelength are found, as well as mobility $\geq 10^7 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at 300 K.

- ⇒ *Ballistic Transport at Room Temperature in Micrometer Size Multigraphene*
S. Dusari, J. Barzola-Quiquia, P. Esquinazi, N. Garcia / Physical Review B (2011) **83** 125402
- ⇒ *Superconducting Behavior of Interfaces in Graphite: Transport Measurements of Micro-Constrictions*
S. Dusari, J. Barzola-Quiquia, P. Esquinazi / Journal of Superconductivity and Novel Magnetism (2011) **24** 401
- ⇒ *Andreev Reflection and Granular Superconductivity Features Observed in Mesoscopic Samples Using Amorphous Tungsten Carbide Superconductors*
J. Barzola-Quiquia, S. Dusari, C. Chilotte, P. Esquinazi / Journal of Superconductivity and Novel Magnetism (2011) **24** 463
- ⇒ *Enhancement of the Ferromagnetic Order of Graphite after Sulphuric Acid Treatment*
J. Barzola-Quiquia, W. Böhlmann, P. Esquinazi, A. Schadewitz, A. Ballestar, S. Dusari, L. Schultze-Nobre, B. Kersting / Applied Physics Letters (2011) **98** 192511
- ⇒ *Electrical Characterization with Atomic Force Microscopy and Low Temperature Transport Properties of Boric Acid Doped Polyaniline with Fe_3O_4 Nanoparticles Composites*
A. Ballestar, F. Yakuphanoglu, B.F. Senkal, M. Munoz, W.A. Farooq / Optoelectronics and Advanced Materials Rapid Communications (2011) **5** 1
- ⇒ *Absence of Field Anisotropy Ferromagnetic Signals of Highly Oriented Pyrolytic Graphite*
A. Ballestar, A. Setzer, P. Esquinazi / Journal of Magnetism and Magnetic Materials (2011) **323** 758
- ⇒ *Experimental Study of the Intrinsic and Extrinsic Transport Properties of Graphite and Multigraphene*
J. Barzola-Quiquia, A. Ballestar, S. Dusari, P. Esquinazi / Book Chapter 8 of Graphene-Synthesis, Characterization, Properties and Applications, ISBN 978-953-307-292-0, Edited by: Jian Ru Gong, Publisher InTech, September 2011



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

Building complex nanostructures for applied catalysis

Prof. Dr. Roger Gläser

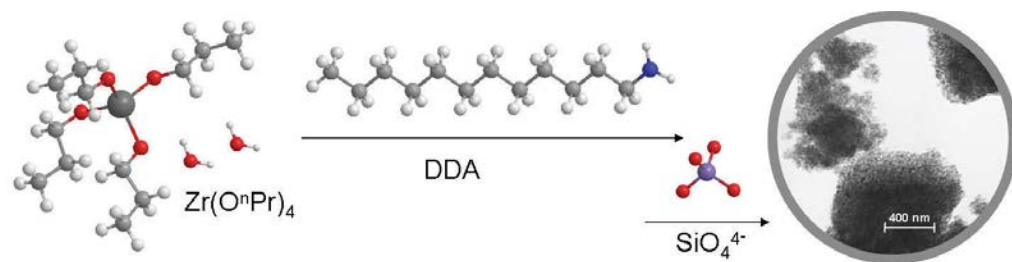
M.Sc. Chem. Thomas Heinze, M.Sc. Chem. Michael Marx, M.Sc. Chem. Dennis Richter,
M.Sc. Chem. Patrick With

The current challenges of modern heterogeneous catalysis include the search for materials with a complex set of properties on different length scales. Our research is centred on nanoporous materials with defined porosity and controllable catalytically active components. Following the principle approaches of the graduate school, we apply different strategies to synthesise novel materials for the use as catalysts and catalyst supports. One example is the preparation of nanoporous materials such as zirconia built from molecular precursors as support for Ni-nanoparticles as active catalysts for the high-temperature conversion of the greenhouse gases methane and carbon dioxide to synthesis gas. Another approach makes use of multifunctional scaffolds in a combined exo- and endotemplating strategy for the preparation of mixed oxides with hierarchically structured pore systems. Moreover, hybrid systems are synthesised with supported ionic liquid-based catalytic redox functionalities on porous inorganic supports opening the general route to introduce chemically diverse active components into the pore systems of these innovative catalytic materials. Catalytic applications range from fine chemical synthesis to environmental protection.



⇒ *Nickel-Loaded Zirconia Catalysts with Large Specific Surface Area for High-Temperature Catalytic Applications*

A. Peters, F. Nouroozi, D. Richter, M. Lutecki, R. Gläser / ChemCatChem (2011) 3 598



↑ Synthesis of Si-stabilised porous zirconia as a support for Ni-catalysts using a molecular Zr-precursor and dodecylamine (DDA) as a structure-directing agent

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

Oxide-based novel electronic and photonic building blocks

Prof. Dr. Marius Grundmann

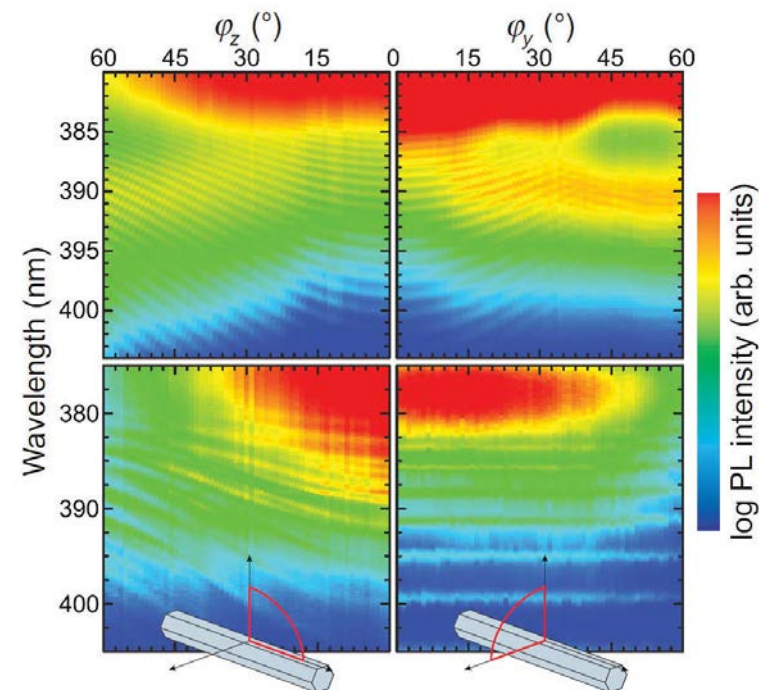
M.Sc. Phys. Michael Bonholzer, Dipl.-Phys. Tammo Böntgen, Dipl.-Phys. Kerstin Brachwitz, Dipl.-Phys. Felix Daume, Dipl.-Phys. Christof Peter Dietrich, Dipl.-Phys. Helena Franke, Dipl.-Phys. Fabian Klüpfel, Dipl.-Phys. Christian Kranert, Dipl.-Phys. Alexander Lajn, Dipl.-Phys. Martin Lange, Dipl.-Phys. Michael Lorenz, Dr. Alexander Müller, Dipl.-Phys. Stefan Puttnins, Dipl.-Phys. Friedrich-Leonhard Schein, Dipl.-Phys. Florian Schmidt, Dipl.-Phys. Marko Stölzel, Dr. Chris Sturm, Dipl.-Phys. Jan Zippel

Zinc oxide (ZnO) and related oxides are fabulous materials for novel electronic and optical devices. In the reporting period novel transistor structures have been synthesised and investigated combining semiconducting ZnO with other oxides. Using extremely thin films of noble metals and noble metal oxides on ZnO, high quality Schottky diodes could be realised that are for the first time also transparent. This offers new possibilities for transparent electronics such as displays on windows and a related German patent has been granted. Also transparent, so called “visible-blind” photodetectors, were designed and fabricated. Using so far unexplored amorphous tungsten trioxide as gate insulator, MOSFET devices with very low switching voltages were realised that perform close to the thermodynamically possible optimum. The abundance of the used oxides, the low processing temperatures (Schottky contacts and WO_3 were fabricated at room temperature) and the energy



efficiency of device operation make these approaches contribute to several aspects of “green technology”.

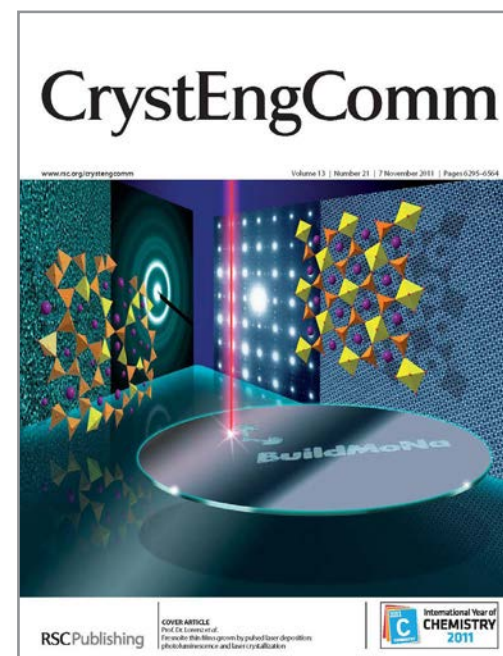
A hundred years ago Lord Rayleigh discussed the phenomenon of (acoustic) whispering gallery modes in St. Paul’s cathedral. Today high quality optical resonators based on whispering gallery modes are an essential element in nano-photonics. Prismatic zinc oxide micro-wires with different polygonal circumference varying from the typically discussed regular hexagon have been investigated. Various whispering gallery modes (triangular, square and hexagonal) have been identified by their characteristic resonance spectra. For the first time Fabry-Pérot modes within the wire cross-section have been found, unambiguously distinguished by their particular angular dispersion. The bending of nanowires leads to a reduction of symmetry, evidenced by local variation of band gap between the tensile and compressive end, and leaves some whispering gallery modes intact. Thus the study of whispering gallery modes remains an active field with applications in nano- and micro-sized optical devices lying ahead. Oxide nanowire heterostructures with large confinement energies have been reported and the first Hall effect measurements on microwires.



↑ Angular-resolved (TE-polarised) photoluminescence spectra at room temperature for the angles along (left) and perpendicular (right) of a ZnO microwire; spectra were recorded at different positions with $d = 16.6 \mu\text{m}$ (top) and $2.6 \mu\text{m}$ (bottom), exhibiting dominantly Fabry-Pérot modes (top) and whispering gallery modes (bottom), unambiguously distinguished by their dispersion perpendicular to the wire

- ⇒ *Tungsten Oxide as Gate Dielectric for Highly Transparent and Temperature-stable Zinc-oxide-based Thin-film Transistors*
M. Lorenz, H. von Wenckstern, M. Grundmann / *Advanced Materials* (2011) **23** 5383
- ⇒ *Fresnoite Thin Films grown by Pulsed Laser Deposition: Photoluminescence and Laser Crystallization*
A. Müller, M. Lorenz, K. Brachwitz, J. Lenzner, K. Mittwoch, W. Skorupa, M. Grundmann, T. Höche / *Cryst-EngComm* (2011) **13** 6377
- ⇒ *One- and Two-dimensional Cavity Modes in ZnO Microwires*
C.P. Dietrich, M. Lange, C. Sturm, R. Schmidt-Grund, M. Grundmann / *New Journal of Physics* (2011) **13** 103021
- ⇒ *Comment on "Exciton-polariton Microphotoluminescence and Lasing from ZnO Whispering-gallery Mode Microcavities"* [*Applied Physics Letters* (2011) **98** 161110]
C.P. Dietrich, M. Grundmann / *Applied Physics Letters* (2011) **99** 136101
- ⇒ *Strain Distribution in Bent ZnO Microwires*
C.P. Dietrich, M. Lange, F.J. Klüpfel, H. von Wenckstern, R. Schmidt-Grund, M. Grundmann / *Applied Physics Letters* (2011) **98**(3) 031105
- ⇒ *Light and Temperature Stability of Fully Transparent ZnO-based Inverter Circuits*
A. Lajn, T. Diez, F. Schein, H. Frenzel, H. von Wenckstern, M. Grundmann / *IEEE Electron Device Letters* (2011) **32**(4) 515
- ⇒ *Electrical Transport and Optical Emission of $Mn_xZr_{1-x}O_2$ ($0 < x < 0.5$) Thin Films*
J. Zippel, M. Lorenz, J. Lenzner, M. Grundmann, T. Hammer, A. Jacquot, H. Böttner / *Journal of Applied Physics* (2011) **110** 043706
- ⇒ *Gate- and Drain-lag Effects in (Mg,Zn)O-based Metal-semiconductor Field-effect Transistors*
F.J. Klüpfel, A. Lajn, H. Frenzel, H. von Wenckstern, M. Grundmann / *Journal of Applied Physics* (2011) **109** 074515
- ⇒ *Defect Properties of ZnO and ZnO:P Microwires*
C.P. Dietrich, M. Brandt, M. Lange, J. Kupper, T. Böntgen, H. von Wenckstern, M. Grundmann / *Journal of Applied Physics* (2011) **109** 013712
- ⇒ *Thermal Stability of ZnO/ZnCdO/ZnO Double Heterostructures Grown by Pulsed Laser Deposition*
M. Lange, C.P. Dietrich, G. Benndorf, M. Lorenz, J. Zúñiga-Pérez, M. Grundmann / *Journal of Crystal Growth* (2011) **328**(1) 13
- ⇒ *Erratum to: Transparent Rectifying Contacts for Visible-blind Ultraviolet Photo Diodes Based on ZnO*
A. Lajn, M. Schmidt, H. von Wenckstern, M. Grundmann / *Journal of Electronic Materials* (2011) **40** 477
- ⇒ *Transparent Rectifying Contacts for Visible-blind Ultraviolet Photo Diodes Based on ZnO*
A. Lajn, M. Schmidt, H. von Wenckstern, M. Grundmann / *Journal of Electronic Materials* (2011) **40** 473
- ⇒ *MgZnO/ZnO Quantum Well Nanowire Heterostructures with Large Confinement Energies*
M. Lange, C.P. Dietrich, J. Zúñiga-Pérez, H. von Wenckstern, M. Lorenz, M. Grundmann / *Journal of Vacuum Science and Technology A* (2011) **29** 03A104
- ⇒ *Exciton-polaritons in a ZnO-based Microcavity: Polarization Dependence and Non-linear Occupation*
C. Sturm, H. Hilmer, R. Schmidt-Grund, M. Grundmann / *New Journal of Physics* (2011) **13** 033014
- ⇒ *Cavity-photon Dispersion in One-dimensional Confined Microresonators with an Optically Anisotropic Cavity Material*
C. Sturm, H. Hilmer, B. Rheinländer, R. Schmidt-Grund, M. Grundmann / *Physical Review B* (2011) **83**(20) 205301
- ⇒ *Nickel-related Defects in ZnO – A Deep-level Transient Spectroscopy and Photo-capacitance Study*
M. Schmidt, K. Brachwitz, F. Schmidt, M. Ellguth, H. von Wenckstern, R. Pickenhain, M. Grundmann, G. Brauer, W. Skorupa / *physica status solidi (b)* (2011) **248**(8) 1949
- ⇒ *Ferrimagnetic $ZnFe_2O_4$ Thin Films on $SrTiO_3$ Single Crystals with Highly Tunable Electrical Conductivity*
M. Lorenz, M. Brandt, K. Mexner, K. Brachwitz, M. Ziese, P. Esquinazi, H. Hochmuth, M. Grundmann / *physica status solidi RRL* (2011) **5**(12) 438

- ⇒ *Semiconducting Oxide Heterostructures*
M. Brandt, H. von Wenckstern, M. Stölzel, H. Hochmuth, M. Lorenz, M. Grundmann / *Semiconductor Science and Technology* (2011) **26** 014040
- ⇒ *Optical Properties of $BaTiO_3/ZnO$ Heterostructures under the Effect of an Applied Bias*
T. Böntgen, S. Schöche, R. Schmidt-Grund, C. Sturm, M. Brandt, H. Hochmuth, M. Lorenz, M. Grundmann / *Thin Solid Films* (2011) **519** 2933
- ⇒ *Determination of the Refractive Index of Single Crystal Bulk Samples and Micro-structures*
R. Schmidt-Grund, P. Kühne, C. Czekalla, D. Schumacher, C. Sturm, M. Grundmann / *Thin Solid Films* (2011) **519** 2777
- ⇒ *Transparente gleichrichtende Metall-Metalloxid-Halbleiterkontaktstruktur und Verfahren zu seiner Herstellung und Verwendung*
H. Frenzel, A. Lajn, H. von Wenckstern, M. Grundmann / DE 10 2009 030 045 B3 (Deutsches Patent- und Markenamt, München, 2011)
- ⇒ *The (Mg,Zn)O Alloy*
H. von Wenckstern, R. Schmidt-Grund, C. Bundesmann, A. Müller, C.P. Dietrich, M. Stölzel, M. Lange, M. Grundmann / *Handbook of Zinc Oxide and Related Materials*, Vol. 1 Materials, Chapter 10, Z.C. Feng, ed. (Taylor and Francis/CRC Press, Florida, USA, 2011), ISBN 978-1439855706
- ⇒ *Metal-semiconductor Field-effect Transistors and Integrated Circuits Based on ZnO and Related Oxides*
H. Frenzel, M. Lorenz, F.-L. Schein, A. Lajn, F.J. Klüpfel, T. Diez, H. von Wenckstern, M. Grundmann / *Handbook of Zinc Oxide and Related Materials*, Vol. 2 Devices and Nano-Engineering, Chapter 11, Z.C. Feng, ed. (Taylor and Francis/CRC Press, Florida, USA, 2011), ISBN 978-1439855744
- ⇒ *Oxide Thin Film Heterostructures on Large Area, with Flexible Doping, Low Dislocation Density and Abrupt Interfaces – Grown by Pulsed Laser Deposition*
M. Lorenz, H. Hochmuth, C. Grüner, H. Hilmer, A. Lajn, D. Spemann, M. Brandt, J. Zippel, R. Schmidt-Grund, H. von Wenckstern, M. Grundmann / *Laser Chemistry* (2011) (Hindawi, New York, 2011) 2011 140976



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

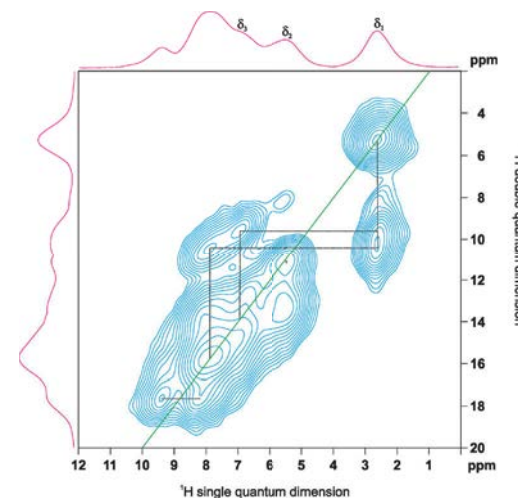
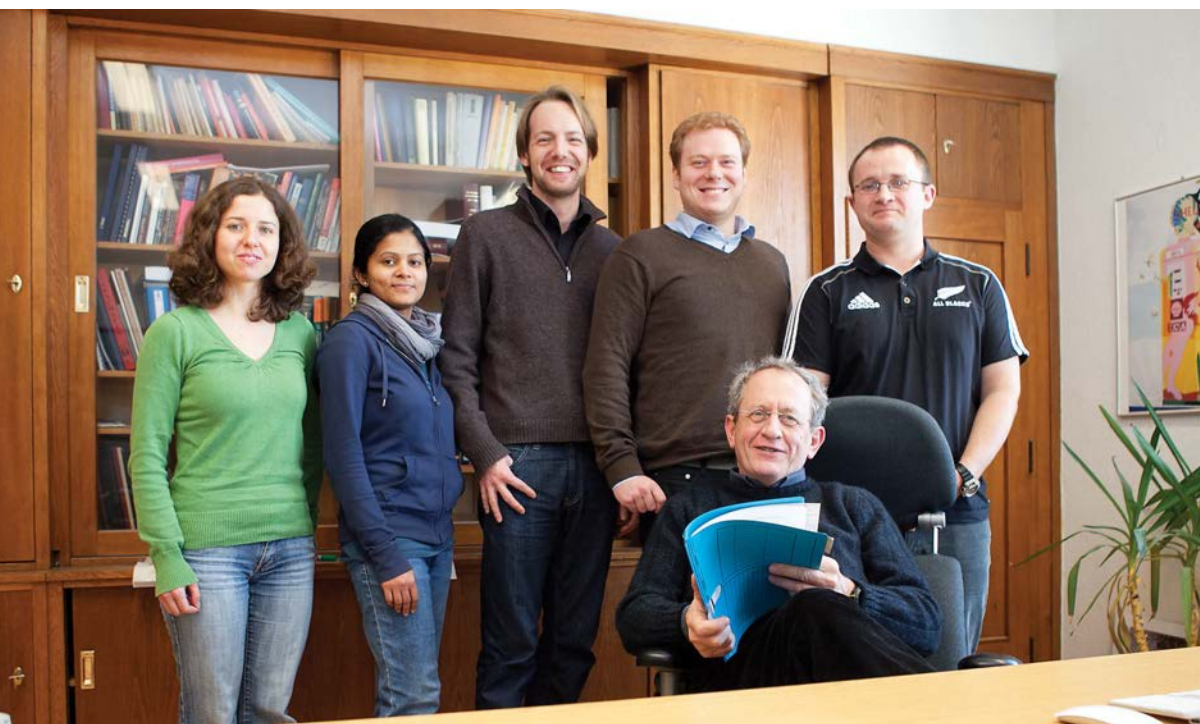
Electronic and chemical structure of modern materials investigated with magnetic resonance

Prof. Dr. Jürgen Haase

M.Sc. Phys. Nataliya Georgieva, M.Sc. Phys. Michael Jurkutat, Dipl.-Phys. Jonas Kohlrutz, M.Sc. Appl. Chem. Anusree Viswanath Kuttatheyil, Dipl.-Phys. Benno Meier

We investigate the electronic properties of quantum materials, as well as the chemical properties of porous media. Of particular current interest are, e.g. high-temperature superconductors and metal organic frameworks (MOFs). These systems have great potential for energy applications as conductors and storage materials. Our group employs predominantly Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR), in particular under extreme conditions, since these are necessary to influence the electronic structure of materials and thus enable us to learn about new states of electronic matter and structural changes. Here the group is world-wide leading.

NMR at the highest magnetic fields (up to 100 Tesla), is developed in cooperation with the Helmholtz Zentrum Dresden Rossendorf and at the highest pressures



2D ^1H SQ-DQ BABA correlation spectra of the MOF, $\text{Zn}(\text{Me}-3\text{py-trz-pba})_2$, recorded at a spinning frequency of 30 kHz

in Leipzig (it originated in a collaboration with the Cavendish Laboratory). Key findings concern two-component physics of high-temperature superconductivity, Lifshitz transitions of the Fermi surface in metals induced by extreme pressures, and characterisation of the local electronic structure metal ions in MOFs.

⇒ NMR Signal Averaging in 62 T Pulsed Fields

B. Meier, S. Greiser, J. Haase, T. Herrmannsdörfer, F. Wolff-Fabris / Journal of Magnetic Resonance (2011) **210** 1

⇒ ^{63}Cu Nuclear Magnetic Resonance Study of $\text{Pr}_{1.85}\text{Ce}_{0.15}\text{Cu}_{1-x}\text{Ni}_x\text{O}_4$: Ni-induced Spin Density Oscillation and Modification of the Low Energy Spin Fluctuations

G.V.M. Williams, M. Jurkutat, D. Rybicki, J. Haase / Journal of Physics: Condensed Matter (2011) **23** 075701

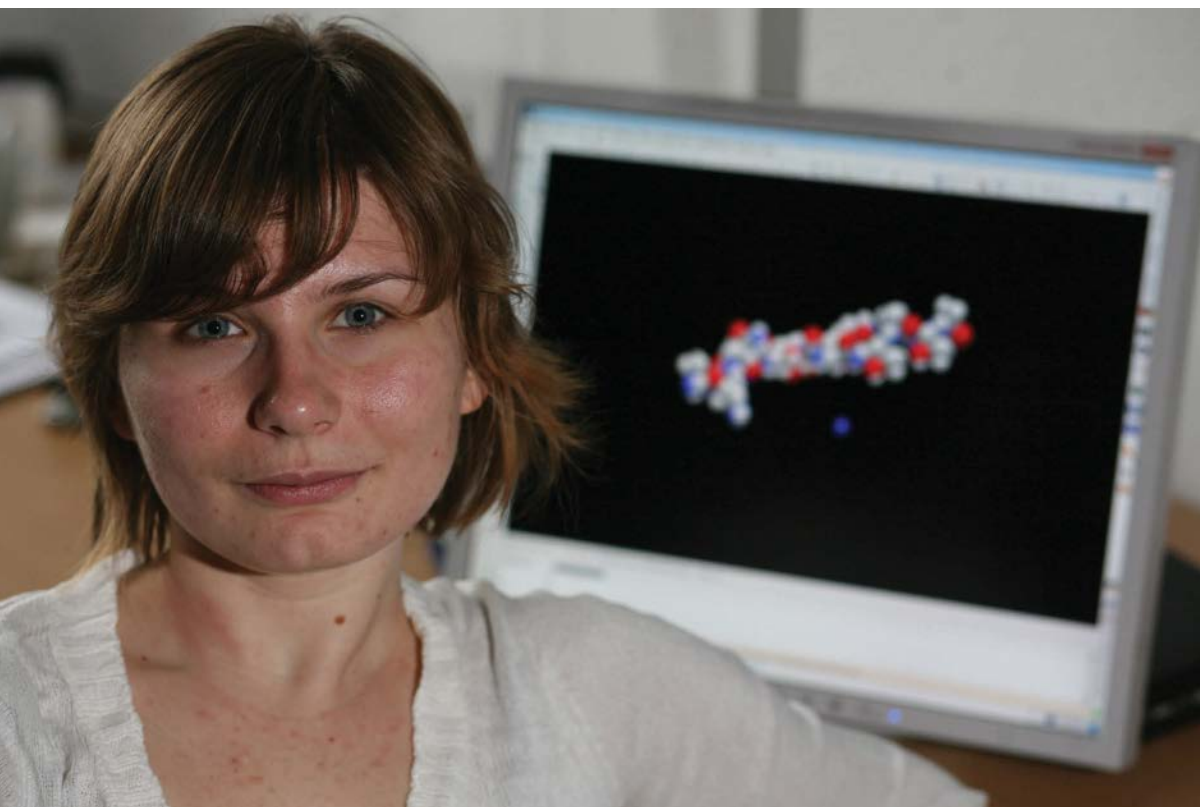
Prof. Dr. Jürgen Haase
Institute for Experimental Physics II
<http://www.uni-leipzig.de/~mqf/>
E-mail: j.haase@physik.uni-leipzig.de
Phone: +49 341 97-32601
Fax: +49 341 97-32649

Multiscale modelling of solvent effects in biomolecular systems

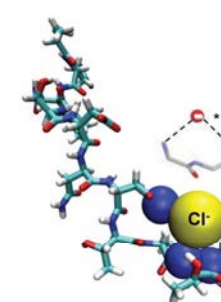
Prof. Dr. Dr. h.c. Wolfgang Hackbusch

M.Sc. Chem. Anastacia Romanova

Our research focus lies at the interface between advanced numerical mathematics and computational molecular sciences. Applying novel modelling techniques to problems in bio and nano sciences we study solvent effects on biologically related molecules. In particular we are interested to understand how solvent components affect molecular structure of peptides, molecule solubility, chemical activity and protein adhesion at interfaces. The effect of the surrounding medium exhibits its influence on biomolecular systems on largely different time and length scales. In order to approach such multiscale phenomena we are developing new theoretical and numerical tools for efficient computation of solvation phenomena on multiple scales. Biological systems require a precise treatment of a large number of weak interactions in order to capture the aggregate effect.

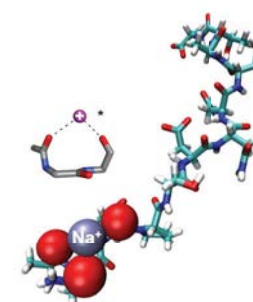


Nests bind anionic atoms



Nest-like bound to Cl⁻

Niches bind cationic atoms



Niche-like bound to Na⁺

*Torrance G. M. et al. J. Mol. Biol. 385 2009, 1076-1090

↑ Ion binding to peptide

Therefore numerical methods efficiently handling large amounts of data are required, which at the same time guarantee a predefined numerical precision. The new methods involve molecular integral equations, molecular dynamics and employ adaptive numerical schemes.

⇒ *Ion Effects on Biomolecule Conformation and Complex Formation in Waters*

M.V. Fedorov, A. Frolov, A.O. Romanova, K. Kirchner, I.V. Terekhova / Abstracts of papers of the American Chemical Society (2011) **241** 317-COMP

⇒ *Effects of Salts on Carbon Nanotubes Dispersions: Understanding Molecular Mechanisms*

A. Frolov, R.N. Arif, A.O. Romanova, A.G. Rozhin, M.V. Fedorov / Abstracts of papers of the American Chemical Society (2011) **242** 245-COLL

⇒ *Ion Effects on α-Cyclodextrin-aromatic Carboxylic Acids in Aqueous Solution : Molecular Mechanisms*

A.O. Romanova / Abstracts of papers of the American Chemical Society (2011) **242** 59-AEI

⇒ *Counter-ion Effects on Ionizable Biomolecules in Aqueous Electrolyte Solutions: Understanding Molecular Mechanisms*

A.O. Romanova, A. Frolov, M.V. Fedorov / Abstracts of papers of the American Chemical Society (2011) **242** 396-COLL

Prof. Dr. Dr. h.c. Wolfgang Hackbusch
Max Planck Institute for Mathematics in the Sciences
<http://www.mis.mpg.de/scicomp/>
E-mail: wh@mis.mpg.de
Phone: +49 341 9959-752
Fax: +49 341 9959-999

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

Prof. Dr. Evamarie Hey-Hawkins

M.Sc. Chem. Solveig Boehnke, M.Sc. Chem. René Frank, M.Sc. Chem. Anne Grundmann, Dipl.-Chem. Julia Haushälter, Dr. Aslihan Kircali, M.Sc. Chem. Anika Kreienbrink, M.Sc. Chem. Martyna Madalska, M.Sc. Chem. Tobias Möller, M.Sc. Chem. Paul Neumann, M.Sc. Chem. Wilma Neumann, M.Sc. Chem. Souvik Pandey, M.Sc. Chem. Julian Pritzwald-Stegmann, Dipl.-Chem. Stefan Richter, Dr. Matthias Scholz, M.Sc. Chem. Markus Streitberger

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

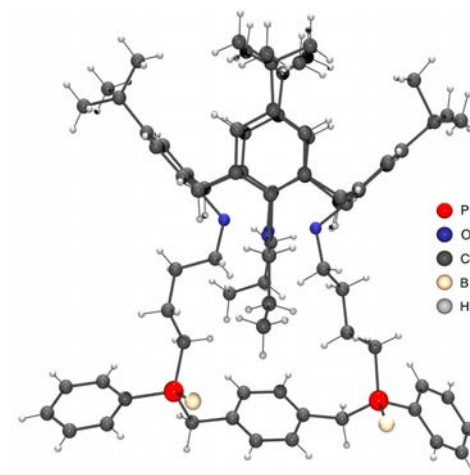
Smart Catalysts: Phosphorus-based ligands play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups (ferrocene, aromatics, heterocycles, etc.) to modify their donor-acceptor properties



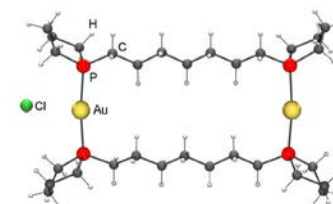
in situ (i.e. electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way “switchable” phosphines for catalytic applications (M. Madalska, P. Neumann). Furthermore, electron-poor *ortho*-carbaboranyl clusters are employed as highly hydrophobic C₂ backbones.

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

From Molecules to Novel Material: Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of functionalised building blocks for organometallic or phosphorus-based polymers are: terminal phosphinidene complexes [LnM=PR] (A. Grundmann), strained inorganic (A. Kreienbrink)



↑ Calix[4]arene-based bis-phosphine container molecule

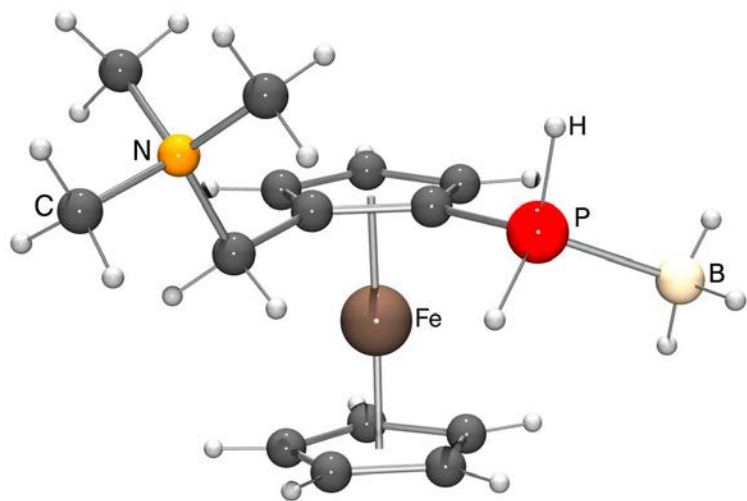


↑ Gold(I)-based nano-frame of 1,7-bis(1-phospholano)heptane

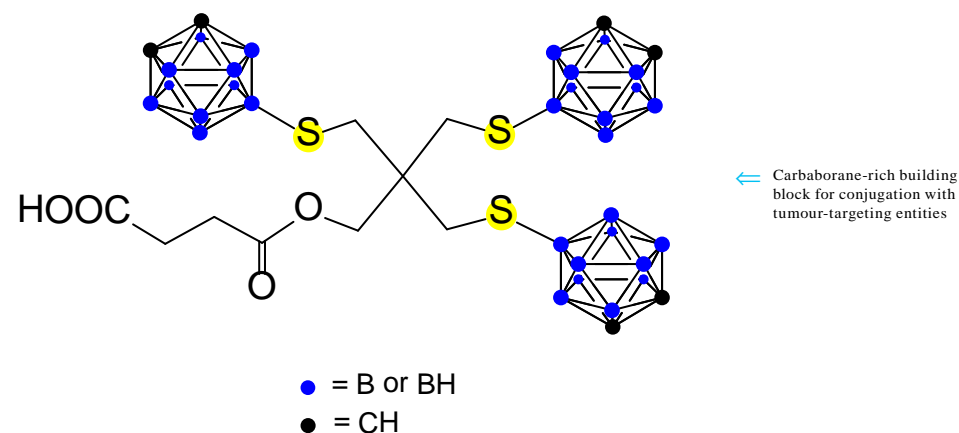
or organic (T. Möller) phosphorus-based rings, or planar-chiral ferrocenylphosphinoboranes (S. Pandey).

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

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



↑ Chiral ferrocenylphosphinoborane as molecular building block for chiral ionic polymers (only the ammonium cation is shown, iodide omitted)



- ⇒ *Asborin Inhibits Aldo/Keto Reductase 1A1*
M. Scholz, M. Steinhagen, J.T. Heiker, A.G. Beck-Sickinger, E. Hey-Hawkins / ChemMedChem (2011) **6** 89
- ⇒ *Pnicogen Bonds: A New Linker for Supramolecular Chemistry?*
S. Zahn, R. Frank, E. Hey-Hawkins, B. Kirchner / Chem. Europ. J. (2011) **17** 6034
- ⇒ *Carboranes as Pharmacophores: Similarities and Differences between Aspirin and Asborin*
M. Scholz, G.N. Kaluderović, H. Kommera, R. Paschke, J. Will, W.S. Sheldrick, E. Hey-Hawkins / Eur. J. Med. Chem. (2011) **46** 1131
- ⇒ *Making and Breaking of P–P bonds with Low-valent Transition Metal Complexes*
S. Gómez-Ruiz, R. Frank, B. Gallego, S. Zahn, B. Kirchner, E. Hey-Hawkins / Europ. J. Inorg. Chem. (2011) 739
- ⇒ *Incorporation of ortho-Carboranyl- N_ϵ -modified L-Lysine into Neuropeptide Y Receptor Y_1 - and Y_2 -Selective Analogues*
V.M. Ahrens, R. Frank, S. Stadlbauer, A.G. Beck-Sickinger, E. Hey-Hawkins / J. Med. Chem. (2011) **54** 2368
- ⇒ *Synthesis and Evaluation of Carborane Derivatives of Indomethacin as Cyclooxygenase Inhibitors*
M. Scholz, A.L. Blobaum, L.J. Marnett, E. Hey-Hawkins / Bioorg. Med. Chem. (2011) **19** 3242
- ⇒ *Carboranes as Pharmacophores: Properties, Synthesis, and Application Strategy*
M. Scholz, E. Hey-Hawkins / Chem. Rev. (2011) **111** 7035
- ⇒ *Carborane-Substituted 1,2-Diphosphetanes*
A. Kreienbrink, M.B. Sárosi, E. Rys, P. Lönnecke, E. Hey-Hawkins / Angew. Chem. (2011) **123** 4798; Angew. Chem. Int. Ed. (2011) **50** 4701; featured in: R.C. Fischer, J.J. Weigand / "Trendbericht Anorganische Molekülchemie 2011", Nachr. Chem. (2012) **60** 216

Prof. Dr. Evamarie Hey-Hawkins
Institute of Inorganic Chemistry
<http://www.uni-leipzig.de/chemie/hh/>
E-mail: hey@rz.uni-leipzig.de
Phone: +49 341 97-36151
Fax: +49 341 97-39319

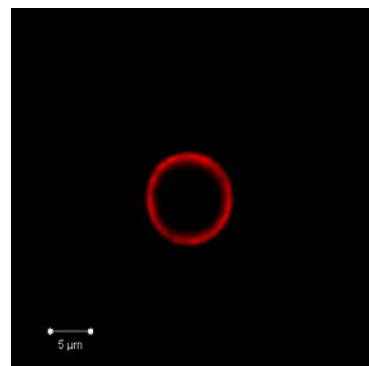
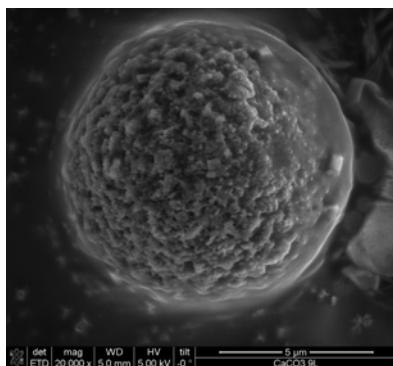
Surface functionalisation of layer-by-layer coated colloidal microcarriers for specific cell uptake

Prof. Dr. Daniel Huster

Dipl.-Phys. Martin-Patrick Göse

The modular construction of Layer-by-Layer (LbL) biopolymer coated microparticles and capsules offer the opportunity to design novel multifunctional drug delivery systems achieving a local, low-dose and time-controlled application of therapeutics into the desired tissue.

Martin Göse focuses his research on the functionalisation of the carrier surface to develop an LbL drug delivery system for a specific carrier / cell interaction with emphasis placed on high biocompatibility. Therefore, a phospholipid bilayer has to be assembled as outermost layer on top of a biocompatible polymer multilayer containing active agents. The integration of a PEG-biotinylated lipid into the lipid bilayer will reduce unspecific cell interaction as well as allow a further surface functionalisation with specific antibodies via streptavidin-biotin binding.



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

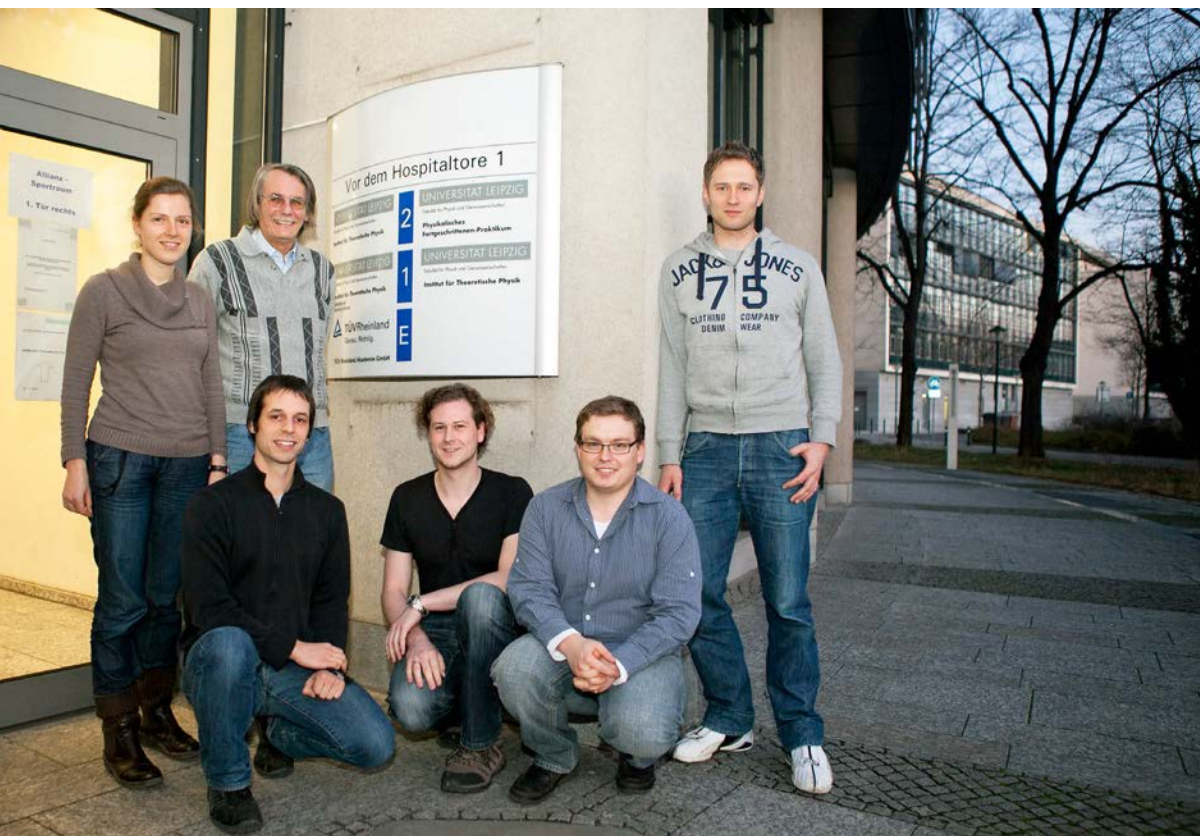
↑ SEM (left) and CLSM (right) images of CaCO_3 microparticles coated with a biopolymer multilayer containing 9 layers protamine sulfate and dextran sulfate; the red fluorescence (right) is based on three layers RITC-labelled PRM as multilayer constituent

Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke

Dipl.-Phys. Niklas Fricke, Dipl.-Phys. Martin Marenz, Dipl.-Phys. Monika Möddel,
Dipl.-Phys. Sebastian Schöbl, Dipl.-Phys. Micha Wiedenmann,
M.Sc. Phys. Johannes Zierenberg

The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on several interrelated subprojects. In all projects, the employed methodology relies mainly on sophisticated Monte Carlo computer simulations based on multicanonical ensembles, parallel tempering techniques and chain-growth algorithms with population control, quantum Monte Carlo simulations based on stochastic series expansions, and thermostated Molecular Dynamics methods, which are adapted by us to the problems at hand and constantly further



improved in order to cope with the complexity of the considered problems:

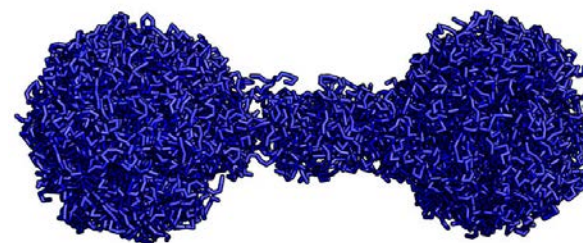
Monika Möddel employs Monte Carlo computer simulations in generalised ensembles for investigations of the conformational mechanics of polymer adsorption transitions and the associated structure formation at attractive, patterned solid substrates.

Sebastian Schöbl and Johannes Zierenberg use chain-growth algorithms and multicanonical simulation methods to explore the conformational statistics of polymers in disordered environments. This is important for a basic understanding of, e.g. the universal properties of the cycloskeleton investigated by several other BuildMoNa groups.

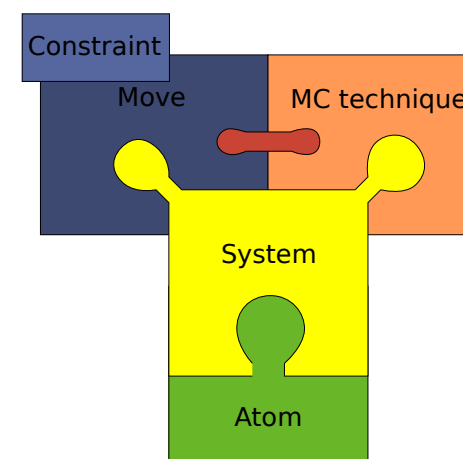
Micha Wiedenmann investigates condensation phenomena at the liquid-gas or solid-gas coexistence described by a simplified lattice gas model, which are of relevance for aggregation processes in general.

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

Martin Marenz aims at developing a tool box ("framework") for multi-scale



← Overlay of 1000 steps using the Monte Carlo simulations framework of a polymer in a barbell confinement



← The five building blocks of our Monte Carlo simulations framework

Monte Carlo computer simulations of mesoscopic and atomistic models of polymers in confined geometries or interacting with a solid substrate. Similar to our previous studies of a generic bead-stick polymer model, the adsorption propensity and structure formation are in the focus of interest.

Niklas Fricke developed a novel renormalisation group inspired complete enumeration method to study the properties of simple polymers modeled by self-avoiding random walks in a disordered environment realised by a percolation cluster. Our method makes it possible to enumerate walks of 1000 steps in a couple of minutes which with standard techniques would take over 10^{170} years.

⇒ *Advanced Multicanonical Monte Carlo Methods for Efficient Simulations of Nucleation Processes of Polymers*

S. Schnabel, W. Janke, M. Bachmann / *Journal of Computational Physics* (2011) **230** 4454

⇒ *Adsorption of Finite Polymers in Different Thermodynamical Ensembles*

M. Möddel, W. Janke, M. Bachmann / *Computer Physics Communications* (2011) **182** 1961

⇒ *Comparison of the Adsorption Transition for Grafted and Non-Grafted Polymers*

M. Möddel, W. Janke, M. Bachmann / *Macromolecules* (2011) **44** 9013

⇒ *Simulating Flexible Polymers in a Potential of Randomly Distributed Hard Disks*

S. Schöbl, J. Zierenberg, W. Janke / *Physical Review E* (2011) **84** 051805

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

From nanometre polymers to microscopic cells – The role of entropic forces in actin network formation

Prof. Dr. Josef Alfons Käs

Dipl.-Phys. Anatol Fritsch, M.Sc. Phys. Markus Gyger, Dipl.-Phys. Chris Händel, Dipl.-Phys. Tina Händler, Dipl.-Phys. Florian Huber, Dipl.-Phys. Tobias Kießling, Dipl.-Math. Melanie Knorr, M.Sc. Phys. David K. Nnetu, Dipl.-Phys. Steve Pawlizak, M.Sc. Phys. Susanne Rönicke, Dipl.-Phys. Jörg Schnauß, Dipl.-Phys. Carsten Schuldt, Dipl.-Phys. Dan Strehle, Dipl.-Phys. Franziska Wetzel

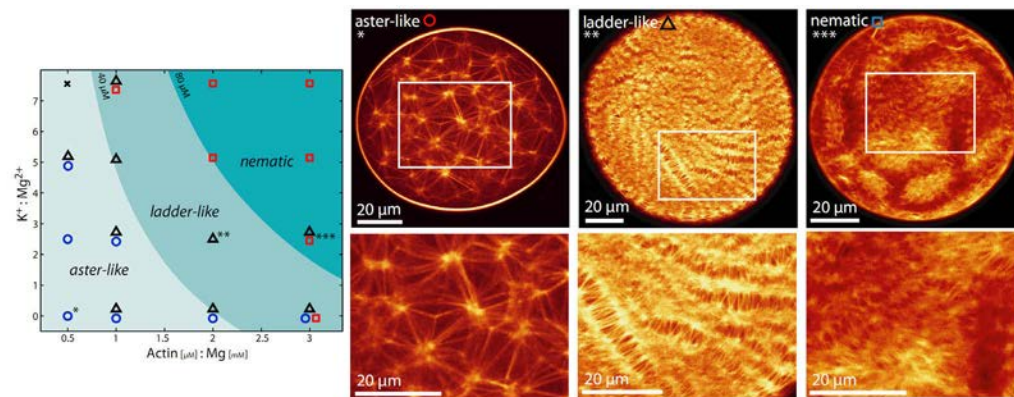
Biopolymer networks contribute mechanical integrity as well as functional organisation to living cells. The protein actin is one of the major constituents of those structures and was found to be present in a large variety of different network architectures ranging from extensive networks to densely packed bundles or fibers.

BuildMoNa students of the Käs group developed a reduced experimental bot-



tom-up system to study the formation of confined actin networks by entropic forces. Experiments based on molecular crowding and counterion condensation allow separating mixing effects from cross-linking effects. This reveals a very general tendency of homogeneous filament solutions to aggregate into regular actin bundle networks connected by aster-like centres. Drastic changes in network architecture directly follow from filament ordering or from flow-induced perturbations of the system.

Complemented by coarse-grained modeling the experiments suggest that regular bundle networks might be a rather general feature of isotropic, homogeneous filament solutions subject to uniform attractive interactions. Due to the fundamental nature of the interactions considered, further severe consequences or restrictions to cytoskeletal network formation on the more complex level of living cells are expected and the aim of future work.



↑ Phase diagram of actin structures; observed network structures are marked by circles, triangles and squares with typical examples of aster-like, ladder-like and nematic structures, respectively, shown on the right; the shading boundaries in the diagram refer to actin concentrations of 40 and 80 μM which correspond to the onset of partial and nematic alignment in F-actin solutions



- ⇒ *Calcium Imaging in the Optical Stretcher*
M. Gyger, D. Rose, R. Stange, T. Kießling, M. Zink, B. Fabry, J.A. Käs / Optics Express (2011) **19** 19212
- ⇒ *Single Cell Viability and Impact of Heating by Laser Absorption*
F. Wetzel, S. Röncke, K. Müller, M. Gyger, D. Rose, M. Zink, J. Käs / European Biophysics Journal (2011) **40** 1109
- ⇒ *Self-regulative Organization of the Cytoskeleton*
F. Huber, J. Käs / Cytoskeleton (2011) **68** 259
- ⇒ *Stochastic Actin Dynamics in Lamellipodia Reveal Parameter Space for Cell Type Classification*
M. Knorr, D. Koch, T. Fuhs, U. Behn, J.A. Käs / Soft Matter (2011) **7** 31923
- ⇒ *Oscillations in the Lateral Pressure of Lipid Monolayers Induced by Nonlinear Chemical Dynamics of the Second Messengers MARCKS and Protein Kinase C*
S. Alonso, U. Dietrich, C. Händel, J.A. Käs, M. Bär / Biophysical Journal (2011) **100** 939
- ⇒ *Robust Organization Principles of Protrusive Biopolymer Networks in Migrating Living Cells*
B. Stuhmann, F. Huber, J.A. Käs / PLoS ONE (2011) **6** e14471

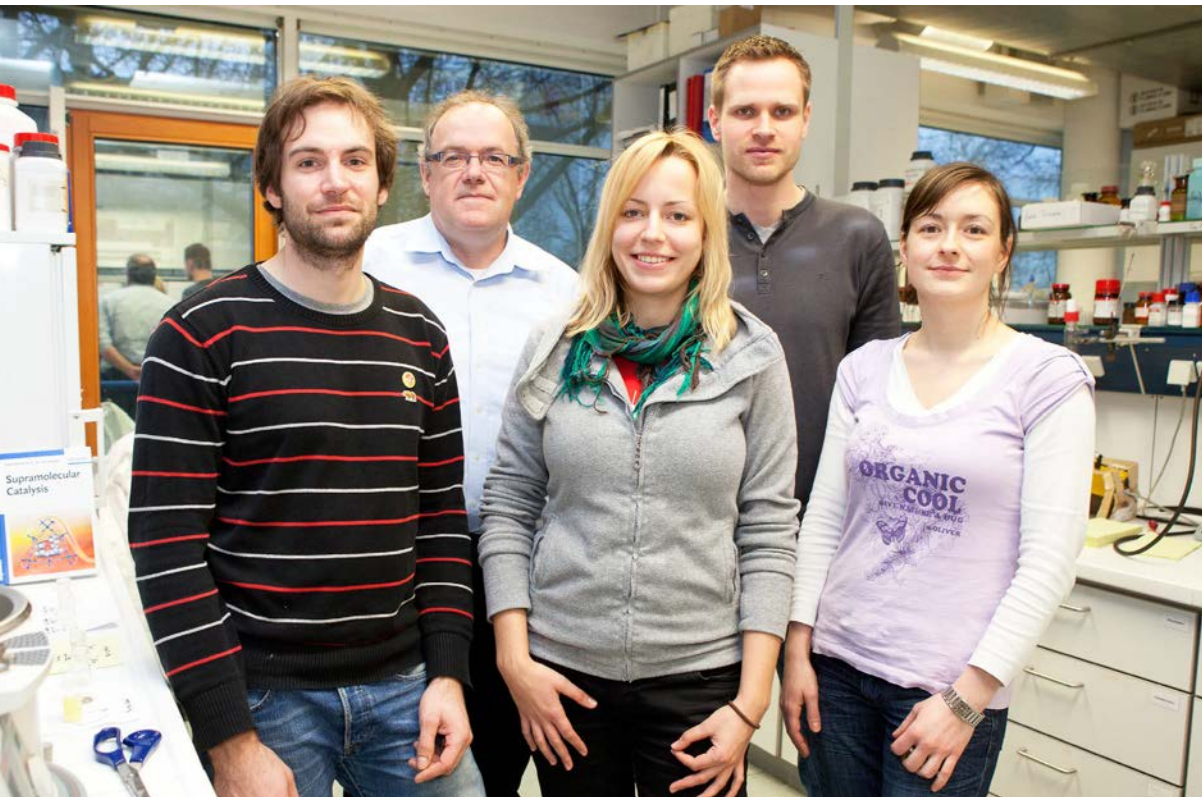
Prof. Dr. Josef Alfons Käs
Institute for Experimental Physics I
<http://www.softmatterphysics.com>
E-mail: jkaes@physik.uni-leipzig.de
Phone: +49 341 97-32471
Fax: +49 341 97-32479

Coordination compounds in supramolecular chemistry and materials chemistry

Prof. Dr. Berthold Kersting

M.Sc. Chem. Matthias Golecki, M.Sc. Chem. Sina Gruschinski, Dipl.-Chem. Jochen Lach, Dr. Ulrike Lehmann, Dipl.-Chem. Ronny Syre

The project “Molecular Magnetism” deals with the development, synthesis and characterisation of novel classes of molecular based magnetic materials. The compounds are characterised by their modular nature, which allows a rational construction of magnetic materials. Particular attention is paid to a basic understanding and the control of magnetic behaviour of polynuclear transition metal complexes. The results are used for the development of polynuclear or polymeric coordination compounds, whose magnetic properties are defined by their constituent building blocks. The research deals with several aspects, as for instance: Synthesis of High-Spin Molecules and Single Molecule Magnets and Deposition of High-Spin-Molecules

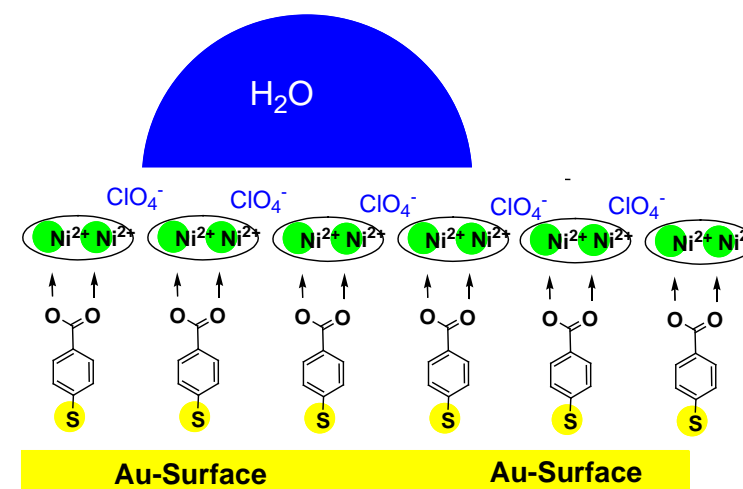


on Surfaces.

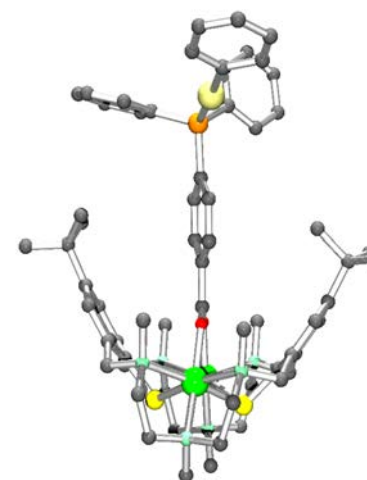
An important goal is the deposition of paramagnetic (high-spin) molecules on surfaces. One aim was to link paramagnetic molecules via ambidentate ligands to a gold surface, as sketched below.

Preliminary contact angle measurements show clear variation of the contact angle, indicating that the complexes bind to the gold surface.

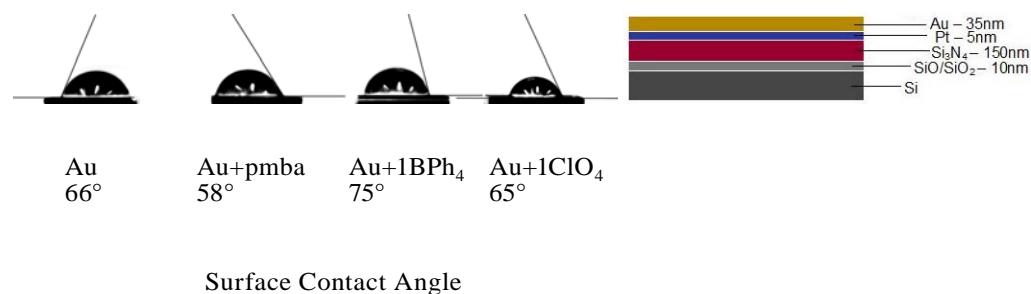
The research activities are also focused on fundamental research at the interface of supramolecular chemistry and nanochemistry with special emphasis on the synthesis of multicomponent nanospheroid assemblies. A key feature is the use of



↑ Formation of a selfassembled monolayer of paramagnetic Ni_2 -complexes with soft SH (1) or PPh_2 (2) functions for attachment to the Au surface



← Molecular structure of a paramagnetic Ni_2Au complex $[\text{LNi}_2-\mu\text{O}_2\text{CC}_6\text{H}_4\text{PPh}_2-\text{AuC}_6\text{H}_5]\text{BPh}_4$ (3BPh₄)



↑ The substrates were immersed in a CH₂Cl₂ solution of free thiol or Ni(II)₂ complex (for at least 12 h) to ensure covalent Au-S bond formation

self-complementary building blocks (e.g. porphyrins, calixarenes, cyclodextrines) which assemble under template-control into hollow nanosized architectures. Possible applications range from storage/slow release of compounds to synthesis of quantum dots (e.g. semiconducting CdTe, GaAs, or metallic Au, Ag) and nanoscale reaction vessels. The size and shape of the assemblies can be controlled by the size of the building blocks, to influence the optical, electronical and magnetic properties of the immobilised particles.

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

Development of novel approaches for the investigation of complex systems

Prof. Dr. Barbara Kirchner

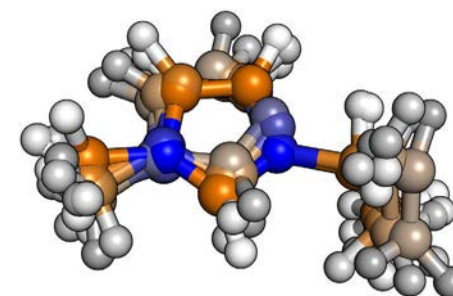
M.Sc. Chem. Martin Brehm, M.Sc. Chem. Eva Perl

For the understanding of complex systems a detailed knowledge on very small time and length scales is required. In that content we are working on two main research areas:

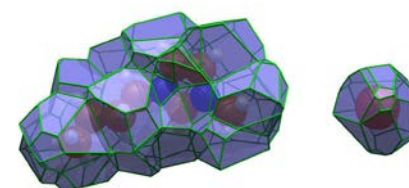
The first is concerned with carrying out ab initio molecular dynamics simulations and with the analysis of the obtained data. The gain of information of these trajectories, especially the reduction of the number of dimensions and the visualisation of the data, are demanding tasks. Therefore, the program package TRAVIS has been developed by Martin Brehm. Although already offering a huge number of possibilities, the program is still improved and extended by further analyses. It has been applied to various studies, most of them dealing with ionic liquids. A second project deals with the implementation of a quantum chemistry code in order to develop alternative optimisation schemes at the molecular level. In the future, this



quantum chemistry code may be embedded into a molecular dynamics program so that these novel approaches may to some extent be applicable to ab initio molecular dynamics simulations. Another approach to apply high-level electronic structure calculations to fluid phases, the Quantum-Cluster-Equilibrium theory, is studied by Eva Perlth.



Temporal development of a selected [Emim] cation in bulk phase



Voronoi cell around one [Bmim] cation and one [Br] anion cut from a bulk phase molecular dynamics simulation

- ⇒ *Singular Value Decomposition for Analyzing Temperature- and Pressure-Dependent Distribution Functions: Decomposition into Grund RDFs (GRDFs)*
Ph.J. di Dio, M. Brehm, B. Kirchner / Journal of Chemical Theory and Computation (2011) **7** 15280
- ⇒ *TRAVIS – A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories*
M. Brehm, B. Kirchner / Journal of Chemical Information and Modeling (2011) **51** 2007
- ⇒ *Ab initio Molecular Dynamics Simulations of a Binary System of Ionic Liquids*
M. Brüssel, M. Brehm, T. Voigt, B. Kirchner / Physical Chemistry Chemical Physics (2011) **13** 13617
- ⇒ *Performance of Quantum Chemically Derived Charges and Persistence of Ion Cages in Ionic Liquids. A Molecular Dynamics Simulation Study of 1-n-Butyl-3-methylimidazolium Bromides*
M. Kohagen, M. Brehm, J. Thar, W. Zhao, F. Müller-Plathe, B. Kirchner / The Journal of Physical Chemistry B (2011) **115** 693
- ⇒ *Binary Systems from Quantum Cluster Equilibrium Theory*
M. Brüssel, E. Perlth, S.B.C. Lehmann, M. v. Domaros, B. Kirchner / The Journal of Chemical Physics (2011) **135** 194113
- ⇒ *Importance of Structural Motifs in Liquid Hydrogen Fluoride*
E. Perlth, J. Friedrich, M. v. Domaros, B. Kirchner / ChemPhysChem (2011) **12** 3474

Prof. Dr. Barbara Kirchner
 Wilhelm Ostwald Institute for Physical
 and Theoretical Chemistry
<http://www.uni-leipzig.de/~quant/>
 E-mail: bkirchner@uni-leipzig.de
 Phone: +49 341 97-36401
 Fax: +49 341 97-36399

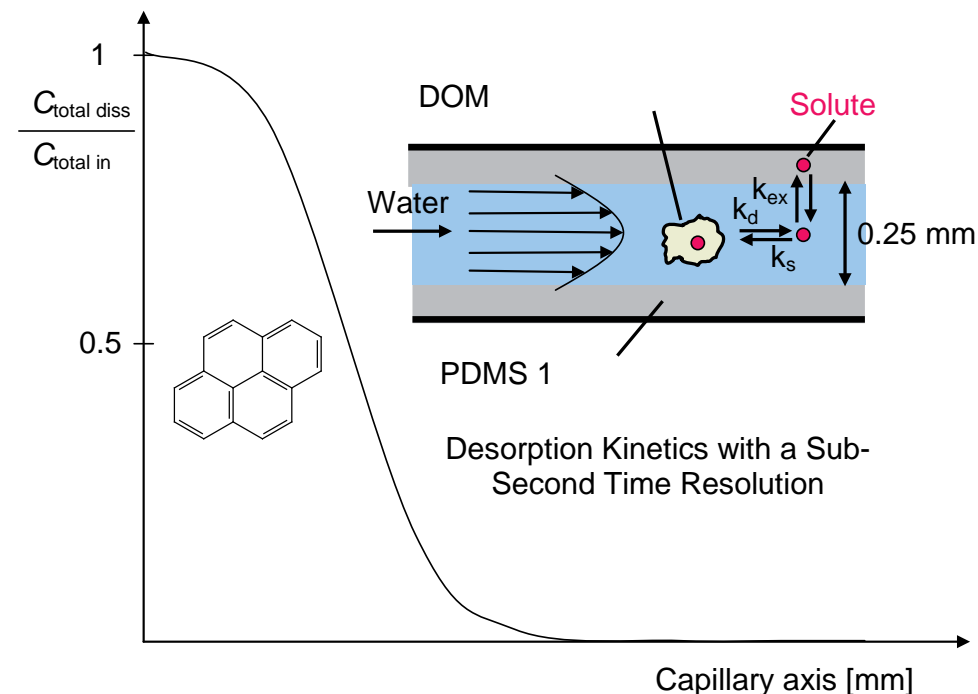
Nano-catalysts for water treatment – nano-catalysis in water

Prof. Dr. Frank-Dieter Kopinke

M.Sc. Chem./Environ. Prot. Ksenia J. Ramus, M.Sc. Chem. Klara Rusevova,
Dipl.-Phys. Jens Schneider

Ksenia Ramus has accomplished her doctoral work on “Influence of Dissolved Organic Matter on the Availability of Organic Compounds: Desorption and Mass Transfer Kinetics”. She wrote a cumulative work on the basis of three papers in highly ranked international journals. The highlight of this work is the development of a new experimental technique – time-resolved in-tube solid phase micro-extraction (TR-IT-SPME) – which is able to measure sorption-desorption-kinetics between any hydrophobic target analytes and colloidally dissolved sorbents such as humic colloids or surfactant micelles in the sub-second time scale.

Klara Rusevova is presently in the final stage of her doctoral work on a new type of nano-catalysts for wet oxidation in water, nano-Perovskites. The figure shows

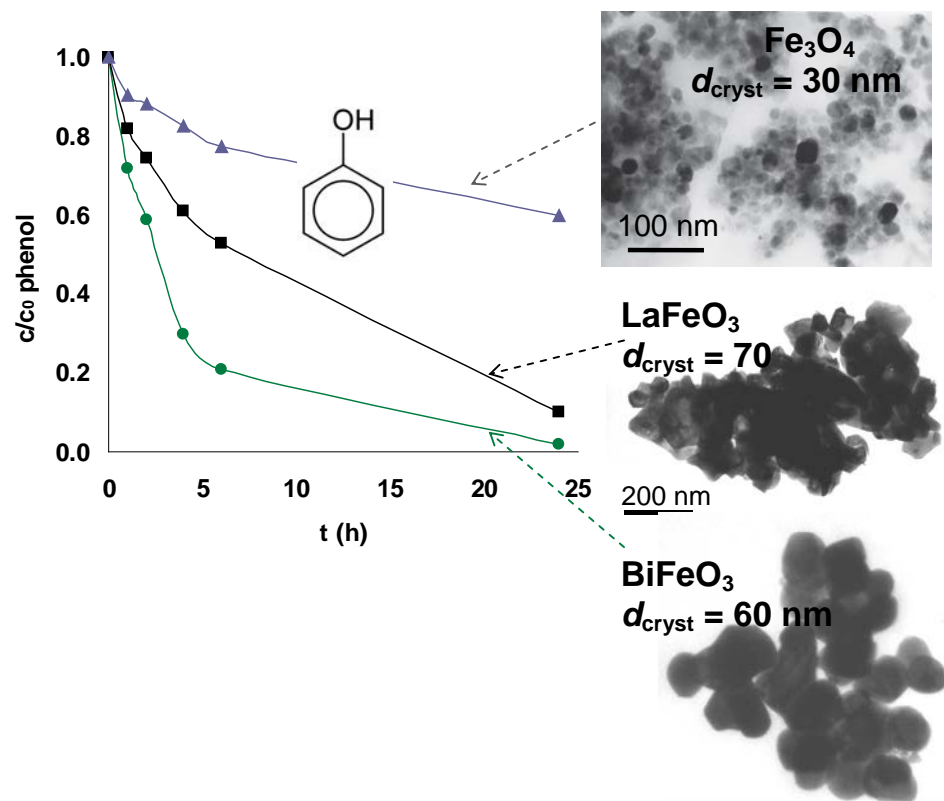


↑ Schematic presentation of the TR-IT-SPME technique for measuring sorption-desorption kinetics in the sub-second time scale



kinetics of phenol oxidation in the presence of three different nano-catalysts. The synthesised nano-Perovskites are clearly superior to the commercial material nano-Magnetite.

Jens Schneider has accomplished his doctoral work with the title “Untersuchungen zur Dissoziation von Wasser durch Einwirkung hochfrequenter elektromagnetischer Felder” in the traditional way, i.e. as a comprehensive monography. He is presently busy with preparing scientific publications on the basis of his doctoral work. The investigated phenomenon which we call “burning water” is not only new. It opens a thrilling perspective on a non-conventional water chemistry.



↑ Oxidation of phenol as a pollutant in neutral aqueous suspension with H_2O_2 at ambient temperature catalysed by three different catalysts: Magnetite and two Perovskites ($C_{\text{cat}} = 0.1$ g L^{-1} , $C_{\text{H}_2\text{O}_2,0} = 3$ g L^{-1} , $C_{\text{phenol},0} = 25$ mg L^{-1})

Prof. Dr. Frank-Dieter Kopinke
Centre for Environmental Research (UFZ)
<http://www.ufz.de/index.php?de=2529>
E-mail: frank-dieter.kopinke@ufz.de
Phone: +49 341 235-1234
Fax: +49 341 235-1471

Metal-organic frameworks – porous materials for gas storage and separation

Prof. Dr. Harald Krautscheid

B.Sc. Chem. Jorge Luis Cholula Díaz, M.Sc. Chem. Dirk Friedrich,
M.Sc. Chem. Marcel Handke, Dr. Daniel Lässig, M.Sc. Chem. Jörg Lincke

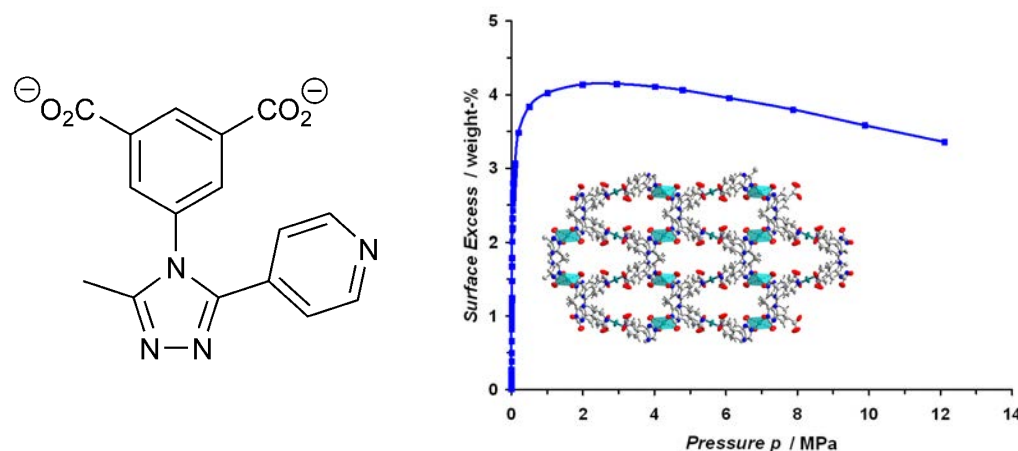
Metal-organic frameworks (MOFs) are a new class of organic-inorganic hybrid materials, in which metal ions are linked by polyfunctional organic ligands to microporous three-dimensional structures. Due to their porosity and their large inner surface these coordination polymers promise interesting applications based on adsorption (gas storage, gas separation and purification, sensorics) and in catalysis. For the synthesis of MOFs we are employing substituted triazolyl benzate linkers



since these ligands exhibit a rich coordination chemistry, provide stability against oxydants, and are prepared from cheap starting materials as many different derivatives.

As an example, the reaction of $\text{H}_2(\text{Me-4py-trz-ia})$ with copper sulfate yields $[\text{Cu}(\text{Me-4py-trz-ia})]$, that can be isolated as single crystals as well as microcrystalline powder in high yield. $[\text{Cu}(\text{Me-4py-trz-ia})]$ forms a flexible 3D coordination polymer with pts topology, a (calculated) porosity of 55 vol.-% and thermal stability up to 250 °C. Comprehensive adsorption studies with different adsorptives reveal remarkable features – the uptake of 9.2 mmol/g (40.5 wt.-%) for CO_2 at 273 K / 0.1 MPa and 15.2 mmol/g, (3.07 wt.-%) for H_2 at 77 K / 0.1 MPa are among the highest reported so far for MOFs. Furthermore, the potential of $[\text{Cu}(\text{Me-4py-trz-ia})]$ in gas separation could be demonstrated.

A second research project deals with the synthesis and properties of new molecular precursors for CuInSe_2 and related materials. These precursors are optimised to react to the desired chalcopyrite semiconductors as thin films at mild conditions in high selectivity. Because of their high absorption coefficients and suitable band gaps, thin layers (ca. 1 μm) of the chalcopyrites CuME_2 ($\text{M} = \text{Ga}, \text{In}; \text{E} = \text{S}, \text{Se}$) are applied in solar cells.



↑ The ligand $[\text{Me-4py-trz-ia}]^{2-}$ (left); 3D crystal structure of $[\text{Cu}(\text{Me-4py-trz-ia})]$ along [001] together with its H_2 adsorption isotherm (excess adsorption, 77 K; right)



- ⇒ *Synthesis and Structural Characterization of New Dinuclear Silver(I) Complexes: Different Coordination Modes of Substituted 1,2,4-Triazine Ligand*
F. Marandi, N. Hosseini, H. Krautscheid, D. Lässig, J. Lincke, M. Rafiee, Y.A. Asl / Journal of Molecular Structure (2011) **1006** 324
- ⇒ *NMR Studies of Benzene Mobility in Metal-Organic Framework MOF-5*
S. Hertel, M. Wehring, S. Amirjalayer, M. Gratz, J. Lincke, H. Krautscheid, R. Schmid, F. Stallmach / The European Physical Journal – Applied Physics (2011) **55** 20702/1 8
- ⇒ *A Microporous Copper Metal-Organic Framework with High H_2 and CO_2 Adsorption Capacity at Ambient Pressure*
D. Lässig, J. Lincke, J. Möllmer, C. Reichenbach, A. Möller, R. Gläser, G. Kalies, K.A. Cychosz, M. Thommes, R. Staudt, H. Krautscheid / Angewandte Chemie (2011) **123** 10528; Angewandte Chemie International Edition (2011) **50** 10344
- ⇒ *Unusual Adsorption Behavior of a Highly Flexible Copper-Based MOF*
C. Reichenbach, G. Kalies, J. Lincke, D. Lässig, H. Krautscheid, J. Moellmer, M. Thommes / Microporous and Mesoporous Materials (2011) **142** 592
- ⇒ *Synthesis, Crystal Structure, and Electron Paramagnetic Resonance Investigations of Heteronuclear Co^{II} / Zn^{II} and Co^{II} / Cd^{II} Coordination Polymers*
D. Lässig, J. Lincke, J. Griebel, R. Kirmse, H. Krautscheid / Inorganic Chemistry (2011) **50** 213
- ⇒ *A Novel Copper-based MOF Material: Synthesis, Characterization and Adsorption studies*
J. Lincke, D. Lässig, J. Moellmer, C. Reichenbach, A. Puls, A. Moeller, R. Gläser, G. Kalies, R. Staudt, H. Krautscheid / Microporous and Mesoporous Materials (2011) **142** 62

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

From glassy dynamics to colloidal drag effects – molecular physics on the nano-scale

Prof. Dr. Friedrich Kremer

Dr. Roxana-Giorgiana Ene, M.Sc. Phys. Ciprian-Ghiorgita Iacob,
Dipl.-Phys. Wilhelm Kossack, M.Sc. Phys. Ilya Semenov, Dipl.-Phys. Tim Stangner,
Dipl.-Phys. Martin Treß, Dipl.-Phys. Olaf Ueberschär, Dipl.-Phys. Carolin Wagner

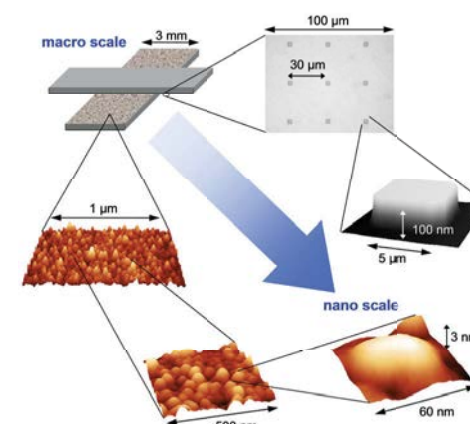
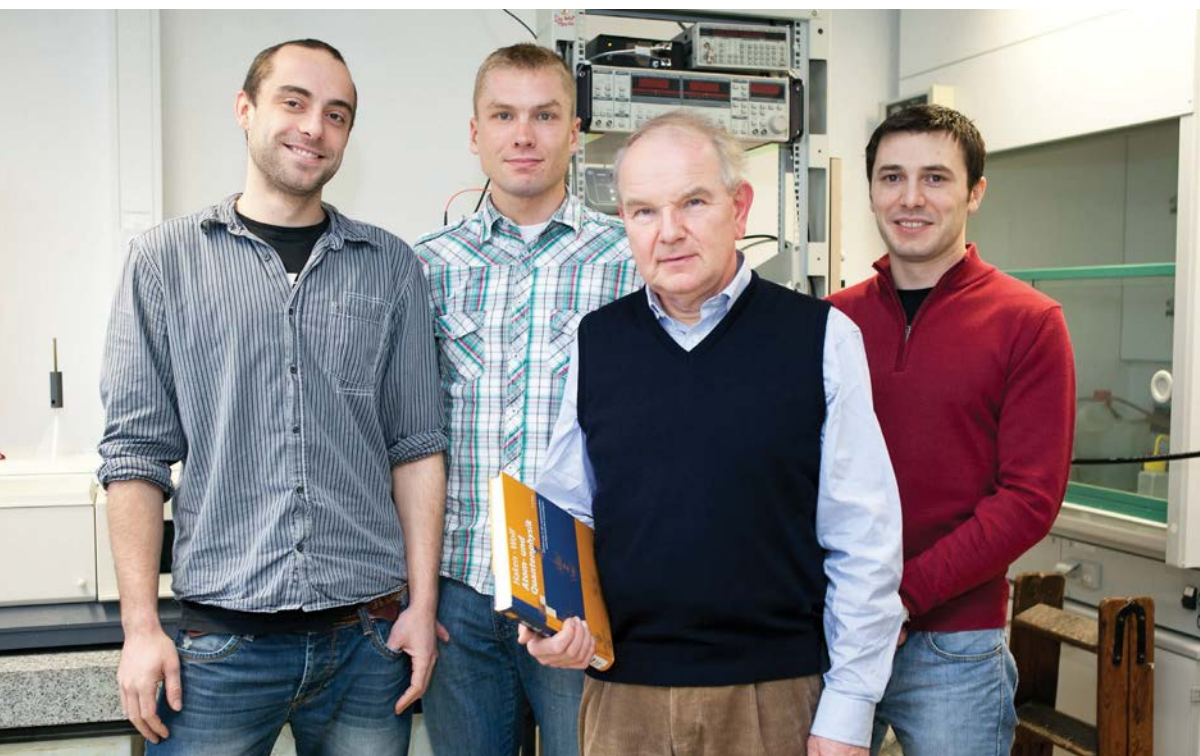
The infrared signature of glassy dynamics: Glassy dynamics reflects a continuous slowing down of molecular fluctuations in a glass forming system. Naturally, this macroscopic effect originates from the individual molecules and their interplay. To unravel the specific signature of a glass forming system we employed IR spectroscopy sensing intramolecular vibrations. Therefore, it is an ideal tool to trace back the glass transition to its microscopic basis by analyzing the temperature dependent spectral features of IR-absorption bands corresponding to the different molecular moieties.

Dynamic force spectroscopy on fluorescence-labeled tau-peptides and monoclonal antibodies: The combination of optical tweezers and dynamic force spectroscopy

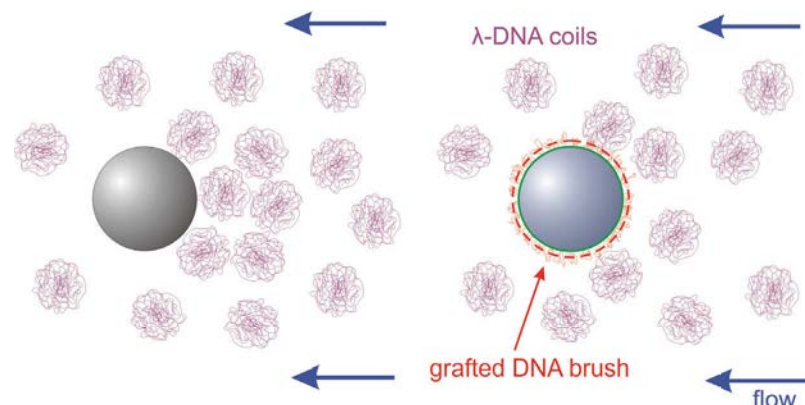
py is a promising approach to gain deep insight into biological systems on the level of single receptor-ligand-interactions. Here we report about the specific binding of an anti-human tau-monoclonal antibody (mAb), HPT-104, interacting with a synthetic fluorescence-labelled tau-peptide. Specific binding events between peptide and mAbs, obtained by dynamic force spectroscopy, are described according to the Dudko-Hummer-Szabo-model. A comparison between labelled and non-labelled tau-peptides and their interactions with mAbs shows that, due to the presence of the fluorescence dye, the bond lifetime and binding length is reduced.

Molecular dynamics of single polymer chains: For the first time, the glassy dynamics of randomly distributed, isolated poly(2-vinylpyridine) polymer coils is studied by means of Broadband Dielectric Spectroscopy (BDS). This is achieved by recently developed nano-structured electrode arrangements where isolated polymer coils are deposited onto ultra-flat, highly conductive silicon electrodes. Atomic Force Microscopy scans prove that the volume of the coils resembles the expected volume of a single chain. The observed dynamics reveals 2 fractions of segments: a fraction which is strongly retarded in its dynamics, possibly due to surface interactions and a bulk-like fraction which disappears not until the polymer coils fall below a certain size. Systematic analysis will enable us to give a certain length of this immobilising effect of the interfacial attraction.

Drag reduction by DNA-grafting for single microspheres in a dilute λ -DNA solution: The fluid resistance of single micrometre-sized blank and DNA-grafted polystyrene microspheres under shear flow is compared in purified water and dilute λ -DNA solutions by means of optical tweezers experiments with a high spatial (± 4 nm) and temporal (± 0.2 ms) resolution. The measurement results show that the drag experienced by a colloid in a dilute λ -DNA solution is significantly decreased if the microsphere bears a grafted DNA brush. The maximum extent of the drag reduction is found to amount to $(60 \pm 20)\%$ compared to the λ -DNA-induced contribution on the drag acting on blank colloids. We propose a theoretical explanation of



this effect, in particular, the solution of the Stokes equation for the studied system yields a numerical prediction that is found to be in full accord with our experimental results within measurement uncertainty.



⇒ *The Effective Hydrodynamic Radius of Single DNA-Grafted Colloids as Measured by Fast Brownian Motion Analysis*

O. Ueberschär, C. Wagner, T. Stangner, C. Gutsche, F. Kremer / *Polymer* (2011) **52** 1829

⇒ *DNA Condensation by TmHU Studied by Optical Tweezers, AFM and Molecular Dynamics Simulations*

C. Wagner, C. Olbrich, H. Brutzer, M. Salomo, U. Kleinekathöfer, U.F. Keyser, F. Kremer / *Journal of Biological Physics* (2011) **37** 117

⇒ *Micro-rheology on (Polymer-grafted) Colloids using Optical Tweezers*

C. Gutsche, M.M. Elmahdy, K. Kegler, I. Semenov, T. Stangner, O. Otto, O. Ueberschär, U.F. Keyser, M. Krüger, M. Rauscher, R. Weber, J. Harting, Y.W. Kim, V. Lobaskin, R.R. Netz, F. Kremer / *J. of Phys. Condensed Mater* (2011) **23** 184114

⇒ *Impact of Initial Solvent on Thermal Stability and Mechanical Properties of Recombinant Spider Silk Films*

K. Spiess, R. Ene, C. Keenan, J. Senker, F. Kremer, T. Scheibel / *J. Mater. Chem.* (2011) **21** 13594

⇒ *Dynamic Force Spectroscopy on the Binding of Monoclonal Antibodies and Tau Peptides*

C. Wagner, D. Singer, O. Ueberschär, T. Stangner, C. Gutsche, R. Hoffmann, F. Kremer / *Soft Matter* (2011) **7** 4370

⇒ *Drag Reduction by DNA-grafting for Single Microspheres in a Dilute λ-DNA Solution*

O. Ueberschär, C. Wagner, T. Stangner, K. Kühne, C. Gutsche, F. Kremer / *Polymer* (2011) **52** 4021

⇒ *Optical Tweezers Setup with Optical Height Detection and Active Height Regulation under White Light Illumination*

C. Wagner, T. Stangner, C. Gutsche, O. Ueberschär, F. Kremer / *Journal of Optics* (2011) **13** 115302

⇒ *IR Transition Moment Orientational Analysis on Semi-crystalline Polyethylene Films*

W. Kossack, P. Papadopoulos, M. Parkinson, F. Prades, F. Kremer / *Polymer* (2011) **52** 6061

⇒ *A Novel Video-based Microsphere Localization Algorithm for Low Contrast Silica Particles under White Light Illumination*

O. Ueberschär, C. Wagner, T. Stangner, C. Gutsche, F. Kremer / *Optics & Lasers in Engineering* (2012) **50** 423

Prof. Dr. Friedrich Kremer

Institute for Experimental Physics I

<http://www.uni-leipzig.de/~mop/>

E-mail: kremer@physik.uni-leipzig.de

Phone: +49 341 97-32550

Fax: +49 341 97-32599

Anomalous Brownian motion of bio-polymers and hot nanoparticles

Prof. Dr. Klaus Kroy

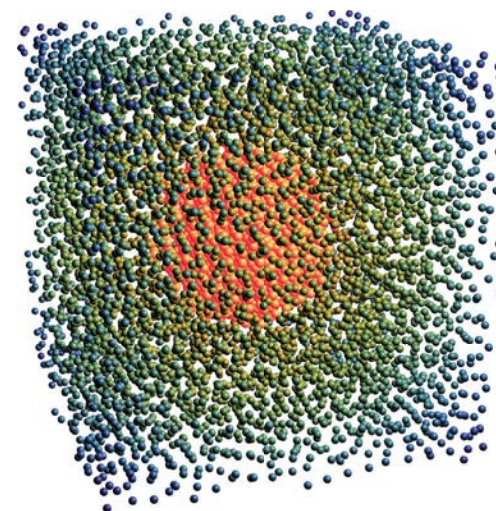
Dipl.-Phys. Jakob Tómas Bullerjahn, Dr. Jens Glaser, Dipl.-Phys. Marc Lämmel,

Dipl.-Phys. Sebastian Sturm, Dr. Lars Wolff

A variety of phenomena in biophysics and nanoscience defy a standard treatment in terms of classical Brownian motion, as thermal noise mixes in with molecular vibration modes or inhomogeneities in temperature or fluid structure. Following up on our recent work, we completed the calculation of the universal spatial heterogeneities found in bulk biopolymer solutions and their effect on Brownian biopolymer dynamics. Further, we developed theories of tracer dynamics wherein the tracer is either polymer-bound and possibly subject to external forces, or driven out of equilibrium by laser heating.

The first scenario generates subdiffusive motion, powered by a complex noise spectrum and serving as a valuable experimental tool in the determination of polymer properties or as a building block in more complex applications such as dynamic force spectroscopy. We provided detailed predictions for experimental observables and an effective equation of motion for the tracer position, suitable for general use.

In the second scenario, particle heating creates large quasi-stationary gradients



⇐ The non-equilibrium Brownian motion of hot nanoparticles obeys a generalised Einstein relation with an effective temperature

in temperature and viscosity, bearing both on the random forces driving the particle and on its viscous drag resistance. Using large-scale MD simulations, we could show that this complex coupling of thermal and hydrodynamic forces can be reduced to an effective equilibrium description governed by a generalised Einstein relation with an effective temperature, for which we could derive a formally exact expression within the theory of fluctuating hydrodynamics.

⇒ *Tube-width Fluctuations of Entangled Stiff Polymers*
J. Glaser, K. Kroy / Physical Review E (2011) **84** 051801

⇒ *Monomer Dynamics of a Wormlike Chain*
J.T. Bullerjahn, S. Sturm, L. Wolff, K. Kroy / EPL (2011) **96** 48005

⇒ *Generalised Einstein Relation for Hot Brownian Motion*
D. Chakraborty, M.V. Gnann, D. Rings, J. Glaser, F. Otto, F. Cichos, K. Kroy / EPL (2011) **96** 60009



Prof. Dr. Klaus Kroy
Institute for Theoretical Physics
<http://www.physik.uni-leipzig.de/~kroy/>
E-mail: klaus.kroy@itp.uni-leipzig.de
Phone: +49 341 97-32436
Fax: +49 341 97-32548

Surface- and materials physics for bio/medical applications

Prof. Dr. Stefan G. Mayr

Dipl.-Phys. Ariyan Arabi-Hashemi, Dipl.-Phys. Jörg Buchwald, Dipl.-Phys. Anja Graumann,
Dipl.-Phys. Marcel Hennes, M.Sc. Phys. Chem. Yanhong Ma

Functional materials offer a wide range of applications and are the main research topic of our group. The evaluation of new application purposes requires a detailed understanding of the underlying physical concepts and processes occurring at the nanoscale and their impact on meso- and macroscopic scales. Performed experiments are compared with results obtained by computer modelling.

Within BuildMoNa, our research focuses on mechanical properties of surfaces at nanoscale (*i*), magnetic shape memory alloys (*ii*) and magnetic nanoclusters (*iii*).

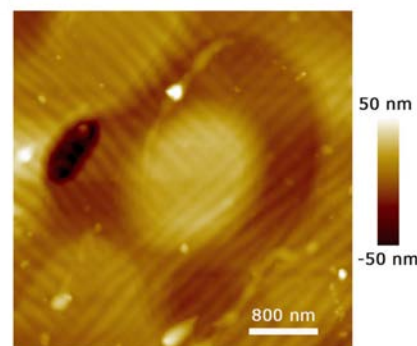
(*i*) Mechanical properties of surfaces fundamentally deviate from within a solid. Similarly, when considering the nanoscale, mechanical response often proves to be different from macroscopic behavior. CR-AFM is a new experimental technique



which allows to analyse these properties. To get a better understanding of the physics at these scales we base the experiments on computer simulations using a multiscale approach including first principle DFT-calculations and classical molecular dynamics.

(ii) In magnetic shape memory alloys internal strains can be induced through the reorientation of easy moveable martensitic twin variants by applying an external magnetic field. Using molecular beam epitaxy (MBE) and sputter deposition single crystalline thin films can be synthesised making these materials also usable for biomedical micro-applications. The investigation focuses on two different magnetic shape memory alloys which have gained great significance in the last years: $\text{Fe}_{70}\text{Pd}_{30}$ and Ni_2MnGa . These two material systems have complementary characteristics. While $\text{Fe}_{70}\text{Pd}_{30}$ is biocompatible and ductile, straining of up to 5% is possible. The biocompatibility of $\text{Fe}_{70}\text{Pd}_{30}$ was proven by cell test studies in collaboration with the Soft Matter Physics Division of Universität Leipzig. Ni_2MnGa has higher achievable strains of up to 10% but it is not biocompatible and brittle. These two material systems offer high potential in various fields e.g. actuators, different kinds of sensors, valves and switches.

(iii) Ultrafine magnetic particles can be employed in a variety of biomedical fields: as contrast enhancer in magnetic resonance imaging, as colloidal mediator in hyperthermia or for precise cell sorting. Providing single component particles with an outer gold layer guarantees biocompatibility and paves the way for further functionalisation. Our research focuses on the synthesis and characterisation of such multicomponent core-shell clusters, using inert gas condensation (IGC) as a versatile and contamination free method for the production of the particles. Self-organisational properties of the employed materials at the nanoscale are put under scrutiny as well as the mechanisms underlying growth and shape forming in order to obtain precisely tailored clusters for future cell tests.



↑ Scheme of twin structure for martensitic thin film on MgO substrate (left); AFM surface topography of as prepared martensitic Fe-Pd film attached on MgO substrate (right)



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

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

Prof. Dr. Harald Morgner

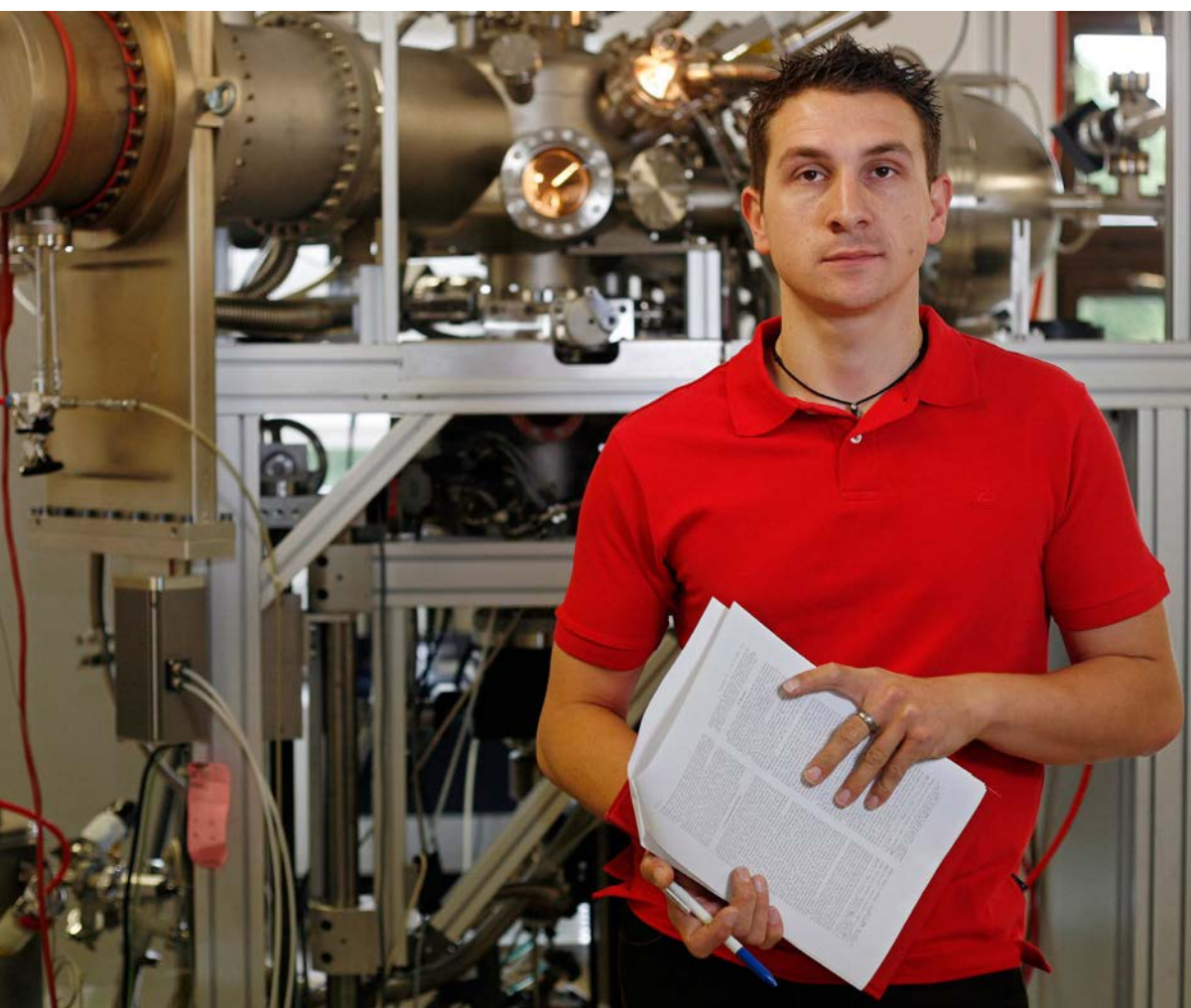
Dr. Tobias Hammer

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 accommodated at the surface. The standard technique of NICISS is able to yield the concen-

tration 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 dimensional 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. A mixture of water with an ionic liquid has been studied with respect to the surface structure. 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.



⇒ *Influence of Water on the Surface Structure of 1-Hexyl-3-methylimidazolium Chloride*
M. Reichelt, T. Hammer, H. Morgner / Surface Science (2011) **605** 1402

Prof. Dr. Harald Morgner
Wilhelm Ostwald Institute for Physical
and Theoretical Chemistry
<http://www.uni-leipzig.de/~pci/>
E-mail: hmorgner@rz.uni-leipzig.de
Phone: +49 341 97-36389
Fax: +49 341 97-39090

Modelling ligand friction in cell adhesion using peptide mimetics

Prof. Dr. Tilo Pompe

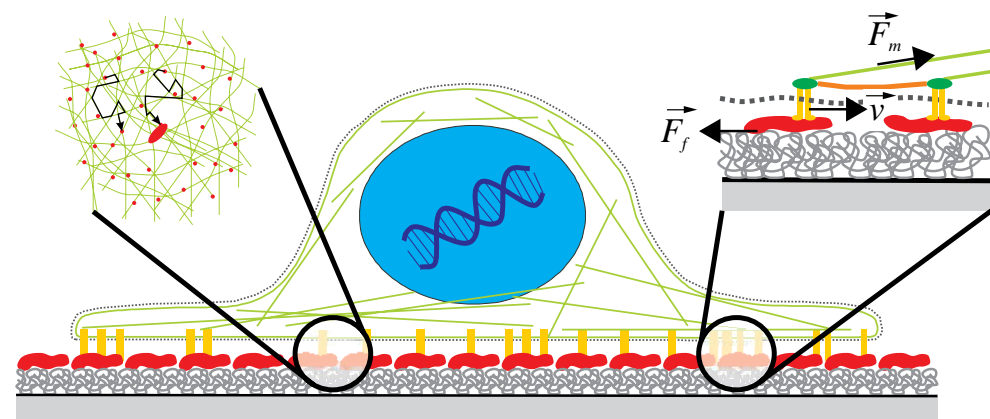
Dipl.-Phys. Andreas Müller

The characteristic of the extracellular microenvironment is of paramount importance in cell growth and differentiation. Recent reports show that mechanical properties of the extracellular matrix and resulting intracellular forces control many of these cellular processes. Therefore, these aspects have to be better understood in engineering of biomaterials scaffolds for applications in tissue engineering and regenerative therapies.

Recently, we demonstrated that besides the elastic characteristic also viscous properties of the extracellular matrix affect mechanical signalling in cell develop-

ment. In this context molecular friction of adhesion ligand proteins on cell culture substrates could be shown to regulate cell traction forces of adherent cells and the subsequent activation of intracellular signalling molecules.

Our current research focuses on the control of the affinity of peptide mimetics of adhesion ligands by the variation of their non-covalent interactions with physico-chemically well-defined materials supports. We aim on the modulation of peptide-substrate interaction in a controlled manner and to study the corresponding cell reaction in terms of cell traction forces, receptor clustering, and activation of signalling proteins of the cell adhesion apparatus. By that we will provide an in-depth understanding of the regulation of cell traction forces by frictional interaction of adhesion ligands with cell culture scaffolds and enable subsequent theoretical modelling approaches.



Model of frictional control of traction forces of adherent cells by non-covalent anchorage of adhesion ligands on surfaces. Schemes of slow, random, (left inset) and fast, directed (right inset) motion of integrin-FN complexes within the interlayer between the cell membrane and the substrate surface. (Left inset) Random reorganisation of FN ligands by a myosin-driven translocation along the actin cortex network. (Right inset) Stationary motion of integrin-FN complexes inside a focal adhesion with equilibrium between molecular friction at the ligand-polymer interface and myosin-motor forces transferred via a link of integrin-ligand complex, proteins inside the focal adhesion, and the cytoskeleton.



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

Synthesis of thin films and nanostructures far from the thermodynamic equilibrium

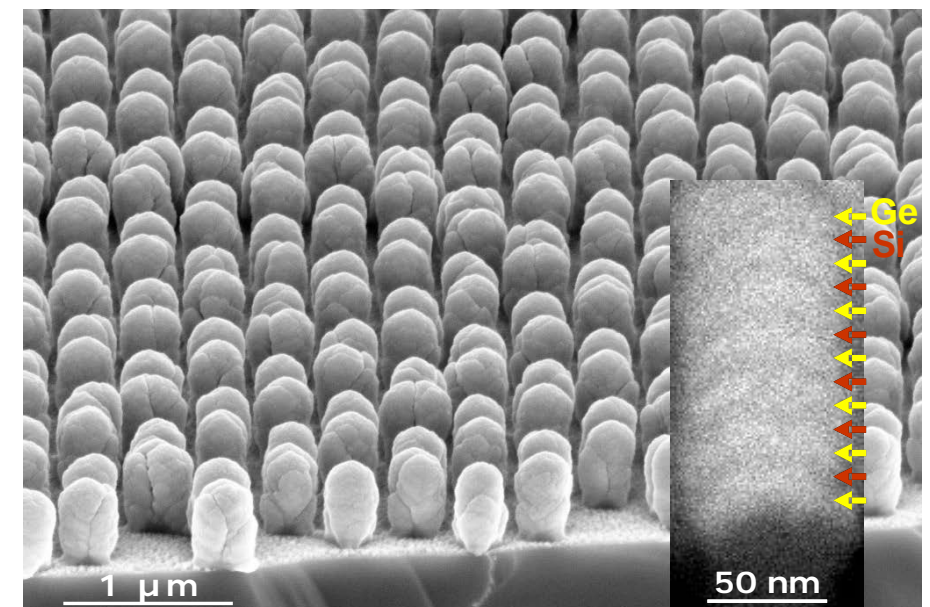
Prof. Dr. Dr. h.c. Bernd Rauschenbach

M.Sc. Chem. Marina Loredana Drob, M.Sc. Phys. Chinmay Khare,
Dipl.-Phys. Lena Neumann, M.Sc. Chem. Eng. Erik Thelander, Dr. Hendrik Zachmann

The research is focused on the formation of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium. Preferentially ion and laser beam techniques are used. These methods influence the nucleation and growth as well as the structural, optical and electrical properties of growing films as a consequence of atomic rearrangement induced by irradiation. A main emphasis of this research was the generation of low-dimensional germanium-silicon nanostructures as thermoelectric materials by ion beam assisted glancing angle deposi-

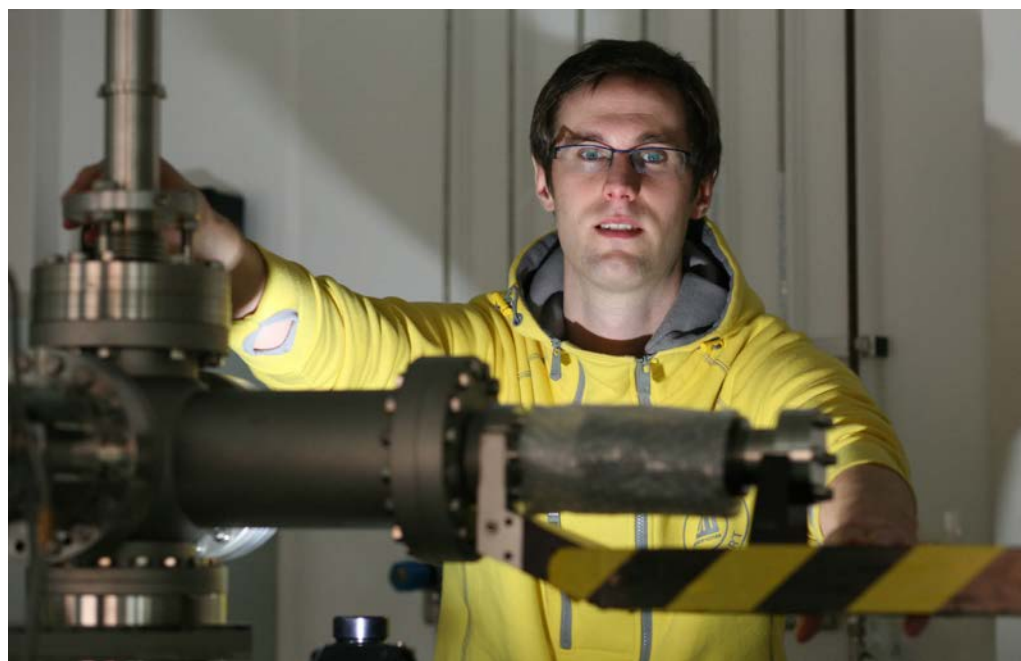
tion. Such heavily doped Si/Ge-nano-columns are predicted to have novel transport properties, because the Pauli principle restricts the heat-carrying electrons to be close to the Fermi energy.

A second research field was the formation of single crystalline gallium nitride films on silicon carbide substrates by ion beam assisted molecular beam epitaxy. The surface is extremely smooth. Atomic steps on the surface are recognised only. The high-resolution electron microscopic cross-section figure shows a perfect interface between the substrate silicon carbide and the gallium nitride layer and demonstrates the transition of hexagonal to the cubic gallium nitride layers within one single atom level.



↑ Cross-sectional scanning electron microscope micrograph of multilayered Si/Ge nano-columns for thermoelectric devices produced by glancing angle deposition

- ⇒ *Growth Temperature Altered Morphology of Ge Nanocolumns*
C. Khare, J.W. Gerlach, M. Weise, J. Bauer, Th. Höche, B. Rauschenbach / *Physica Status Solidi A* (2011) **208** 851
- ⇒ *Experimental Evidence for an Angular Dependent Transition of Magnetization Reversal Modes in Magnetic Nanotubes*
O. Albrecht, R. Zierold, S. Allende, J. Escrig, C. Patzig, B. Rauschenbach, K. Nielsch, D. Görlitz / *Journal of Applied Physics* (2011) **109** 0939104
- ⇒ *Glancing Angle Deposition of Ge Nanorod Arrays on Patterned Si Substrates*
C. Khare, R. Fechner, J. Bauer, M. Weise, B. Rauschenbach / *Journal of Vacuum Science Technology A* (2011) **29** 041503
- ⇒ *Optimized Growth of Ge Nanorod Arrays on Si Patterns*
C. Khare, B. Fuhrmann, H.S. Leipner, J. Bauer, B. Rauschenbach / *Journal of Vacuum Science Technology A* (2011) **29** 051501
- ⇒ *Sensitivity of Surface Plasmon Resonance Sensors Based on Metallic Columnar Thin Films in the Spectral and Angular Interrogations*
A. Shalabney, C. Khare, B. Rauschenbach, I. Abdulhalim / *Sensors & Actuators: Chemical B* (2011) **159** 201



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

NanoBioengineering – novel immuno-based multielectrode arrays and field potential recording systems for Life Sciences

Prof. Dr. Andrea A. Robitzki

Dipl.-Biochem. Sina Haas, Dr. Dana Krinke, Dipl.-Biochem. Anja Steude



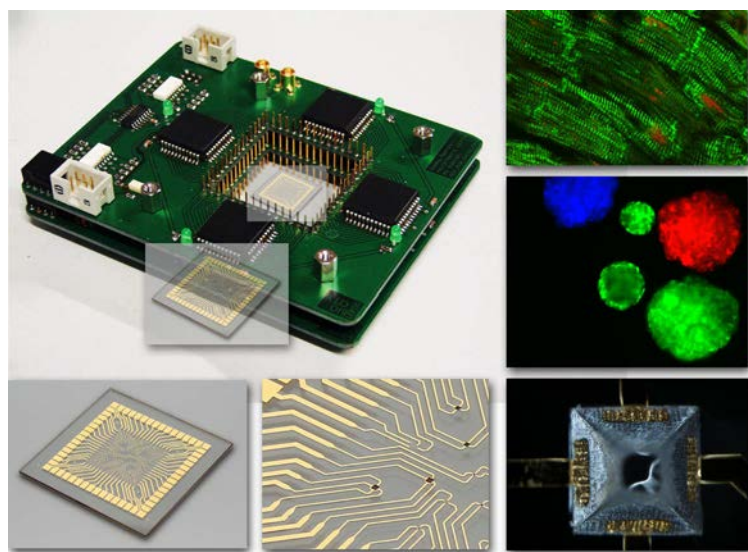
Research in 2011 focused on (i) proteome analysis of gender dependent ischemic processes in cardiomyocytes, (ii) monitoring of ion channel activity, and (iii) electrochemical immune-sensing of the extracellular brain tumour marker tenascin C.

Anja Steude successfully developed an electrochemical, immune-based biosensor to be applied in the field of solid tumour characterisation. The sensor detects tenascin C impedimetrically and indicates the cell cycle progression of neuronal

cells. It mainly consists of gold measuring electrodes, a platinum counter electrode and a pinholder with Ag/AgCl reference electrodes.

Dana Krinke could successfully deepen her understanding of neurodegenerative processes in 3D in vitro neuronal organotypic tissues.

Sina Haas investigated the proteomics of viable cardiomyocytes and the changes they undergo during ischemia and regeneration and correlated the results with field potential measurements.



← Example of an electronic board for the uptake of a glass based microcavity array with an 4-electrode configuration (left) used for real time bioelectronic monitoring of 3D spheres (right); Cardiomyocyte spheres were characterised via impedance spectroscopy and immunohistochemical staining (right, top; actinin)

⇒ *A Cell-Based Impedance Assay for Monitoring Transient Receptor Potential (TRP) Ion Channel Activity*
O. Pänke, W. Weigel, S. Schmidt, A. Steude, A.A. Robitzki / Biosensors and Bioelectronics (2011) **26** 2376

⇒ *An Electrode Array for Electrochemical Immuno-Sensing in High Throughput Applications Using the Example of Impedimetric Tenascin C Detection*
A. Steude, S. Schmidt, A.A. Robitzki, O. Pänke / Lab-On-Chip, (2011) **11** 2884

Prof. Dr. Andrea A. Robitzki
Centre for Biotechnology and Biomedicine and
Institute of Biochemistry
<http://www.uni-leipzig.de/~dmpt/>
E-mail: andrea.robitzki@bbz.uni-leipzig.de
Phone: +49 341 97-31241
Fax: +49 341 97-31249

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

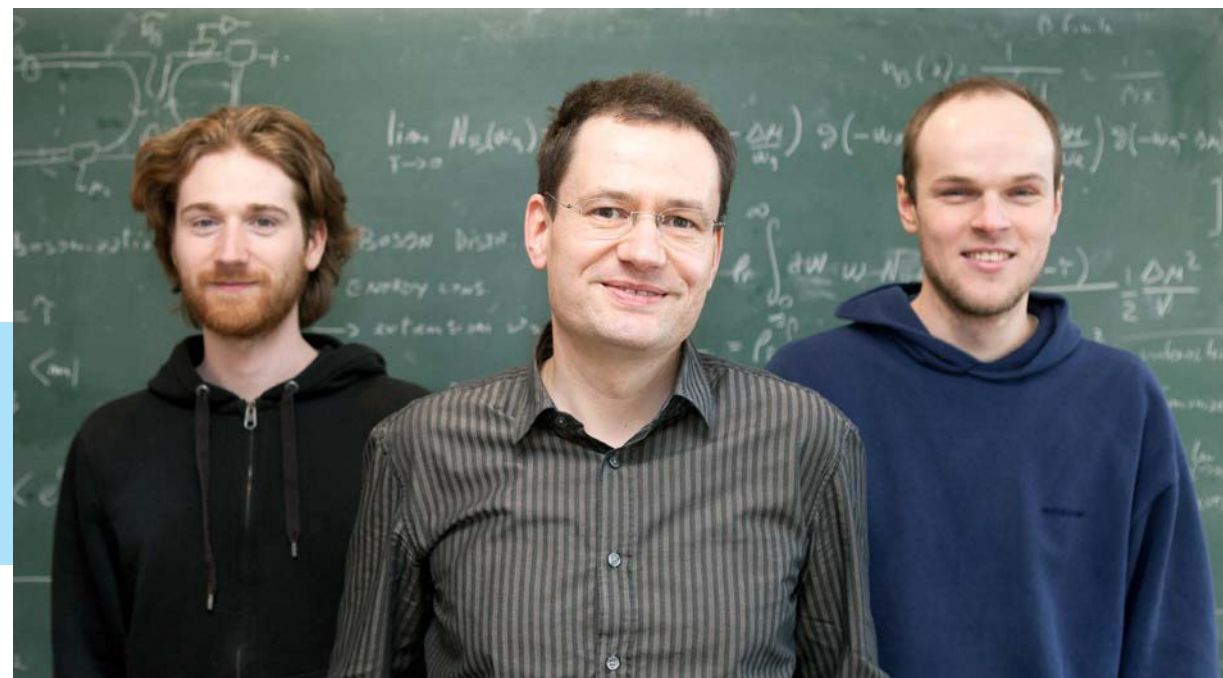
Prof. Dr. Bernd Rosenow

Dipl.-Phys. Alexander Janot, M.Sc. Phys. Martin Treffkorn

Research in the group is focused on the analysis of quantum condensates and their low-energy excitations.

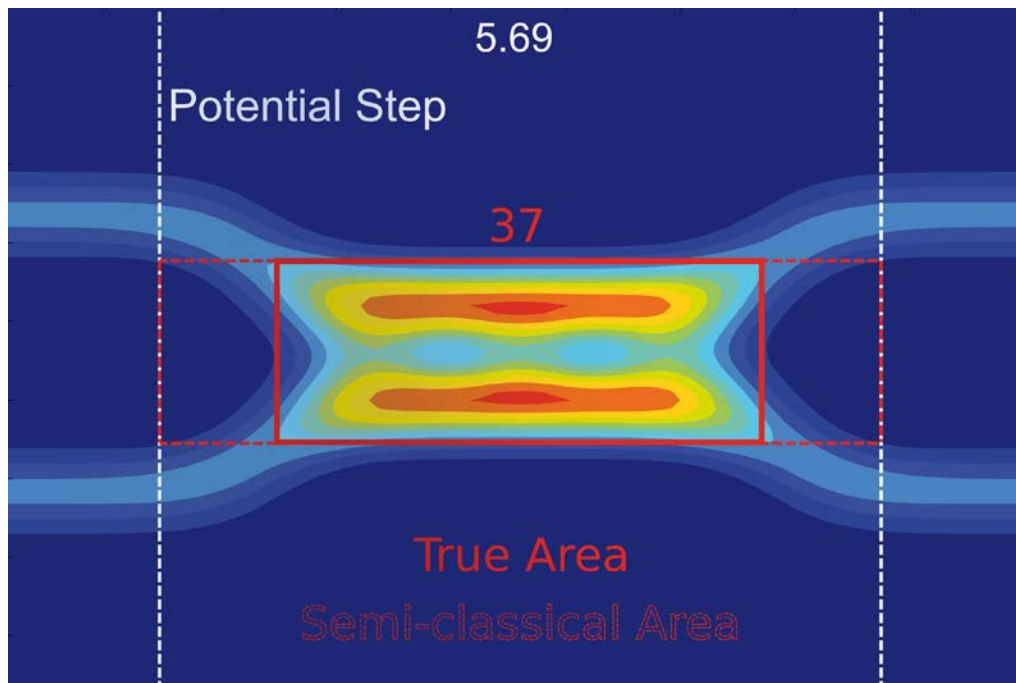
Examples for quantum condensates are exciton condensates, quantum Hall fluids, and superconductors. The common characteristic of these states of matter is the existence of a macroscopic wave function which describes the collective quantum dynamics of the system. Examples for experimental observables are the coherent emission of light from exciton-polariton condensates, and the dissipationless counterflow and Josephson-like interlayer current for exciton condensates in quantum Hall double layers.

For the case of exciton-polaritons, we have been studying the superfluid density in the presence of pumping and cavity disorder. We have found that on short length



scales the disorder is screened by fluctuations of the condensate density, while on long length scales as the condensate consists of domains with different quantum mechanical phases. The superfluid density decreases rapidly once the disorder is sufficiently strong to nucleate local regions with an emission frequency different from that of the condensate.

The low energy excitations of the quantum Hall condensate at filling factor $5/2$ are believed to be quasiparticles with non-abelian statistics, an exotic generalisation of bosonic and fermionic statistics. Currently, experimental efforts are under way to proof the existence of these particles through interference experiments in submicron scale devices. An important building block of such interferometers are quantum point contacts, which allow tunneling between counter-propagating edge states. By numerically implementing the recursive Green function algorithm, we were able to demonstrate that interference occurs even within a single point contact (as compared to two point contacts generically used in interferometers), opening a path towards further miniaturisation of interference devices.



↑ Electron density distribution in a quantum point contact with harmonic confinement in transverse direction and a potential step in longitudinal direction (dashed white lines); there are back-scattering paths both at the left and right side of the QPC, whose interference gives rise to magneto-oscillations of the conductance; the quantum mechanical interference area (full red line) is significantly smaller than the semi-classical one (dashed red line)



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

Experiences

BuildMoNa's fourth year – a principal investigator's view Different perspectives on the same matter

Prof. Dr. Frank-Dieter Kopinke, Prof. Dr. Hauke Harms



BuildMoNa has passed its fourth year, a very important one with respect to its future. The proposal for extension of the graduate school until 2017 has been prepared. Many thanks to the participants in the presentation for the board of DFG reviewers in Bonn in February 2012. They have done a great job. Whatever the final outcome will be, we have done our best.

BuildMoNa can be considered as a melting pot where ingredients from different institutions are mixed – those from the university and those from non-university institutions. Hence, it is clear that different perspectives on the common work come together. This is intended and a possible source of benefits. Scientists from both institutions benefit from the broader set of common resources, such as experimental facilities, scientific expertises, a pool of excellent students. Possibly, there are even more buried sources of benefits which just wait to be dug up.

We would like to start the search for further benefits from the perspective of a Helmholtz researcher. Helmholtz institutions get a sound basic funding from the

Federal Ministry of Education. Sometimes, this might be a matter of disapproval from the university colleagues – not totally incomprehensible. However, another aspect of Helmholtz research is sometimes overlooked: Helmholtz researchers are not as free as their university colleagues with respect to their choice of research subjects. Helmholtz research is organised in 5-year periods wherein research fields, strategic goals, milestones, products, etc. are clearly defined. University teachers may possibly gently smile on these terms. The keyword we would like to extract for identification of potential BuildMoNa benefits is “products”. Do we have clearly defined common products in our graduate school? Certainly, our main product are well-educated young scientists – chemists, biochemists, and physicists. This is quite a lot! Nevertheless, common products beyond excellent papers are scarce – products beyond the range of interests of the scientific community, which the society or even the German industry are eager to get. They would certainly be a good additional feature of BuildMoNa.

As a member of several advisory boards we have the opportunity to gain insight into the many facets of nanoscience-based communities. We have used this opportunity extensively during the last 12 months. Most of the running projects and networks, such as NanoNature and NanoCare in Germany, NanoSan in Austria or NanoObservatory in Switzerland, are strictly product oriented. New materials or nano-based devices (such as a portable ng-balance) are in the focus.

We are not sure whether excellent science and a stringent product orientation are compatible without making compromises. But isn't it worth considering that in BuildMoNa II?

Prof. Dr. Frank-Dieter Kopinke

Prof. Dr. Hauke Harms

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

M.Sc. Chem. Anika Gladytz



The interdisciplinary training offers unique chances for young scientists as it is urgently needed to serve the needs of today's society and industry. However, considering that undergraduate study programmes usually still focus on one of the classical disciplines, cutting-edge interdisciplinary postgraduate education has to face the problem that the candidates usually have very different background knowledge. To solve this problem, BuildMoNa has successfully established scientific modules that summarise the basics of physics, chemistry or biochemistry that are needed in order to follow the high-level interdisciplinary modules.

In addition to the scientific education BuildMoNa offers a variety of different soft skills training modules. These modules are very well adapted to the needs of the doctoral candidates. The benefit for the doctoral candidates is especially high if there is a direct link to their every-day work. As very positive examples I would like to mention the module "Advanced presentation skills" which prepares the participants for the BuildMoNa workshop and the module "Scientific writing and publish-

ing research" which helps to overcome difficulties when writing papers.

A huge advantage of the educational programme of the graduate school is its enormous flexibility. The content and the time schedule of the educational programme can be adapted to the individual needs and goals of each doctoral candidate. I have chosen to attend the majority of the scientific modules at the beginning of my doctoral research. For me, this strategy implied several important advantages. First, I gained valuable knowledge which I could implement in my work on my research topic. Secondly, I made contact to other doctoral candidates and principal investigators and got to know their research interests and methods. This opened doors for fruitful cooperations and methodology exchange. Finally, this strategy allows attending fewer modules now. Some months ago I gave birth to my little daughter. As my project contains a lot of theoretical work I have now the freedom to work mainly at home and according to my own schedule. Additionally the flexible child care programme of the graduate school offers great advantages. During meetings or when I need to work in the lab, the nanny employed by BuildMoNa takes care of my daughter. Additionally she joins us during conferences, workshops or symposia. This allows combining doctoral research and the family life.

The high-level interdisciplinary education, the very well chosen soft skills training opportunities and the top-level research are the basis of the success of the graduate school. In combination with a high degree of flexibility it ensures that every doctoral candidate can largely benefit from the training programme. Accordingly over the last years more and more highly motivated and excellent applicants, who enrich and improve the graduate school, could be attracted.

M.Sc. Chem. Anika Gladytz

Training

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

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

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



TRAINING CONCEPT

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

BuildMoNa training programme: M, 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 (2010-M09)

10 / 11 November 2011,

written exam, 2 credit points, yearly recurrence with modification, 43 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. J. Käs

Lecturers:

Prof. Dr. J. Käs, Universität Leipzig, Germany; Prof. Dr. J. Spatz, Universität Heidelberg, Germany; Prof. Dr. H. Fuchs, Universität Münster, 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 inflammation, analytics will include AFM and solid-state NMR

Nano-manipulations: From self-propelled particles to molecular motors (2011-M01)

11 / 12 April 2011,

written exam, 2 credit points, yearly recurrence with modification, 38 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 gives an introduction into materials and methods behind local force generation.

Responsible Scientists:

Prof. Dr. F. Cichos, Prof. Dr. J. Käs

Lecturers:

Prof. Dr. F. Cichos, Universität Leipzig, Germany; Prof. Dr. J. Käs, Universität Leipzig, Germany; Prof. Dr. R. Golestanian, University of Oxford, UK; I. Tolic-Norrelykke, MPI CBG Dresden, Germany; S. Grill, MPI CBG Dresden, Germany

Contents:

- ⇒ Molecular motors, biological motors, biological force generation
- ⇒ Self-propelled particles, propulsion mechanisms
- ⇒ Experimental mobility characterisation

Methods:

- ⇒ Optical tweezer, optical stretcher, laser dissection, magnetical tweezers
- ⇒ Scanning force microscopy and spectroscopy, optical microscopy
- ⇒ Single particle tracking
- ⇒ Experimental data analysis

From molecules to materials: Solid state inclusion compounds (2011-M02)

15 / 16 September 2011,

written exam, 2 credit points, yearly recurrence with modification, 31 participants

Link molecular science and materials science. Understand how porous molecular-based materials with voids in the crystal lattice are obtained from molecules or molecular precursors. Understand the properties and application of these solids.

Responsible Scientists:

Prof. Dr. H. Krautscheid, Prof. Dr. B. Kersting

Lecturers:

Prof. Dr. B. Kersting, Universität Leipzig, Germany; Prof. Dr. H. Krautscheid, Universität Leipzig, Germany; Prof. Dr. N.B. McKeown, Cardiff, UK; Prof. Dr. N.R. Champness, Nottingham, UK; Prof. Dr. J. Hulliger, Bern, Switzerland; Prof. G. Day, Cambridge, UK; Prof. Dr. S. Cohen, UCSD, San Diego, USA; Prof. Dr. R. Feile, TU Darmstadt, Germany; Dr. M. Haeckel, Leibniz-Institut für Meereswissenschaften, Kiel, Germany

Contents:

- ⇒ Absorption and storage of small molecules in molecular crystals
- ⇒ Supramolecular networks
- ⇒ Organic zeolithes
- ⇒ MOFs
- ⇒ Clathrate hydrates
- ⇒ Co-crystallisation, polymorphism
- ⇒ Storage of gases in marine sediments
- ⇒ Inclusion chemistry of container molecules

Methods:

- ⇒ Molecular crystals
- ⇒ Clathrate formation
- ⇒ Synthesis
- ⇒ Synthesis of designer clathrates
- ⇒ Handling and characterisation of solid state inclusion compounds

Theory: Structure and mechanics of foams and cellular matter (2011-M03)

22 / 23 September 2011,

written exam, 2 credit points, yearly recurrence with modification, 11 participants

The module aimed at providing the scientific background required to study foams and other synthetic and natural cellular materials. Participants learned about the basic physical principles to understand foams and cellular structures on the basis of their microstructure and topology, and about their significance for biological tissues and morphogenesis.

Responsible Scientists:

Prof. Dr. W. Janke, Prof. Dr. K. Kroy

Lecturers:

Prof. Dr. S. Hilgenfeldt, University of Illinois, USA; Dr. A. Kraynik, Sandia National Labs, USA; D.B. Staple, MPPKS Dresden, Germany

Contents:

- ⇒ Physical principles of foams and cellular materials
- ⇒ Review of basic principles of soft matter physics
- ⇒ Structure and mechanics/dynamics of foams and cellular matter
- ⇒ Mechanics of networks; introduction to surface evolver and foam structure exercises
- ⇒ Physical principles responsible for the structure of cell assemblies, growth and morphogenesis

Methods:

- ⇒ Statistical mechanics and theoretical modelling of cellular structures and topologies, rheology and mechanics, Minkowski functionals, free energies, variational principles, computer simulations

From biomolecules to cells: Monitoring and imaging of molecule alterations in cellular pathologies (2011-M04)

13 / 14 April 2011,

oral exam, 2 credit points, yearly recurrence with modification, 19 participants

The basics of proliferation, differentiation, migration, apoptosis of neuronal cell biology and cell-matrix interactions were presented. Got insight in processes of directed axonal out growth dependent on guidance molecules correlated with receptor expression profile. Also, novel methods and techniques for optical and bio-electronic monitoring were demonstrated. Another focus were principles of bio-hybrid systems such as micro-electronic microarrays and viable cell and tissue models. A series of tutorials on flow cytometry, slide-based cytometry, multiparametric analyses, etc. were also made available.

Responsible Scientist:

Prof. Dr. A. Robitzki

Lecturers:

Prof. Dr. A. Robitzki, BBZ, Germany; H.-G. Jahnke, BBZ, Germany; F. Preijers, Radboud University Nijmegen, The Netherlands; R.F. Murphy, Carnegie Mellon University, Pittsburgh, USA; G. Nolan, University of Stanford, CA, USA; N. Senghaas, Nikon GmbH, Germany; C. Vallan, Celeza GmbH, Switzerland

Contents:

- ⇒ Neuronal cellbiology, guidance molecules and axonal out growth
- ⇒ Stem cell biology and differentiation
- ⇒ Cell and tissue models on multielectrode-microarrays, e.g. Morbus Alzheimer on a chip
- ⇒ Impedance based spectroscopy and measurement methods
- ⇒ Super-microscope and high resolution microscopy

Methods:

- ⇒ Impedance spectroscopy, cytometry, high resolution microscopy of cells and tissues

Smart molecules: Ionic liquids – From physical properties to applications (2011-M05)

12 / 13 October 2011,

written exam, 2 credit points, yearly recurrence with modification, 25 participants

This module aimed at giving a basic background on ionic liquid (IL) research. Links between different IL disciplines like molecular sciences as well as topics from industry and physics, homogeneous, heterogeneous, and bio-catalysis were provided.

Responsible Scientists:

Prof. Dr. E. Hey-Hawkins, Prof. Dr. B. Kirchner, Prof. Dr. F. Kremer

Lecturers:

Prof. Dr. F. Kremer, Universität Leipzig, Germany; Prof. Dr. A. Abbot, University of Leicester, UK; Dr. M. Deetlefs, The Queen's University of Belfast, UK; Prof. Dr. F. Endres, University of Clausthal, Germany; Prof. Dr. K. Seddon, The Queen's University of Belfast, UK; PD Dr. A. Stark, Universität Leipzig, Germany; Dr. V. Strehml, University of Potsdam, Germany; Prof. Dr. K. Massonne, BASF, Ludwigshafen, Germany

Contents:

- ⇒ Basics about ionic liquids
- ⇒ Physics of ionic liquids
- ⇒ Handling ionic liquids and their synthesis
- ⇒ Application of ionic liquids

Methods:

- ⇒ Synthesis, Characterisation of IL properties by different spectroscopic methods (IR, NMR, UV-Vis, etc.)

Magnetic resonance: Fundamentals and applications (2011-M06)

6 / 7 September 2011,

written exam, 2 credit points, yearly recurrence with modification, 24 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 were provided that layed the foundation for its application. Due to the exceptional breadth of applications, advanced courses focus on current research needs.

Responsible Scientist:

Prof. Dr. S. Berger

Lecturers:

Prof. Dr. S. Berger, Universität Leipzig, Germany; Dr. Findeisen, Universität Leipzig, Germany

Contents:

- ⇒ Basic principles of NMR
- ⇒ NMR of liquids and of solids as a basic analytical tool
- ⇒ Advanced methods: in biological systems, quantum solids, surfaces
- ⇒ Hardware development for special applications

Methods:

- ⇒ Given the great expertise in magnetic resonance, interdisciplinary teaching will provide first-hand knowledge from leading experts in various fields; the teaching will also profit from a long-standing experience with GDCh courses where we combine lectures on various subjects with concrete experimental training at instruments, which provides hands-on education in complicated methods
-

Complex nanostructures: Nanoparticles and catalysis (2011-M07)

25 / 26 October 2011,

oral exam, 2 credit points, yearly recurrence with modification, 19 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, Universität Leipzig, Germany; Prof. Dr. F.-D. Kopinke, UFZ, Germany; Prof. Dr. H. Harms, UFZ, Germany; Dr. K. Schirmer, EAWAG Zürich, Switzerland; Prof. C.H. Christensen, Haldor Topsøe, Lyngby, Denmark; Prof. Dr. S. Kureti, TU Freiberg, Germany; Prof. K. Tryantafyllidis, Aristotle University Thessaloniki, Greece; Dr. A. Georgi, UFZ, Germany, Dr. K. Mackenzi, UFZ, Germany

Contents:

- ⇒ Nanostructures and nanoparticles are two basic 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, upcoming 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: Preparative methods in chemistry (2011-M08)

7 / 8 July 2011,

oral exam, 2 credit points, yearly recurrence with modification, 29 participants

Getting familiar with synthesis methods in solid-state chemistry. Synthesis of new materials via molecular precursors, chemical transport, sol-gel processes and solvothermal reactions. Understanding and application of the different methods to prepare complex systems and nanomaterials.

Responsible Scientists:

Prof. Dr. B. Kersting, Prof. Dr. H. Krautscheid

Lecturers:

Prof. Dr. B. Kersting, Universität Leipzig, Germany; Prof. Dr. H. Krautscheid, Universität Leipzig, Germany; Prof. Dr. N. Hüsing, University of Salzburg, Austria; Prof. Dr. P. Schmidt, HS Lausitz, Germany; Prof. Dr. J.J. Schneider, TU Darmstadt, Germany

Contents:

- ⇒ Synthesis of solid-state compounds and nanomaterials
 ⇒ Understanding the chemical aspects of preparative methods
 ⇒ Introduction: reactions in solid state
 ⇒ Materials synthesis and functional properties
 ⇒ Sol-gel methods
 ⇒ Nanostructured metals, oxides, carbon and their hybrids
 ⇒ High-temperature species in synthesis
 ⇒ Hydrothermal/solvothermal synthesis
 ⇒ Templated synthesis
 ⇒ Chemical transport reactions

Methods:

- ⇒ Introducing the synthetic tools for solid state and nanomaterials, a selection of typical methods in preparative solid-state chemistry
 ⇒ Preparation and characterisation of nanomaterials
-

Multifunctional scaffolds: From model systems to living cells (2011-M10)

29 / 30 September 2011,

written exam, 2 credit points, yearly recurrence with modification, 26 participants

The module aimed at providing the scientific background required to study and manipulate biopolymers, biopolymer networks, proteins and protein networks, including the highly dynamic polymer scaffolds in living tissues as an organising matrix for smart nanoelements, molecular motors, mechano-sensing, in natural and artificial nanoscopic devices for force-generation, motile polymeric machines, biomimetic devices, etc.

Responsible Scientist:

Prof. Dr. K. Kroy

Guest Lecturers:

Prof. Dr. K. Kroy, Universität Leipzig, Germany; Dr. T. Betz, Institute Curie, France; Dr. D. Heinrich, LMU Munich, Germany; Prof. Dr. G. Koenderink, AMOLF, NL; Prof. Dr. U. Schwarz, University of Heidelberg, Germany

Contents:

- ⇒ Physical, chemical and biological perspectives onto various multifunctional scaffolds as well as to modern experimental techniques
- ⇒ General soft matter background, statistical physics and simulation approaches, protein assembly and aggregation, the complex interactions in aqueous media, biopolymers and biopolymer networks, including molecular motors, cytoskeleton and extra-cellular matrix, living cells

Methods:

- ⇒ Single molecule imaging/tracking
- ⇒ Advanced microscopy
- ⇒ Rheology
- ⇒ Micro-rheology
- ⇒ In vitro 3-dimensional scaffolds
- ⇒ Statistical mechanics
- ⇒ Theoretical modelling
- ⇒ Computer simulations

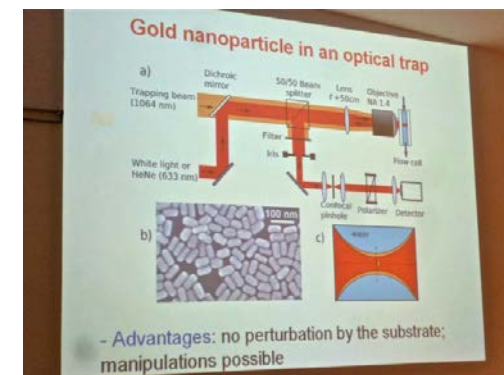
Scientific minisymposium

Hot nanoparticles and nanostructures

11 / 12 October 2011

The second BuildMoNa Minisymposium was organised by the research groups of Prof. Dr. F. Cichos, Prof. Dr. K. Kroy and Prof. Dr. B. Rauschenbach.

The symposium centred on the physics of laser-heated nanoparticles and nanostructures to touch on various aspects of physical chemistry and technological and medical applications. It gathered leading experts from a rapidly emerging and highly interdisciplinary field at the intersection of nanophotonics and nanoscale nonequilibrium stochastic thermodynamics. The aim was to promote the development of new concepts of nanoparticle manipulation, such as hot Brownian motion, self-propelled nanoparticle transport, nanoscale thermophoresis, thermal nanoconductance and innovative technologies, such as nanoparticle tracking, trapping and



steering, (dual-focus) photothermal correlation spectroscopy, and nanoparticle surgery. Speakers of the minisymposium were:

- ⇒ Prof. Dieter Braun, Ludwig Maximilians Universität München, Germany: *Thermophoresis for medicine and evolution*
- ⇒ Prof. Alois Würger, Université Bordeaux I, France: *Leidenfrost droplets on a ratchet*
- ⇒ Prof. Haw Yang, Princeton University, USA: *3D tracking of single heated colloidal particles in solution*
- ⇒ Prof. Masaki Sano, University of Tokyo, Japan: *Active colloids: from external to self-control of nonequilibrium transports of colloids*
- ⇒ Prof. Ramin Golestanian, University of Oxford, UK: *Collective thermotaxis of self-thermophoretic active colloids*
- ⇒ Dr. Giovanni Volpe, Universität Stuttgart, Germany: *Behaviour of microswimmers in complex environments*
- ⇒ Dr. Matthias Krüger, MIT, USA: *Casimir interactions between hot and cold nanoparticles*
- ⇒ Prof. Peter Reimann, Universität Bielefeld, Germany: *Anisotropic diffusion in square lattice potentials: giant enhancement and control*
- ⇒ Dr. Ralf Vogelgesang, MPI for Solid State Research, Stuttgart, Germany: *Farfield control of optical nearfields at plasmonic nanostructures*
- ⇒ Prof. Gregory Hartland, University of Notre Dame, USA: *Transient absorption microscopy studies of single metal and semiconductor nanostructures*
- ⇒ Dr. Markus Lippitz, MPI for Solid State Research, Stuttgart, Germany: *An optical antenna for spectroscopy of a nano-particle's breathing mode*
- ⇒ Prof. Michel Orrit, University of Leiden, The Netherlands: *Alignment and hot Brownian motion of a single nanorod in an optical trap*
- ⇒ Prof. Jean-Louis Barrat, Université Joseph Fourier Grenoble, France: *Nanoscale heat transfer: what can we learn from molecular simulation*
- ⇒ M.Sc. Phys. Markus Selmke, Universität Leipzig, Germany: *Hot nanoparticle diffusion probed by twin-focus photothermal correlation spectroscopy*
- ⇒ Dr. Dipanjan Chakraborty, Universität Leipzig, Germany: *Generalized Einstein relation for hot Brownian motion*
- ⇒ Prof. Dr. Werner Köhler, Universität Bayreuth, Germany: *Transient cage formation around laser-heated gold colloids in polymer solutions*
- ⇒ Dr. Claire Cobley, MPI for Intelligent Systems Stuttgart, Germany: *Gold Nanocages: A New Platform for Biomedical Applications*
- ⇒ Prof. Dr. Brahim Lounis, Université Bordeaux I, France: *Photothermal detection of nanometre-sized absorbing objects*

Transferable skills workshops

Scientific writing and publishing research, part II

Dr. Dorothea Sommerfeldt,

3 / 4 February 2011, 8 participants

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

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

Peter James Witchalls, Golin Wissenschaftsmanagement,

25 February 2011, 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.

Scientific writing and publishing research, part I

Dr. Dorothea Sommerfeldt,

4 / 5 July 2011, 11 participants

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

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Mastering the selection process: Developing job application strategies for business and industry

Uni support,

18 / 19 August 2011, 10 participants

Having personal initiative and preparing intensively for the application process are absolutely essential for anyone applying for top positions in business and industry. Central elements of this process include sounding out one's chances on the job market, developing solid application strategies, and carefully preparing a successful self-presentation in initial job interviews, selection interviews or in selection and assessment centres.

The target of this seminar was to help participants steer systematically towards positions that match their individual career aspirations and to show them how to place themselves as closely as possible to the top of applicant ranking lists. Participants developed targeted application strategies and learnt valuable details about selection criteria and various selection procedures used in business and industry. By informing themselves about the situation in specific companies and learning more about the demands of business and industry, participants will be in a position to apply both their outstanding professional qualifications and their soft skill competencies appropriately and effectively.

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Advanced presentation skills

Prof. Dr. Roger Gläser, Universität Leipzig,

19 / 26 / 28 September 2011 within the Workshop for doctoral candidates, 10 participants

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

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Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Peter B. Littlewood	<i>Department of Mechanical Science Cavendish Laboratory, University of Cambridge, UK</i>	A condensate of matter and light: Bose Einstein condensation of polaritons	31 January 2011	<i>Faculty of Physics and Earth Sciences</i>
Dr. Christian Schütz	<i>Institute for Nuclear Chemistry, Johannes Gutenberg-University Mainz, Germany</i>	Boron analysis in the BNCT project of the University of Mainz	24 March 2011	<i>Faculty of Chemistry and Mineralogy</i>
Prof. Dr. Ramin Golestanian	<i>Department of Physics and the Rudolf Peierls Centre for Theo- retical Physics, St. Cross College, Oxford, UK</i>	From microswimmers to nanoswimmers: The role of fluctuations	12 April 2011	<i>Faculty of Physics and Earth Sciences</i>
Dr. Paul Eastham	<i>Trinity Colleg Dublin, Ireland</i>	Polariton condensation and lasing in semi- conductor microcavities – coherence and dynamics	10 June 2011	<i>Faculty of Physics and Earth Sciences</i>
Prof. Dr. Helma Wennemers	<i>Department of Chemistry, Univer- sity of Basel, Switzerland</i>	Peptides as molecular allrounders – Asym- metric catalysis, synthetic collagen and Ag-nanoparticles	14 June 2011	<i>Faculty of Biosciences, Pharmacy and Psychology</i>
Prof. Dr. Lothar Weber	<i>Universität Bielefeld, Fakultät für Chemie, Germany</i>	Leuchtende Borverbindungen	15 June 2011	<i>Faculty of Chemistry and Mineralogy</i>
Dr. Stephan Schmidt	<i>Fraunhofer Institute of Biomedical Technology, Potsdam; Max-Planck Institute of Colloids and Interfaces, Potsdam-Golm, Germany</i>	Interaction forces between bioactive surfaces and soft colloidal particles as AFM force probes	17 June 2011	<i>Faculty of Biosciences, Pharmacy and Psychology</i>
Dr. Klemens Massonne	<i>BASF SE Ludwigshafen, Germany</i>	Ionic liquids at BASF SE: Introduction and technical applications	29 June 2011	<i>Faculty of Chemistry and Mineralogy</i>
Prof. Dr. Bertrand I. Halperin	<i>Department of Physics, Harvard University, USA</i>	Defects with character – Majorana states in condensed matter systems	5 July 2011	<i>Faculty of Physics and Earth Sciences</i>
Prof. Dr. Randall Q. Snurr	<i>Department of Chemical and Bio- logical Engineering, Northwestern University, Evanston, USA</i>	Computational design of metal-organic frameworks for energy and environmental applications	23 September 2011	<i>Faculty of Chemistry and Mineralogy</i>
Prof. Susumu Kitagawa	<i>Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Shimogyo-ku, Kyoto, Japan</i>	Chemistry and application of porous coordination polymers/metal-organic frameworks	23 September 2011	<i>Faculty of Chemistry and Mineralogy</i>
Prof. Dr. Ady Stern	<i>Department of Condensed Matter Physics, Weizmann Institute of Sci- ence, Rehovot, Israel</i>	Proposed experimental probes of non- abelian anyons	1 November 2011	<i>Faculty of Physics and Earth Sciences</i>
Prof. Dr. Georg Papastavrou	<i>Universität Bayreuth, Germany</i>	Biopolymers at interfaces	1 November 2011	<i>Faculty of Biosciences, Pharmacy and Psychology</i>

Events

4th Scientific symposium

The fourth scientific symposium of the Graduate School “Leipzig School of Natural Sciences – Building with Molecules and Nano-objects” (BuildMoNa) was held on 21 March 2011 at the Helmholtz Centre for Environmental Research (UFZ). Interdisciplinary topics from the current research on the development and investigation of new materials were presented. Renowned guest speakers from science gave talks on current topics of BuildMoNa. During the poster session, as one part of the symposium, doctoral candidates presented their scientific topics and discussed them with the international guests, receiving further inspiration for their work at the Graduate School BuildMoNa.

Invited speakers were:

- ⇒ Prof. Dr. Flemming Besenbacher, Aarhus University, Denmark: *Self-assembly of DNA nanostructures: Dynamics, self-organisation of DNA bases and DNA-boxes*
- ⇒ Prof. Dr. Ulf Diederichsen, Georg-August-Universität Göttingen, Germany: *Building with peptide secondary structure*
- ⇒ Dr. Manfred Buck, University of St Andrews, UK: *Nanoscience in flatland: Molecular assemblies and electrochemistry*
- ⇒ Prof. Dr. Alan E. Rowan, Radboud University Nijmegen, The Netherlands: *Polymeric nano-worms: From solar cells to drug delivery*



↑ Participants of the 4th scientific symposium



4th Workshop for doctoral candidates

30 doctoral candidates presented their scientific results with short talks on the 4th BuildMoNa Workshop on 26 and 27 September 2011 in Dresden. About 100 BuildMoNa participants followed the lectures in the Moritzburg and Altendresden conference room, the conference venue of the NH Hotel Dresden. Presentations covered the whole research profile of the graduate school: Development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. Mechanisms of material formation from building blocks, e.g. self-organisation, were also included.

For the 10 participants of the 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. At the end of the workshop a jury selected three presentations given by the doctoral candidates.

The first prize was awarded to Tobias Möller for his presentation “P-chiral polymeric phosphines”, the second to Verena Ahrens for her presentation “Carbaborane containing neuropeptide Y analogs for breast cancer therapy” and the third to Martin Brehm for “TRAVIS – A free analyser and visualiser for Monte Carlo and molecular dynamics trajectories”.



← Participants of the workshop in front of the “Frauenkirche”



↑ Winners of the presentation awards at the 4th Workshop:
Tobias Möller, Verena Ahrens and Martin Brehm
(from left to right)

4th Annual reception

On 7 December 2011, BuildMoNa celebrated its fourth anniversary. The reception was opened by welcoming addresses of the speaker of the graduate school Professor Evamarie Hey-Hawkins followed by a lecture of Prof. Dr. Dr. h.c. mult. Helmut Schwarz (President of the Alexander von Humboldt-Foundation) called “Chemistry with methane: Concepts rather than recipes”.

At this event, the BuildMoNa Awards were given to doctoral candidates to recognise their outstanding scientific achievements.

Daniel Lässig (Institute of Inorganic Chemistry) received the first prize for the synthesis and comprehensive characterisation of a novel material, published in:

A Microporous Copper Metal-Organic Framework with High H_2 and CO_2 Adsorption Capacity at Ambient Pressure

D. Lässig et al. / Angew. Chem. Int. Ed. (2011) **50** 10344

and

Synthesis, Crystal Structure, and Electron Paramagnetic Resonance Investigations of Heteronuclear Co^{II}/Zn^{II} and Co^{II}/Cd^{II} Coordination Polymers

D. Lässig et al. / Inorg. Chem. (2011) **50** 213

Martin Brehm (Wilhelm Ostwald Institute for Physical and Theoretical Chemistry) received the second prize for the conception on an innovative software package published in:

TRAVIS – A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories

M. Brehm et al. / J. Chem. Inf. Model. (2011) **51** 2007

Christof P. Dietrich (Institute for Experimental Physics II) was awarded the third prize for his work on differentiation of Whispering-Gallery and Fabry-Perot-Modes in ZnO-nanowires, which led to the following publication:

One- and Two-Dimensional Cavity Modes in ZnO Microwires

C.P. Dietrich et. al. / New J. Phys. (2011) **13** 103021

as well as two further papers on ZnO-nano-wires:

Strain Distribution in Bent ZnO Microwires

C.P. Dietrich et al. / Appl. Phys. Lett. (2011) **98** 031105

and

Defect Properties of ZnO and ZnO:P Microwires

C.P. Dietrich et al. / J. Appl. Phys. (2011) **109** 013712

Congratulations again to the winners!



↑ The winners of the BuildMoNa Awards:
Daniel Lässig, Martin Brehm and Christof P. Dietrich
(from left to right)

↓ Prof. Dr. Dr. h.c. mult. Helmut Schwarz



Childcare

Flexible childcare services at BuildMoNa

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



Funding of doctoral candidates



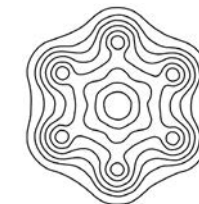
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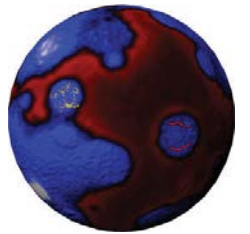
Europa fördert Sachsen.



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