UNIVERSITÄT LEIPZIG



Graduate School Building with Molecules and Nano-objects



Cover image

- ⇒ Left: Schematic representation of a dense network of topologically entangled stiff polymers
- \Rightarrow *Right*: Scanning transmission ion micro-tomogram of PMMA screw created by proton beam writing from 3 directions
- \Rightarrow *Bottom:* Model of NPY with carbaborane cluster



Annual Report 2010

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- $89 \Rightarrow$ From molecules to materials: Magnetic nanoparticles (2010-M02)
- $90 \Rightarrow$ Theory: Probability in physics (2010-M03)
- $91 \Rightarrow$ From biomolecules to cells: Ligands, receptors and signal transduction (2010-M04)
- $92 \Rightarrow$ Smart molecules: Biomolecules (2010-M05)
- $93 \Rightarrow$ Magnetic resonance: Fundamentals and applications (2010-M06)
- $94 \Rightarrow$ Complex nano-structures (2010-M07)
- $95 \Rightarrow$ Synthesis: Synthesis of thin films and nanostructures (2010-M08)
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- $100 \Rightarrow$ Project management for young scientists: Taking off as project pilot
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Leipzig school of natural sciences – the third year of building with molecules and nano-objects

Preface Prof. Dr. Evamarie Hey-Hawkins

Established in 2007 as one of the projects within the Excellence Initiative the Graduate School BuildMo-Na focuses on interdisciplinary graduate education through top-level, synergistic research.

To meet the increasingly broad skill demands in science and industry the interdisciplinary graduate training includes both research and a well-structured curriculum. The independent research work carried out by doctoral candidates, under thorough supervision, represents a major part of the gradu-



ate training. In addition, individual scientific training in key areas and soft skills contributes to a highly valuable and lasting education. Moreover, the training programme profits from the involvement of international and industrial partners.

While chemistry and physics often orient their interdisciplinary efforts towards biology this graduate school strives not only for a biological perspective but moreover for a strong connection between chemistry and physics, which is rarely found. Our materials research concept is based on a "bottom-up" approach. Progressive building blocks, such as smart molecules, peptides, active proteins, polymeric scaffolds, and nano-objects, will be combined – preferentially by self-organisation – to create fundamentally new classes of materials that are inspired by active, adaptive living matter, and that 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 the future knowledge transfer from fundamental to applied sciences.

At the end of the year 2010, 94 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 17 young scientists have already finished their doctoral studies. Today, 26 doctoral candidates were awarded a BuildMoNa scholarship and 36 doctoral candidates are financed by means of third-party funds. Additionally, 18 candidates are funded by ESF doctoral positions, and 14 doctoral candidates as well as two postdocs are promoted within two ESF young researchers groups affiliated with the graduate school.

The scientific training includes the annual organisation of ten scientific and methods modules according to the overall research concept. Additionally, the minisymposium "Physics of Cancer" was organised by Prof. Josef Käs. The minisymposium gathered worldwide the pioneering groups that are concerned with the physics of cancer.

Science related events included the 3rd BuildMoNa Symposium and the 3rd BuildMoNa Workshop for doctoral candidates.

On 8 December, the ceremonial event for the third-year anniversary of Build-MoNa took place. The lecture of Prof. Klaus Kern, MPI of Solid State Research, dealt with "Current at the nanoscale". On this occasion, the annual "BuildMoNa Awards" were presented to three doctoral candidates for their scientific publications resulting from their doctoral research.

During the year 2011, the graduate school will apply for its continuation in 2012.

Prof. Dr. Evamorie Hey-Hawkins

Organisation and management



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

Dipl.-Biochem. Marco Glaß

M.Sc. Chem. Martyna Madalska

Dipl.-Phys. Martin Lange

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

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
DiplBiochem. Verena Ahrens	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	Modified peptides for biotechnology
DiplPhys. Tobias Andrea	Prof. Dr. T. Butz / Prof. Dr. J. Käs	3D-visualisation of intracellu- lar drug delivery systems by ion micro-tomography and 3D-inverse tomography sculpting
M.Sc. Phys. Ana Isabel Ballestar Balbas	Prof. Dr. P. Esquinazi / Prof. Dr. T. Butz	Intrinsic anisotropy of multigra- phene and transport properties of graphite interfaces
DiplBiochem. Lars Baumann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	Structure-activity relation of che- mokines
DiplChem. Kathrin Bellmann-Sickert	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	Improvement of the bioavailability of neuropeptides and chemokines
DiplPhys. Tammo Böntgen	Prof. Dr. M. Grundmann / Prof. Dr. FD. Kopinke	Optical investigation of BaTiO ₃ - heterostructures with ellipsometry and Raman-scattering
DiplPhys. Kerstin Brachwitz	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	Materials of ferroic order and their interaction
M.Sc. Chem. Martin Brehm	Prof. Dr. B. Kirchner / Prof. Dr. R. Gläser	Development of a program package for efficient simulation of complex chemical systems
B.Sc. Chem. Jorge Luis Cholula Díaz	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmann	Properties of novel precursor based materials
M.Sc. Chem. Murali Dama	Prof. Dr. S. Berger / Prof. Dr. J. Haase	Organo gels as an alignment media for RDC measurements
DiplPhys. Christof Peter Dietrich	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	Growth and charactisation of ZnO- based microstructures
M.Sc. Chem. Marina Loredana Drob	Prof. Dr. B. Rauschenbach / Prof. Dr. M.R. Buchmeiser	Biopolymeric materials for regen- erative medicine
M.Sc. Phys. Srujana Dusari	Prof. Dr. P. Esquinazi / Prof. Dr. H. Morgner	Measurements of the mean free path and spin diffusion length in multigraphene
M.Sc. Phys. Susanne Ebert	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	The development of a novel tech- nique to measure the proteomic content of biological cells by com- bining microfluidics, laser-based nano-manipulation and optical high-resolution tomography

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Sylvia Els	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	Gastrointestinal peptides related to obesity
DiplPhys. Roxana-Giogiana Ene	Prof. Dr. F. Kremer / Prof. Dr. E. Hey-Hawkins	Structural levels of organisa- tion in spider silk as studied by time-resolved polarised rheo-FTIR spectroscopy
DiplPhys. René Feder	Prof. Dr. T. Butz / Prof. Dr. P. Esquinazi	Defect production by single ions tra- versing multigraphene
M.Sc. Chem. René Frank	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Carbaboranyl amino acids for applications in BNCT
M.Sc. Chem. Dirk Friedrich	Prof. Dr. H. Krautscheid / Prof. Dr. M. Grundmannn	Synthesis, characterisation and deposition of CIGS precursors
DiplPhys. Anatol Fritsch	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	Growth of soft breast tumour cells in micro- and nanostructured hard environments
M.Sc. Chem. Anika Gladytz	Prof. Dr. B. Abel / Prof. Dr. A.G. Beck-Sickinger	Nanospectroscopy near chemical and biological interfaces
DiplPhys. Jens Glaser	Prof. Dr. K. Kroy / Prof. Dr. S. Müller	Theory of semiflexible polymers
DiplBiochem. Marco Glaß	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	HP-Bioforce: An integrated and automated screening plattform for functional force measurement at cell and tissue layers for pharmaceutical research
M.Sc. Chem. Matthias Golecki	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	Encapsulation of catalytically active metal complexes
M.Sc. Phys. Markus Gyger	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	Active and passive biomechanical measurements for characterisation and stimulation of biological cells
DiplBiochem. Sina Haas	Prof. Dr. A. Robitzki / Prof. Dr. J. Käs	Development of a bioforce microar- ray sensor for measuring cellular biomechanical forces of ischemic cell layers
M.Sc. Chem. Tobias Hammer	Prof. Dr. H. Morgner / Prof. Dr. A.G. Beck-Sickinger	Investigation of aqueous solutions with ion-scattering-spectroscopy
DiplBiochem. Rayk Hassert	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. M. Grundmann	Peptides for specific adhesion to hard matters
DiplChem. Julia Haushälter	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	Phosphine-baskets – ligands for selective catalysis
M.Sc. Chem. Thomas Heinze	Prof. Dr. R. Gläser / Prof. Dr. B. Kirchner	Noble metal nanoparticles on or- dered porous supports for the in-situ synthesis and conversion of H_2O_2 in supercritical carbon dioxide

Title and Name	First / Second Supervisor	Working title of doctoral thesis
DiplPhys. Helena Hilmer	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	Growth and characterisation of UV- microcavities
DiplPhys. Florian Huber	Prof. Dr. J. Käs / Prof. Dr. M. Grundmann	Artificial cell motility
M.Sc. Phys. Ciprian-Ghiorghita Iacob	Prof. Dr. F. Kremer / Prof. Dr. R. Gläser	Molecular dynamics of organic ma- terials confined in nano-pores
M.Sc. Chem. Cathleen Juhl	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	Investigation of the function of adiponektin receptors by peptide segmentation
M.Sc. Phys. Michael Jurkutat	Prof. Dr. J. Haase / Prof. Dr. W. Janke	Investigation of the electronic properties of high-temperature su- perconductors by means of NMR
M.Sc. Phys. Chinmay Khare	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	Glancing angle deposition
DiplPhys. Tobias Kießling	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	Molecular marker free isolation of pluripotent haematopoetic stem cells and metastatic cancer cells from blood
M.Sc. Chem. Aslihan Kircali	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	Phosphorus-rich complexes as pre- cursors for binary or ternary metal phosphides $M_x P_y$ or $M_x M'_y P_z$
DiplPhys. Fabian Klüpfel	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	Transparent active multi-electrode arrays for the measurement of nerve cell signals
DiplMath. Melanie Knorr	Prof. Dr. J. Käs	Role of stochasticity in a moving thin polymer film
DiplPhys. Wilhelm Kossack	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	IR-spectroscopy for the analysis of structure and dynamic of polymers
M.Sc. Chem. Anika Kreienbrink	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	Synthesis and reactions of carba- borane-substitued 1,2-diphosphe- tanes and other phosphorus-rich heterocycles
DiplBiochem. Dana Krinke	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	Development of an impedance- based HTS screening on novel neuronal 2D and 3D cell culture models for testing drugs against neurodegenerative diseases
M.Sc. Appl. Chem. Anusree Viswanath Kuttatheyil	Prof. Dr. J. Haase / Prof. Dr. H. Krautscheid	Structure determination and host-guest interactions in porous metal-organic frameworks studied by solid-state NMR
DiplChem. Jochen Lach	Prof. Dr. B. Kersting / Prof. Dr. P. Esquinazi	Thin films of redox-active high-spin molecules

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Daniel Lässig	Prof. Dr. H. Krautscheid / Prof. Dr. J. Haase	Synthesis and characterisation of porous coordination polymers with N-donor-ligands
DiplPhys. Alexander Lajn	Prof. Dr. M. Grundmann / Prof. Dr. J. Käs	Fabrication and characterisation of transparent field-effect transistors
DiplPhys. Martin Lange	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	Growth and characterisation of quantum wire heterostructures
M.Sc. Chem. Ulrike Lehmann	Prof. Dr. B. Kersting / Prof. Dr. E. Hey-Hawkins	Hydrogenation of CO ₂ by supported container molecules
M.Sc. Chem. Jörg Lincke	Prof. Dr. H. Krautscheid / Prof. Dr. R. Gläser	Coordination polymers with nitrogen-rich ligands
DiplPhys. Michael Lorenz	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	Investigations on the stability of zinc oxide based metal-semi-conductor field-effect-transistors
M.Sc. Chem. Martyna Madalska	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	Immobilised switchable phosphine- based catalysts
M.Sc. Chem. Veronika Mäde	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	Modified pancreatic polypeptide for treatment of obesity
M.Sc. Phys. Tuhin Subhra Maity	Prof. Dr. P. Esquinazi / Prof. Dr. B. Kersting	Electronic transport in meso and nanoscopic magnetic nanostruc- tures
DiplPhys. Benno Meier	Prof. Dr. J. Haase / Prof. Dr. S. Berger	Ultra-high field magnetic resonance of modern materials
DiplPhys. Monika Möddel	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	Modelling and computer simulations of adsorption specifity of synthetic peptides
M.Sc. Chem. Tobias Möller	Prof. Dr. E. Hey-Hawkins / Prof. Dr. S. Berger	Synthesis of P-chiral phosphorus compounds derived from low-valent phosphorus species
DiplPhys. Alexander Müller	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	Investigation of carrier dynamics in ZnO films and microcavities
DiplPhys. Karla Müller	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	The use of scanning probe tech- niques and laser nanomanipulation to isolate and mechanostimulate highly potent mesenchymal stem cells
DiplPhys. Nils Neubauer	Prof. Dr. F. Cichos / Prof. Dr. K. Kroy	Photothermal fluctuation spectros- copy on gold nanoparticle dimers
DiplPhys. Lena Neumann	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	Hyperthermal ion assisted atomic assembly
M.Sc. Phys. K. David Nnetu	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	The use of biomechanics to reduce metastatic aggressiveness

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Souvik Pandey	Prof. Dr. E. Hey-Hawkins / Prof. Dr. B. Kersting	P-based polymers: synthesis and applications in materials science
M.Sc. Chem. Julian Rodger Frederic Pritzwald-Stegmann	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	Phosphorus-based organometallic/ inorganic hybrid materials
M.Sc. Chem. / M.Sc. Environmental protection Ksenia Jolanta Ramus	Prof. Dr. FD. Kopinke / Prof. Dr. R. Gläser	Thermodynamic activity versus total concentration of xenobiotics as predictors of bioavailability
DiplChem. Daniel Rathmann	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. A. Robitzki	Structure activity relationships of RF-amide peptide receptors with chemical modified peptides
M.Sc. Chem. Dennis Richter	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	Heterogeneous photocatalysis: water splitting with visible-light irradiation
M.Sc. Chem. Anastacia Romanova	Prof. Dr. W. Hackbusch / Prof. Dr. M. Grundmann	Molecular simulations of ion effects on structural and thermodynamical properties of biopolymers
DiplPhys. Martin Rothermel	Prof. Dr. T. Butz / Prof. Dr. M. Grundmann	Spatially resolved characterisa- tion of the composition, structural disorders and electronic properties of inorganic nanostructures
M.Sc. Chem. Klara Rusevova	Prof. Dr. FD.Kopinke / Prof. Dr. R. Gläser	Iron-based nanoparticles catalysts for oxidation of pollutants in water
DiplPhys. Florian Schmidt	Prof. Dr. M. Grundmann / Prof. Dr. R. Gläser	Characterisation of defects in het- ero- and nanostructures
DiplPhys. Jens Schneider	Prof. Dr. FD. Kopinke / Prof. Dr. M. Grundmann	Studies of dissociation processes of water exposed to high-frequency electromagnetic fields
DiplPhys. Sebastian Schöbl	Prof. Dr. W. Janke / Prof. Dr. M. Grundmann	Modelling and computer simulations of molecular pattern recognition
DiplChem. Matthias Scholz	Prof. Dr. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Imitation and modification of bioac- tive lead structures via integration of clusters
DiplPhys. Carsten Schuldt	Prof. Dr. J. Käs / Prof. Dr. B. Abel	Cellular force generation on the single molecule level
M.Sc. Phys. Ilya Semenov	Prof. Dr. F. Kremer / Prof. Dr. K. Kroy	Dynamics of DNA under tension and in confinement
DiplBiochem. Max Steinhagen	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. E. Hey-Hawkins	Enzyme analytics
DiplBiochem. Anja Steude	Prof. Dr. A. Robitzki / Prof. Dr. A.G. Beck-Sickinger	Development and fabrication of novel peptide based biosensors for neuronal diagnostic tools
DiplPhys. Marko Stölzel	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	Time-resolved spectroscopy on ZnO based micro- and nanowire hetero- structures and -cavities

Title and Name	First / Second Supervisor	Working title of doctoral thesis
DiplPhys. Dan Strehle	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	Mechanical and dynamic properties of actin bundles
M.Sc. Chem. Markus Streitberger	Prof. Dr. E. Hey-Hawkins / Prof. Dr. R. Gläser	Building catalytically active bi- metallic nano-frames with flexible bisphosphine ligands
DiplPhys. Chris Sturm	Prof. Dr. M. Grundmann / Prof. Dr. W. Janke	Investigation of the cw optical prop- erties of ZnO cavities
DiplPhys. Sebastian Sturm	Prof. Dr. K. Kroy / Prof. Dr. F. Kremer	Nonequilibrium dynamics of forced and confined semiflexible polymers
DiplChem. Ronny Syre	Prof. Dr. B. Kersting / Prof. Dr. M. R. Buchmeiser	Photo-induced electron tranfer in multimeric capsule complexes
M.Sc. Chem. Eng. Erik Thelander	Prof. Dr. B. Rauschenbach / Prof. Dr. M. Grundmann	Synthesis of nanostructures using laser ablation
DiplPhys. Martin Treß	Prof. Dr. F. Kremer / Prof. Dr. F. Cichos	Molecular dynamics in nanometre- thick polymer layers studied by means of broadband dielectric spectroscopy
DiplPhys. Olaf Ueberschär	Prof. Dr. F. Kremer / Prof. Dr. W. Janke	Investigating stochastic thermody- namics by means of optical tweezer
DiplPhys. Carolin Wagner	Prof. Dr. F. Kremer	Investigation of the interaction of receptors and ligands by optical tweezers
DiplPhys. Franziska Wetzel	Prof. Dr. J. Käs / Prof. Dr. K. Kroy	Direct staging of primary mamma- carcinomas by determining their cellular composition including metastatically competent cells, dormant cancer cells and cancer stem cells
DiplPhys. Micha Wiedenmann	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	Cluster aggregation and condensa- tion of nano-objects
M.Sc. Chem. Patrick With	Prof. Dr. R. Gläser / Prof. Dr. E. Hey-Hawkins	Preparation, physico-chemical characterisation and testing of sup- ported metal (oxide) catalysts
DiplPhys. Lars Wolff	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	Plasticity and active remodelling of cells
DiplPhys. Hendrik Zachmann	Prof. Dr. B. Rauschenbach	Electrical defects in ion beam as- sisted deposition of Cu(In,Ga)Se ₂ thin film solar cells
DiplPhys. Jan Zippel	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	Magnetic tunnel junctions

Alumni 2010

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Dalia Angeles-Wedler	Prof. Dr. FD. Kopinke	Environmental application of palla- dium catalyst for hydrodechlorina- tion reactions
Dr. rer. nat. Heiko Frenzel	Prof. Dr. M. Grundmann / Prof. Dr. H. Morgner	Transport investigations on ZnO based field-effect structures
Dr. rer. nat. Nicole Jahr	Prof. Dr. S. Berger / Prof. Dr. A.G. Beck-Sickinger	NMR-investigations at modified ubiquitines
Dr. rer. nat. Markus Kraus	Prof. Dr. FD. Kopinke	Application of coupled temperature- and concentration pulses for effi- cient adsorptive catalytic elimina- tion of pollutants from contaminated exhaust air
Dr. rer. nat. Carolin Limburg	Prof. Dr. E. Hey-Hawkins / Prof. Dr. H. Krautscheid	Ferrocenylphosphanides and phos- phanediides as building blocks for heterometallic complexes
Dr. rer. nat. Johanna Lutz	Prof. Dr. B. Rauschenbach	Phase formation and diffusion be- haviour for ion implanted austenitic metal alloys
Dr. rer. nat. Marisa Mäder	Prof. Dr. B. Rauschenbach	Substrate-bound nanostructures by diffraction mask projection laser ablation
Dr. rer. nat. Santhosh-Kumar Podiyanachari	Prof. Dr. M.R. Buchmeiser / Prof. Dr. B. Rauschenbach	Cyclopolymerisation of 1,6-hepta- diynes
Dr. rer. nat. Franziska Weichelt	Prof. Dr. M.R. Buchmeiser / Prof. Dr. B. Kersting	Synthesis und characterisation of new composite and hybrid materials based on functionalised nano- und microparticles of metal oxides and salts

Mini-projects

Student name	Doctoral candidate (supervisor)	Title of mini-project
Tobias Diez	DiplPhys. Alexander Lajn	Enhancement of data evaluation, measurement automatisation and characterisation of transparent oxide semiconductor based devices
Pierre Eckold	M.Sc. Chem. Daniel Lässig	Synthesis and characterisation of metal-organic frameworks
Annika Eisenschmidt	M.Sc. Chem. Martyna Madalska	Switchable ferrocenyl phosphines
Marcel Handke	M.Sc. Chem. Jörg Lincke	Synthesis and characterisation of metal-organic frameworks
Tobias Kühl	DiplBiochem. Sina Haas	Electrophysiological screening of potential drug candidates against cardiovascular diseases and ischemia
Marc Lämmel	DiplPhys. Sebastian Sturm	Fluidisation in crosslinked actin networks
Wolfram Pönisch	DiplMath. Melanie Knorr	Role of stochasticity in a moving thin polymer film
Steven Reichardt	M.Sc. Phys. Michael Jurkutat	Coupled resonator probe for nanoscale distance measurements with NMR
Axel Straube	DiplChem. Julia Haushälter	Phosphane baskets
Sudarsan Venkat Ramani	M.Sc. Chem. Souvik Pandey	Synthesis and characterisation of chiral polyferrocenylphosphines
Ralf Wunderlich	DiplPhys. René Feder	Defect production by single ions tra- versing multigraphen
Johannes Zierenberg	DiplPhys. Sebastian Schöbl	Semiflexible polymers in a disorder landscape of soft discs

Statistics



Research Topics

ORIGIN OF DOCTORAL CANDIDATES:



Ultrafast spectroscopy and nanoscopy

Prof. Dr. Bernd Abel

M.Sc. Chem. Anika Gladytz

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



Specific project of A. Gladytz:

Atomic Force Microscopy (AFM) of Peptide-Silicon and Peptide-Mica Hybrid Interfaces (Coopertation with A. Beck-Sickinger group)

One strategy to induce biocompatibility of inorganic surfaces is the application of peptide coatings. In this work the binding behaviour and surface layer formation of promising amino acid sequences to silicon and mica have been investigated by a combination of atomic force microscopy (AFM) and fluorescence microscopy. Both, silicon and mica, were incubated at ambient temperatures with peptides containing RHTRK sequences (see Fig., [1]), an amino acid sequence with electrostatic surface affinity, once (peptide au13) and fourfold (peptide bk18) and a biotin residue for fluorescence labelling.

The coverage is a concentration dependent phenomenon that might be quantised by an optical measurement (absorption, fluorescence). We investigated the fluorescence of fluorescein labelled peptides for silicon surfaces. Due to autofluorescence of mica in the visible region we applied a NIR fluorescence label (DyLight750streptavidin) for measurements on mica. Both measurements, AFM and fluorescence, confirm that the fourfold repetition of RHTRK in bk18 result in an increase of the surface affinity compared to au13 by two orders of magnitude (complete surface coverage above a EC50 concentration, see Fig., [2]). The affinity to mica is even bigger (EC50 = 2.0 ± 0.1 nM).

The aim of the current efforts is to study the morphology of the peptide layers and their formation principles. Although the size of the two peptides differs substantially, they form disc shaped clusters of 2–3 nm in height and 40–50 nm in diameter barely dependent on the concentration (apart from multilayer formation.) Clusters of similar size are found in measurements on mica coverage suggesting it to be a property of the peptide formed prior to deposition or induced by the surface.

[1] Peptides bk18 (sequence RTHRKRTHRKRTHRKRTHRK-OH) and au13 (sequence VRTRDDARTHRK-OH) were provided by Rayk Hassert (AG Beck-Sickinger, Biochemistry Department at Universität Leipzig).

[2] Ming Zhou, Atomic Force Microscopy of Synthetic Peptides bound to a Silicon Surface, Master Thesis, Universität Leipzig, 2010.

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Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger

Dipl.-Biochem. Verena Ahrens, Dipl.-Biochem. Lars Baumann, Dipl.-Chem. Kathrin Bellmann-Sickert, M.Sc. Chem. Sylvia Els Dipl.-Biochem. Rayk Hassert, M.Sc. Chem. Cathleen Juhl, M.Sc. Chem. Veronika Mäde, Dipl.-Chem. Daniel Rathmann, Dipl.-Biochem. Max Steinhagen, Dr. Denise Zwanziger

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 (Dipl.-Chem.), Kathrin Bellmann-Sickert (Dipl.-Chem.) and Daniel Rathmann (Dipl.-Chem) synthesise chemically modified peptide hormones that are modified by nonnatural amino acids, lipid or polyethylene glycol moieties to improve stability in biological system. They address ghrelin, neuropeptide Y, pancreatic polypeptide and neuropeptide FF, respectively.

Verena Ahrens and Denise Zwanziger work on the development of novel antitumour peptides by conjugation with carbaboranes or radionuclide chelating com-





pounds. 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 2010 was the proof of principle by Khan, Zwanziger et al. for the successful targeting of breast cancer tumours in human. Denise Zwanziger finished her doctoral thesis in October 2010.

In the field of chemical modification of proteins, Cathleen Juhl (Dipl.-Chem), Kathrin Bellmann-Sickert (Dipl.-Chem.) 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. Successful labelling could be published by different strategies.

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.

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Biomolecular problems studied by NMR

Prof. Dr. Stefan Berger M.Sc. Chem. Murali Dama, Dr. Nicole Jahr

Murali Dama has started a project to synthesise molecules which could induce magnetic alignment in organic solvents. Whereas this kind of alignment has been already established for biomolecular NMR, i.e. in water as the solvent, convincing solutions for the organic phase are lacking. Murali Dama has focused in the last year on so called LMOG's (low molecular weight organic gelators) with the hope

that the introduction of extended π -systems will promote the orientation of the gelphase and transfer this alignment to dissolved organic molecules. Murali Dama has succeeded in the synthesis of several LMOG's and characterised their gelation by diffusion NMR measurements, however, so far, we could not yet observe the desired alignment within the magnetic field.

A closely related project carried out by Lisett Valentin tries to induce such an align-



ment with the help of the anisotropy of the electron cloud of paramagnetic lanthanide ions. For this, suitable lanthanide complexes have to be synthesised and the organic compound of interest has to be covalently linked to such a lanthanide complex. Similarly to the project of Murali Dama this work is still in its early stages.



The desired goal: left NMR tube: an organic molecule (strychnine) randomly oriented; right NMR tube: orientation induced by an aligned gel

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

Prof. Dr. Tilman Butz

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

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

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.

René Feder is part of the ESF-Nachwuchsforschergruppe "funktionale multiskalige Strukturen". His research topic is the defect production by single ions traversing multi-graphene. Therefore resistance-measurements were performed before, during and after the irradiation of multi-graphene samples by high energy hydrogen and helium ions. The setup was modified to measure under vacuum conditions and different gas atmospheres and pressures. Depending on these parameters, the sample showed different behaviors in the resistance change. Next intention will be the sample preparation on Si_3N_4 -windows or SU-8-grids (produced with proton beam writing) to detect the transmitted ions.

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



Single photon generation from semiconductor nanostructures

Prof. Dr. Frank Cichos

Dipl.-Phys. Nils Neubauer

The controlled generation of single photons is one of the important fundamentals for quantum in-formation processing and other optical applications such as direct absorption measurements.

Single photon emission occurs under zero shot noise and thus provides the ideal source i.e. for quantum cryptography where information is encoded in the polarisation state of a single photon. Single photon generation is possible by exploiting a single two-level quantum system, which is excited by a resonant laser. Such single quantum systems can be realised using single organic molecules, single semiconductor nanostructures or even single atoms. Here we employ single semiconductor nanoparticles and nanorods to generate single photons. As materials we have selected cadmium-selenide (CdSe) quantum dots with zinc-sulfide (ZnS) capping layers as well as zinc oxide/zinc magnesium oxide (ZnO/ZnMgO) nanorods (collaboration with AG Prof. M. Grundmann). Further a special laser scanning confocal microscope for excitation and detection of single photons in the ultraviolet

spectral region has been built. The microscope uses evanescent wave excitation to reduce background fluorescence photons. Emitted photons are collected in a laser scanning confocal mode and detected by a Hanbury Brown Twiss dual detector configuration with a single photon counter. The setup has recently test with the help of CdSe/ZnS quantum dots embedded in polymers and studied at room temperature. The calculated second order intensity autocorrelation function of the emitted photons clearly displays a dip at zero delay between two detected photons. This provides proof of the single photon emission of the studied CdSe/ZnS quantum dots. The in-



crease in the correlation function delivers further information on the excited state lifetime of the two-level system. Current experiments now aim at the UV excitation and detection of single photons from ZnO/ZnMgO nanorods, which would pave the ways for single photon generation in the ultraviolet spectral region.





Confocal fluorescence image of single CdSe/ ZnS colloidal quantum dots embedded in a polymer (image size $10 \times 10 \mu m$); the image has been recorded in a special home-built laser scanning confocal microscope for UV exciation and detection Second order intensity autocorrelation of a single quantum dot in the left image; the dip at zero time delay clearly reveals the so called antibunching of photons and thus the single photon emission

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New findings in graphite: getting closer to its intrinsic electronic properties

Prof. Dr. Pablo D. Esquinazi

M.Sc. Phys. Ana Isabel Ballestar Balbas, M.Sc. Phys. Srujana Dusari, M.Sc. Phys. Tuhin Subhra Maity

Although graphite has been widely investigated within the last 50 years, the intrinsic electronic properties of the graphene layers within graphite are still under discussion. Within our research we are interested to study the intrinsic properties of graphene layers within graphite. Due to the natural packing of the graphene layers within graphite, their natural shielding from the environment and their weak coupling we expect that they behave more ideal than single layers. Experimental results indicate that graphene layers within graphite show outstanding two-dimensional ballistic properties with a very low carrier density already at room temperature, overwhelming those in single graphene layers. The resistivity measured in bulk graphite samples is not intrinsic but comes from internal interfaces or grain boundaries running parallel to the graphene layers. Due to disorder and/or hydrogen doping these boundaries can have an enhanced carrier density, short-circuiting the parallel running graphene layers. In the last years there were several published hints for the existence of granular superconductivity in bulk graphite, which is still under discussion. Our work's aim is to study the electronic properties of these graphite interfaces and to show that superconductivity is localised in patches embedded in a semiconducting-like graphene matrix within the interfaces.

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Scanning electron microscope images of a graphite ~15 nm thick sample with a constriction and the four contact electrodes for resistance measurements; the white dashed line indicates the sample borders

The picture shows a 500 nm constriction on the same sample; the change of the electrical resistance vs. constriction width is used to check the ballistic or diffusive behavior of the carriers within the graphene layers

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Complex nanomaterials for innovative catalysis

Prof. Dr. Roger Gläser

M.Sc. Chem. Thomas Heinze, 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. We apply combined templating strategies and scaffolding approaches to synthesise novel materials for the use as catalysts and catalyst supports. For instance, porous carbon spheres are used as scaffolds and nanoreactors for the surfactant-assisted preparation of ziroconia spheres with hierarchically structured pore systems (Figure). Moreover, chemically diverse active components are introduced into the pore systems of these materials. Moreover, the distinct and





Carbon sphere used as an exotemplate (*left*) for the preparation of zirconia spheres with hierarchically structured pore system (*right*)

tunable properties of novel solvent systems such as supercritical fluids and ionic liquid phases under nanconfinement within the pore space of the materials are applied to control the selectivity of catalytic conversions on the level of molecules and molecular assemblies.

The concepts of these complex nanomaterials are applied to contemporary fields of heterogeneous catalysis. Applications in environmental catalysis such as selective catalytic reduction of nitrogen oxides (SCR-DeNO_x) by transport-optimised pore systems and energy-related catalysis such as photocatalytic water splitting or high-temperature conversions for hydrogen production such as the dry reforming of methane with carbon dioxide are typical examples.

⇒ Zirconia with Defined Particle Morphology and Hierarchically Structured Pore System Synthesized via Combined Exo- and Endotemplating

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ZnO-based alloys for nano-scale optoelectronic devices

Prof. Dr. Marius Grundmann

Dipl.-Phys. Tammo Böntgen, Dipl.-Phys. Kerstin Brachwitz, M.Sc. Phys. Christof Peter Dietrich, Dr. Heiko Frenzel, Dipl.-Phys. Helena Hilmer, Dipl.-Phys. Fabian Klüpfel, Dipl.-Phys. Alexander Lajn, Dipl.-Phys. Martin Lange, Dipl.-Phys. Michael Lorenz, Dipl.-Phys. Alexander Müller, Dipl.-Phys. Florian Schmidt, Dipl.-Phys. Marko Stölzel, Dipl.-Phys. Chris Sturm, Dipl.-Phys. Jan Zippel

ZnO based heterostructures are very promising candidates for photonic and optoelectronic applications in the UV spectral range. To obtain efficient emitters a deep understanding of the properties of the applied materials is essential. Wurtzite $Mg_xZn_{1-x}O$, a suitable barrier material, has therefore been investigated to understand the dynamic carrier processes and their interaction properties with light.

In ZnO, electron-hole pairs form a nanometre-sized hydrogen-like bound state, the so-called exciton. However, this simple model cannot thoroughly explain light absorption and emission in $Mg_xZn_{1-x}O$ alloys. Therefore, model wave functions of 1D excitons have been calculated by solving the two-particle Schrödinger equation for electron and hole within the effective mass approximation. The computations



Probability amplitudes of calculated 1D electron-hole wavefunctions; the electron position is plotted horizontally, the hole position vertically ↑ Scheme and electron microscopy image of a core/shell nanowire heterostructure and luminescence spectra for two QW-thicknesses



show a downward trend for the transition probabilities into single electron-hole states with increasing energy. While mostly the "bright" low-energy states take part in the luminescence emission, much more "dark" high-energy states are available for absorption processes as the density of states increases for increasing energy. This contributes to the large Stokes shift between absorption and emission maxima observed for these alloys.

In order to realise emitters as a building block for nano-scale devices, core/shell nanowire heterostructures were grown with pulsed laser deposition. The integration of a quantum well (QW) in the $Mg_xZn_{1-x}O$ shell around the ZnO nanowire core allowed an enhancement of the emission properties and a tunable QW-energy. Due to the usage of an $Mg_xZn_{1-x}O$ barrier with a large Mg-content of 25%, the QW emission energy was tuned between 3.42 eV and 3.68 eV by changing the QW-thickness. The core/shell structures show a larger QW energy range compared to reports in the literature. Besides a small region near the tip, the QW-energy is very homogeneous along the wire axis, which is also result of the expertise in $Mg_xZn_{1-x}O$ thin film growth and the understanding of the exciton-localisation that occurs.

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 G. Zimmermann, M. Lange, B. Cao, M. Lorenz, M. Grundmann / phys. stat. sol. RRL (2010) 4 82
- ⇒ Observation of Strong Light-Matter Coupling by Spectroscopic Ellipsometry
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- ⇒ Donor-Acceptor Pair Recombination in Non-Stoichiometric ZnO Thin Films C.P. Dietrich, M. Lange, G. Benndorf, H. von Wenckstern, M. Grundmann / Sol. Stat. Comm. (2010) 150 379
- ⇒ Homoepitaxial Mg_xZn_{1-x}O (0 ≤ x ≤ 0.22) Thin Films Grown by Pulsed Laser Deposition
 M. Lorenz, M. Brandt, M. Lange, G. Benndorf, H. von Wenckstern, D. Klimm, M. Grundmann / Thin Solid
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- ⇒ Tuning the Lateral Density of ZnO Nanowire Arrays and its Application as Physical Templates for Radial Nanowire Heterostructures

B. Cao, J. Zúñiga-Pérez, C. Czekalla, H. Hilmer, J. Lenzner, N. Boukos, A. Travlos, M. Lorenz, M. Grundmann / J. Mat. Chem. (2010) **20** 3848

- ⇒ p-Type Phosphorus Doped ZnO Wires for Optoelectronic Applications
 B.Q. Cao, M. Lorenz, G. Zimmermann, C. Czekalla, M. Brandt, H. von Wenckstern, M. Grundmann / in: Nanowires. ed. P. Prete (2010) 117 ISBN 978-953-7619-79-4
- Interface Effects in ZnO Metal-Insulator-Semiconductor- and Metal-Semiconductor-Structures
 H. Frenzel, H. von Wenckstern, A. Lajn, M. Brandt, G. Biehne, H. Hochmuth, M. Lorenz, M. Grundmann / AIP Conf. Proc. (2010) 1199 469



⇒ Ag Related Defect State in ZnO Thin Films
 H. von Wenckstern, A. Lajn, A. Laufer, B.K. Meyer,
 H. Hochmuth, M. Lorenz, M. Grundmann / AIP Conf.
 Proc. (2010) 1199 122

⇒ Two-Dimensional Electron Gases in MgZnO/ ZnO Heterostructures

H. von Wenckstern, J. Zippel, A. Lajn, M. Brandt, G. Biehne, H. Hochmuth, M. Lorenz, M. Grundmann / AIP Conf. Proc. (2010) **1199** 99

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NMR and EPR investigations of the electronic properties of modern materials

Prof. Dr. Jürgen Haase

M.Sc. Phys. Michael Jurkutat, M.Sc. Chem. Anusree Viswanath Kuttatheyil, Dipl.-Phys. Benno Meier

Our group investigates the electronic properties of materials with the methods of solid- state nuclear magnetic resonance (NMR) and electron-paramagnetic resonance (EPR). In NMR, we are working under the highest magnetic fields and highest pressures. Within the Graduate School BuildMoNa we focus on three areas of research, development of magnetic resonance in pulsed magnetic fields (up to 80 T) (B. Meier), high-temperature superconductors (M. Jurkutat) as well as modern porous coordination polymers, i.e. metal-organic frameworks (MOF) (A.V. Kuttathey-il).





In cooperation with the Helmholtz-Zentrum Dresden-Rosendorf, where the highest magnetic fields generated with pulsed magnets can be achieved, we are working on NMR investigations to expand the potential applications of NMR. Although the magnetic field strength is changing on a timescale of milliseconds, we were able to reproducibly record NMR signals and accumulate the spectra as a function of magnetic field strength. We were also able to differentiate two signals in a mixture of $_{19}$ F-containing liquids.

The investigation of high-temperature superconductors by NMR is a valuable tool since elementselective information about the electron density can be obtained and compared to existing theories. ₁₇O-enriched samples show two different resonances that show signal overlap. By sophisticated NMR techniques we are able to differentiate those two signals and get a more detailed picture that give rise to a two-liquid scenario in those electron-doped materials.

Metal-organic frameworks (MOFs) offer high potential for many applications such as catalyis, separation, and gas-storage. Solid-state NMR and EPR can deliver important information on the interaction between small adsorbed guest molecules and the host frame including the location of the adsorption site and the determination of the adsorption strength. Among others, we investigate mixed-metal MOFs containing zinc and cobalt with unconventional triazole linkers.

⇒ New Approach to High-Pressure Nuclear Magnetic Resonance with Anvil Cells
 T. Meissner, S.K. Goh, J. Haase, B. Meier, D. Rybicki, P.L. Alireza / J. Low Temp. Phys. (2010) 159 284

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

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

Proteins are the basic building blocks for all living organisms we know. In Living Nature, proteins work very efficiently as selective catalysts, sensors, controllers, etc.; moreover, proteins are biodegradable. All of this brings protein-based devices (where proteins are used as functional blocks of man-made equipment) to one of the most prospective technology of the 21st century.

However, there is a big lack in our understanding of the molecular-level mechanisms of how proteins work. We know that the activity of a protein depends on its structure. It is also known, that solvent and various background compounds (salts, auxiliary solvents, surfactants, other macromolecules, etc.) can make dramatic effects on protein/peptide structure in solution as well as on biomoleculebiomolecule and biomolecule-surface interactions. However, currently we are still far from complete understanding of the basic mechanisms which govern protein folding and conformational stability upon changes in the protein environment. Once we un-



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





Protein-ion binding in aqueous solution

of the complexes with similar complexes found in crystal structures of natural proteins (Torrance G.M. et al., J. Mol. Biol. (2009) **385** 1076) we may conclude that the ion-peptide complexes are stable during aggregation and precipitation. This finding gives a new route for designing basic physical-chemical tools to control geometry of protein/peptide aggregates by changing the background compounds during biomacromolecule precipitation.

⇒ Selective Na⁺/K⁺ Effects on the Formation of alpha-Cyclodextrin Complexes with Aromatic Carboxylic Acids: Competition for the Guests

I.V. Terekhova, A.O. Romanova, R.S. Kumeev, M.V. Fedorov / The journal of physical chemistry / B (2010) 114 12607

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derstood these mechanisms, we could make a significant step forward to controllable and sustainable production of peptide/protein-based devices. Good candidates to explore these mechanisms are small synthetic peptides due to their relative simplicity.

In our work we investigate interactions of small synthetic peptides with water and buffered aqueous solutions. We found that these peptides can form complexes with ions or water molecules in solution. Comparing the characteristic structures



Smart molecular precursors for novel materials, catalysis and biosciences

Smart molecular precursors for novel materials, catalysis and biosciences

Prof. Dr. Evamarie Hey-Hawkins

M.Sc. Chem. René Frank, Dipl.-Chem. Julia Haushälter, M.Sc. Chem. Aslihan Kircali,

M.Sc. Chem. Anika Kreienbrink, Dr. Carolin Limburg, M.Sc. Chem. Martyna Madalska, M.Sc. Chem. Tobias Möller, M.Sc. Chem. Souvik Pandey,

M.Sc. Chem. Julian Rodger Frederic Pritzwald-Stegmann, Dipl.-Chem. 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).

Phosphorus-rich transition metal complexes were developed as *molecular precursors for novel materials*. Thus, thermal decomposition gave phosphorus-rich binary metal phosphides MP_x (x > 1) whose optical, electronic and magnetic properties are now being studied (Aslihan Kircali).

Polymers are typically the fundamental building blocks of scaffolds but more and more they also play a role as smart molecules.

Strained phosphorus-containing heterocycles are highly suitable precursors for the synthesis of novel chiral phosphorus-based polymers. At present we are focusing on the stereoselective synthesis of chiral heterocyclic precursors (Anika Kreienbrink, Tobias Möller).

Inorganic P-based chiral polymers that also include redox-active transition metals in the side chain or the polymer backbone will be obtained from chiral primary and secondary ferrocenyl phosphine–borane adducts via catalytic dehydrogenation (Souvik Pandey) or by employing highly reactive terminal transition metal phoshinidene complexes ($L_nM=PR$ moieties) in copolymerisation reactions. These P-based



Organometallic rhodium-phosphorus complex as suitable precursor for RhP₂



polymers are expected to exhibit NLO properties besides electrical conductivity and possibly superconductivity.

Furthermore, chiral primary and secondary ferrocenyl phosphines are prepared as useful precursors for organometallic/inorganic metal-phosphorus-based hybrid materials, which can exhibit unusual structures (*clusters, polymers, 2D or 3D networks*) in the solid state, as well as unusual electronic, magnetic and optical properties (Carolin Limburg, Julian Pritzwald-Stegmann).

In *catalysis*, an important goal is to combine the best of all areas – homogeneous, heterogeneous, and bio-inspired catalysis. Phosphorus-based container molecules (*phosphine baskets*, Julia Haushälter) or dinuclear molecular squares (Markus Streitberger) are promising candidates in this respect as they allow for interplay





of molecular recognition (bio-inspired) and transition-metal catalysis. *Switchable catalysts* based on chiral ferrocenyl phosphines (redox-active ferrocenyl unit, UV-active π system) are developed as ligands in catalytically active complexes. Suitable precursors are grafted on silica or graphite and their applications are explored (Martyna Madalska). Furthermore, novel chiral phosphorus-based *ionic liquids* are prepared as chiral scaffolds for catalysts or stabilisation of catalytically active nanoparticles.

In *biosciences, carbaborane clusters* are either used as pharmacophoric entities in the cyclooxygenase (COX) inhibitors aspirin (asborin) and indomethacin (indoborin) to influence the electronic structure and increase the bulkiness of the inhibitor (Matthias Scholz) or as conjugates with tumour-targeting entities, such as a Y_1 receptor-selective neuropeptide Y (NPY) derivative, to allow selective delivery of boron into tumour cells, which is one of the major requirements for boron neutron capture therapy (René Frank).



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Carbaborane conjugate of a neuropeptide Y (NPY) derivative

- ⇒ A Sodium Ferrocenylphosphanide Polymer Based on Racemic Primary Aminoalkyl(bisphosphanyl)ferrocene C. Limburg, S. Gómez-Ruiz, E. Hey-Hawkins / Dalton Trans. (2010) **39** 7217
- ⇒ Synthesis of Racemic Aminoalkylferrocenyldichlorophosphanes and -dialkyl Phosphonites and their Conversion to Primary Phosphanes
 - C. Limburg, P. Lönnecke, S. Gómez-Ruiz, E. Hey-Hawkins / Organometallics (2010) 29 5427

Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke

Dipl.-Phys. Monika Möddel, Dipl.-Phys. Sebastian Schöbl, Dipl.-Phys. Micha Wiedenmann

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

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

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

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



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

Two other BuildMoNa doctoral candidates have very successfully completed their doctoral thesis in 2009 and are now working as postdocs at EPF Lausanne, Switzerland (Sandro Wenzel) and the University of Georgia, USA (Stefan Schnabel). With both there are still ongoing collaborations exploiting some of the material in their theses:

Sandro Wenzel performed research into the physics of quantum phase transitions in dimerised Heisenberg models and other quantum effects for patterned spin systems, for which he has identified an unconventional universality class. Further results for the quantum compass models are of relevance for certain aspects of quantum computing.

Stefan Schnabel developed novel simulation methods for the classification of symmetry properties governing the crystallisation of single flexible polymers and studied the relation to compact hydrophobic-core formation and the collapse transition.

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





Adsorption phase diagram for a 40mer and representative polymer conformations in each phase, where ε_s parametrises the substrate attraction strength and T is the temperature

⇒ Re-Examining the Directional-Ordering Transition in the Compass Model with Screw-Periodic Boundary Conditions

S. Wenzel, W. Janke, A. Läuchli / Phys. Rev. E (2010) 81 066702

⇒ Systematic Microcanonical Analyses of Polymer Adsorption Transitions M. Möddel, W. Janke, M. Bachmann / Phys. Chem. Chem. Phys. (2010) 12 11548

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

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

Prof. Dr. Josef Alfons Käs

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

The investigation of physical, i.e. material, properties of cells is an emerging field in physics which connects biophysics, cell biology and medical research. Understanding cytoskeletal, i.e. actin structural arrangement, as well as the influence of cytoskeletal alterations on cellular mechanical properties is the scope of the BuildMo-Na students of the Soft Matter Physics Division. During malignant transformation of cells changes in their cytoskeleton and the cell membrane occur. Such processes are mirrored in the viscoelastic properties, viz. BuildMoNa students investigated that primary breast tumour cells are softer than normal breast cells. Interestingly,





softening correlates with cell proliferation, as well as with lamellipodial dynamics. Furthermore, some cells were obtained which actively contract when they are treated with the laser beams in the Optical Stretcher. From such active cell reaction the cell gains the ability to adapt its mechanical properties to the environment which can enhance the possibility of the cell to leave the primary tumour and form distant metastasis. This new insights were published in Nature Physics and were discussed at the international BuildMoNa minisymposium "Physics of Cancer", October 2010.

 \Rightarrow Stiffening of Human Skin Fibroblasts with Age

C. Schulze, F. Wetzel, T. Kueper, A. Malsen, G. Muhr, S. Jaspers, T. Blatt, K.-P. Wittern, H. Wenck, J.A. Käs / Biophys. J. (2010) **99** 2434

- ⇒ Are Biomechanical Changes Necessary for Tumour Progression?
 A. Fritsch, M. Höckel, T. Kiessling, K.D. Nnetu, F. Wetzel, M. Zink, J.A. Käs / Nat. Phys. (2010) 6 730
- ⇒ Mesenchymal Stem Cells in Cartilage Repair: State of the Art and Methods to monitor Cell Growth, Differentiation and Cartilage Regeneration

J. Galle, A. Bader, P. Hepp, W. Grill, B. Fuchs, J.A. Käs, A. Krinner, B. Marqua, K. Muller, J. Schiller, R.M. Schulz, M. von Buttlar, E. von der Burg, M. Zschar-

nack, M. Loffler / Current Medicinal Chemistry (2010) **17** 2274

 ⇒ Probing the Physics of Tumor Cells from Mechanical Perspectives
 M. Zink, A. Fritsch, F. Wetzel, K.D. Nnetu, T.
 Kielling, LA, Kög (Cell Name, Neurolattor of the

Kießling, J.A. Käs / Cell News – Newsletter of the German Society for Cell Biology (2010) **36** 17 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

Metalated container molecules in catalysis and molecular magnetism

Prof. Dr. Berthold Kersting

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

We investigate various aspects of the chemistry of metalated container molecules. Our studies are devoted to the encapsulation of catalytically active transition metal complexes within self-assembled molecular capsule complexes. One project aims at the development and use of catalysts which unite novel aspects of supramolecular chemistry and transition metal catalysis for the activation and transformation of small molecules (M. Golecki, U. Lehmann). The encapsulation of the catalyst and the substrates will increase their effective concentration and decrease their solvation, both of which can have a marked influence on the activity of the system or may result in novel patterns of reactivity.

Another project deals with the development, synthesis and characterisation of novel classes of molecular based magnetic materials (J. Lach, R. Syre). The com-





The cover picture shows a schematic representation of the procedure used for the determination of the magnetic properties of the macrocyclic dinickel complex [Ni₂L(μ -SCN₄Me)]BPh₄•2MeCN. On the left, the complex is depicted in the form of its two nickel atoms, their first coordination sphere and the 1-methyltetrazole-5-thiolate coligand as obtained from the crystal structure determination. The found N(3),N(4)-bridging coordination mode is hitherto unknown for 1-R-tetrazole-5-thiolates. In addition, theoretical calculations were carried out in order to study the coordination features of the complex. Details are discussed in the article by S.V. Voitekhovich, B. Kersting et al., p. 5343.

pounds 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.

 $\Rightarrow Magnetic Properties of Mixed Ligand Ni^{ll}_{2} and Ni^{ll}_{4} Complexes Composed of Macrocyclic Hexaamine-Dithiophenolato and Bridging Tetrazolato Ligands$

J. Lach, S.V. Voitekhovich, V. Lozan, P.N. Gaponik, O.A. Ivashkevich, J. Lincke, D. Lässig, B. Kersting / Z. Anorg. Allg. Chem. (2010) **636** 1980

⇒ Dependence of the Chemical Properties of Macrocyclic $[Ni^{II}_{2}L(u-O_{2}CR)]^{+}$ Complexes on the Basicity of the Carboxylato Coligands (L = Macrocyclic $N_{6}S_{2}$ Ligand)

U. Lehmann, J. Klingele, V. Lozan, G. Steinfeld, M.H. Klingele, S. Käss, A. Rodenstein, B. Kersting / Inorg. Chem. (2010) 49 11018

⇒ A Novel Metal Binding Mode of 1-R-5-Thiotetrazolates: N(3),N(4)-Bridging. Synthesis, X-Ray Diffraction, Magnetic Properties and Quantum-Chemical Study of a Macrocyclic Dinickel Complex Coligated by 1-Methyl-5-thiotetrazolate

S.V. Voitekhovich, R. Syre, J. Lach, V. Matulis, P. Gaponik, O.A. Ivashkevich, B. Kersting / Eur. J. Inorg. Chem. (2010) 5343

 \Rightarrow Two-Step Spin Crossover in the Mononuclear Iron(II) Complex [Fe^{II}(L)₂(NCS)₂] (L = 2,5-di-(2-pyridyl)-1,3,4-thiadiazole)

J. Klingele, D. Kaase, M.H. Klingele, J. Lach, S. Demeshko / Dalton Trans. (2010) 1689

 ⇒ High-Field ESR and Magnetization Study of a Novel Macrocyclic Chelate Trinuclear Ni(II) Complex
 Y. Krupskaya, A. Parameswaran, A. Alfonsov, R.
 Klingeler, V. Kataev, N. Beyer, J. Lach, M. Gressenbuch, B. Kersting, B. Büchner / J. Low Temp. Phys. (2010) 159 84 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

Smart molecules from theoretical calculations

Prof. Dr. Barbara Kirchner

M.Sc. Chem. Martin Brehm

As trajectories from MD simulations are paths through the high-dimensional phase space, it is essential to perform steps for dimension reduction in order to gain insight into the simulated system. Because the choice of these dimension reduction algorithms is so important, we continued to develop our own trajectory analysing and visualising programme package, called TRAVIS, in 2010. Travis will be published in 2011 and will be freely available in the internet as an open source project.

Many of the analyses that are available in TRAVIS have been applied to the systems we simulated. Among these systems are a classical MD simulation of the ionic liquid [Bmim][Br], ab initio MD simulations for several mixtures of the very important ionic liquid [Emim][OAc] with water, and a gas phase study of $[\text{Emim}][\text{EtSO}_4]$. These studies will also be published in 2011. Some snapshots of the analyses' results are shown below.





 Defining a hydrogen bond criterion in a combined distance/angle histogram





Movement of single ion pairs over time

Temporal development of hydrogen bonds

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Wastewater treatment with colloids and nanocatalysts

Prof. Dr. Frank-Dieter Kopinke

Dr. Dalia Angeles-Wedler, Dr. Markus Kraus, M.Sc. Chem./Environ. Prot. Ksenia J. Ramus, M.Sc. Chem. Klara Rusevova, Dipl.-Phys. Jens Schneider

Klara Rusevova has continued her work on Fe-based Nano-Catalysts for Oxidation of Organic Pollutants in Water. The application of iron-based nano-catalysts is a new tool for advanced oxidation processes (AOPs) for treating pollutated wastewaters. The activation of H₂O₂ on the surface of Fe-based nano-particles (NPs) at neutral pH avoids problems related to classical Fenton-reaction with dissolved





TEM image of Fe₃O₄

↑ TEM image of LaFeO₃

iron as catalyst which needs strongly acidic conditions. We synthesised and tested nano-particulate Fe-catalysts such as magnetite (Fe_3O_4) and perovskite minerals in the Fenton-like oxidation of organic pollutants at neutral pH in batch experiments: $LaFeO_3$ and $BiFeO_3$ perovskites show significantly higher specific activities for phenol oxidation with H₂O₂ and use it more efficiently than the predescribed catalyst magnetite. TEM analyses show crystallite sizes in the nanometre range for



— Temperature profile within a water flow (upwards in a glass reactor) which is exposed to an external field of radiowaves, visualised by means of an IR-camera; at the bottle neck (light spot) water is dissociated into H₂ and O₂ at about 100 °C

perovskites and magnetite (see figures). However, BET analyses revealed relatively low specific surface areas for LaFeO₃ (5.2 m²/g) and BiFeO₃ (3.2 m²/g) in comparison with magnetite (95 m²/g).

Jens Schneider has continued his studies on Burning Water and Nano-Particles. Water can be dissociated into the elements hydrogen and oxygen at relatively low temperatures under the impact of an external high frequency electromagnetic field. The resulting gas burns with a coloured flame ("burning water"). This phenomenon has been first described in the internet a couple of years ago by an American researcher, but it has never been verified nor scientifically investigated. We were able to reproduce this finding with radio-waves (13.56 MHz) in a home-made experimental arrangement.

The aim of our study is to reveal the nature of the water dissociation. The bridge between 'burning water' and the goals of BuildMoNa is built by the introduction of various nano-particles (NPs) in external HF-fields, which are micro-waves and ultrasound (beyond radio-waves). We study the interactions between external fields and the catalytic properties of NPs such as Pd-NPs and magnetite-NPs. As probe reaction we use the hydrodechloribnation of chlorobenzene. The results are scientifically new.

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Pd-Catalyzed Hydrodechlorination of Chlorinated Aromatics in Contaminated Waters – Effects of Surfactants, Organic Matter and Catalyst Protection by Silicone Coating
 F.-D. Kopinke, D. Angeles-Wedler, D. Fritsch, K. Mackenzie / Appl. Catal. B Environ. (2010) 96 323

⇒ Radio-Wave-Induced Thermo-Chromatographic Pulses – Experimental Evidence M. Kraus, U. Trommler, F. Holzer, F.-D. Kopinke, U. Roland / Modelling and Applications. Proc. HES-10 International Symposium on Heating by Electromagnetic Sources (2010) 337, Servizi Grafici Editoriali, Padova (ISBN 978-88-89884-13-3)

Single-source precursors for chalcopyrite semiconductors $CuME_2$ (M = Ga, In; E = S, Se)

Prof. Dr. Harald Krautscheid

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

Thin-film chalcopyrite photovoltaic (PV) technology based on Cu(Ga,In)(S,Se)₂ semiconductor materials ("CIGS") has attracted increasing interest in the past two decades. This PV technology is suitable for large-scale production, offers high efficiency (up to 19,9 % on laboratory scale devices) and stability comparable to that of crystalline silicone. The bandgaps of the ternary compounds range between 1.04 eV (CuInSe₂) and 2.43 eV (CuGaS₂), hence they well match to the solar spectrum and are furthermore tunable by substitution between Ga and In or S and Se. Nevertheless, the current production of such solar cell devices is based on high vacuum and high temperature methods. For these reasons, it is interesting to develop low-cost, high-throughput and reliable PV production techniques.





Thermogravimetry and differential thermal analysis for [ⁱPr₃PCu(SC₂H₄S)InMe₂]₂

Our aim is to prepare polynuclear complexes containing copper, group-13-metal and chalcogen atoms in the ratio 1:1:2, that can be used as precursors for the formation of CIGS layers. We were able to synthesise and characterise several complexes with this ratio, e.g. the series of bimetallic 1,2-ethylenedithiolates [${}^{i}Pr_{3}PCu(SC_{2}H_{4}S)$ MR₂]₂ (M = Ga, In; R = Me, Et, ${}^{i}Pr$). These tetranuclear complexes can be conveniently prepared in high yield and good purity. Their thermal decomposition to CIGS under mild conditions is monitored by thermoanalytical methods like simultaneous thermal analysis (thermogravimetry, DTA) and temperature dependent power X-





Thermolysis of ['Pr3PCu(SC2H4S)InMe2]2 observed by temperature dependent powder X-Ray diffractometry

Ray diffraction (see figure).

As alternative approaches to CIGS thin films we are currently developing spray pyrolysis and aerosol-assisted chemical vapour deposition experiments, in which an organic solution of a single-source precursor (SSP) is nebulised and then transferred onto a heated substrate, where the thermolysis of the SSP into the desired product takes place. These SSPs (e.g. $[iPr_3PCu(SC_2H_4S)InMe_2]_2)$ have the CuGaE₂ or CuInE₂ (E=S, Se) components "built in", giving the advantage to yield the correct stoichiometry in the final product.

⇒ Metal Oxide-Organic Frameworks (MOOFs), a New Series of Coordination Hybrids Constructed from Molybdenum(vi) Oxide and Bitopic 1,2,4-triazole Linkers
A.P. Lucanko, C.A. Sanchuk, L.Lingko, D.Läczig, A.A. Fokin, F.D. Butava, P.B. Schreiner, H. Krautsch

A.B. Lysenko, G.A. Senchyk, J. Lincke, D. Lässig, A.A. Fokin, E.D. Butova, P.R. Schreiner, H. Krautscheid, K.V. Domasevitch / Dalton Trans. (2010) 4223

- ⇒ Magnetic Properties of Mixed Ligand Ni^{II}₂ and Ni^{II}₄ Complexes Composed of Macrocyclic Hexaamine-Dithiophenolato and Bridging Tetrazolato Ligands
 J. Lach, S.V. Voitekhovich, V. Lozan, P.N. Gaponik, O.A. Ivashkevich, J. Lincke, D. Lässig, B. Kersting / Zeitschrift für Anorganische und Allgemeine Chemie (2010) 636 1980
- \Rightarrow Highly Functionalised 3,4,5-Trisubstituted 1,2,4-Triazoles for Future Use as Ligands in Coordination Polymers

J. Lincke, D. Lässig, H. Krautscheid / Tetrahedron Lett. (2010) **51** 653

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From the glassy dynamics of mono-molecular layers to Infrared transition moment orientational analysis (IR-TMOA) – molecular biophysics in basic research and application

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From the glassy dynamics of monomolecular layers to Infrared transition moment orientational analysis (IR-TMOA) – molecular biophysics in basic research and application

Prof. Dr. Friedrich Kremer

Dipl.-Phys. Roxana-Giogiana Ene, M.Sc. Phys. Ciprian-Ghiorghita Iacob, M.Sc. Phys. Wilhelm Kossack, M.Sc. Phys. Ilya Semenov, Dipl.-Phys. Martin Treß, Dipl.-Phys. Olaf Ueberschär, Dipl.-Phys. Carolin Wagner

Glassy dynamics of mono-molecular layers of poly(2-vinyl pyridine): Recently, a preparation method using ultra-flat, highly doped silicon wafers as electrodes, which are covered with strongly insulating silica nano-structures as spacers was developed in our group. This enables us to apply Broadband Dielectric Spectros-



copy to study samples, which do not exhibit a full surface coverage; in particular, the investigation of the glassy dynamics of ultrathin layers of polymers down to and below the mono-molecular limit (where the polymer chains form sub-layers). In the case of poly(2-vinyl pyridine), it will be possible to study the dynamics of isolated coils which do not interact with each other and hence, can be treated as a statistical average over different conformations of a single polymer chains.

The effective hydrodynamic radius of single DNA-grafted colloids as measured by fast Brownian motion analysis: Optical tweezers accomplished with fast position detection, enable one to carry out Brownian motion analysis of single DNA-grafted colloids in media of varying NaCl concentrations. By that the effective hydrodynamic radius of the colloid under study is determined and found to be strongly dependent on the conformation of the grafted DNA chains. The observed scaling of the brush height with the ion concentration is in full accord with the pertinent theoretical predictions by Pincus, Birshtein and Borisov.

Receptor/ligand-interaction as studied on a single molecule level: Optical tweezers-assisted dynamic force spectroscopy is employed to investigate specific receptor/ligand-bonds on a single contact level. The specific binding of two monoclonal antibodies, HPT-110 and HPT-104, to synthetic tau-peptides with different phosphorylation pattern is analysed. The specificity of HPT-110 to the tau-peptide containing a phosphorylation at Ser235 and of HPT-104 to the tau-peptide containing a phosphorylation at Thr231 is confirmed. Additionally, our approach allows for a detailed characterisation of the unspecific interactions that are observed between HPT-104 and the peptide phosphorylated only at Ser235 and between HPT-110 and



From the glassy dynamics of mono-molecular layers to Infrared transition moment orientational analysis (IR-TMOA) – molecular biophysics in basic research and application

the peptide phosphorylated only at Thr231. By analyzing the measured ruptureforce distributions it is possible to separate unspecific from specific interactions. Thereby for the latter characteristic parameters like the lifetime of the bond without force τ_0 , the characteristic length x_{ts} and the free energy of activation ΔG are determined. The results are in accordance with conventional ELISA tests but offer a much more refined insight.

Hierarchies in the structural organisation of spider silk: Polarised IR-spectroscopic and mechanical measurements are combined to analyse the conformational changes in hydrogenated and partially deuterated major ampullate spider silk of Nephila edulis. Special attention is given to supercontraction and to the case where the latter is hindered by mechanical constraints. Crystal stress can be measured from the frequency shift of main-chain vibrations. The results show that in both states of silk a serial arrangement between the crystalline and amorphous phase dominates the nanostructure. The determination of the molecular order parameters of the different moieties proves that the amide hydrogen exchange is a selective process, taking place at the surface of β -sheet nanocrystals, implying that these regions are accessible by water. The mechanical properties change dramatically when the fiber is wet ("supercontraction") due to the fact that the pre-stress of the chains interconnecting the nanocrystals is irreversibly released. A novel network of H-bonds formed in the process, can be suppressed if supercontraction is hindered. A three-component combined model of crystals in serial arrangement with amorphous chains and a fraction of chains by passing them can describe all states of spider silk, assuming hydrogen bonding of worm-like chains at low pre-strain.



Infrared transition moment orientational analysis: A novel spectroscopic approach, that reveals a complete characterisation of the quadratic averaged orientation of the different infrared transition dipole moments in any IR translucent material has been developed. Using a rotary measurement setup, the electric field in the sample can be varied in all three dimensions. Since, the absorption coefficient is explicitly dependent on the relative orientation of the transition dipoles and the electric polarisation, one is enabled to quantify the fraction of ordered molecular moieties and their orientation. Based on this technique, thin substrate supported, polymer films are studied in order to investigate their interaction with solid-state interfaces according to their specificity and range for different combinations of polymers and substrates, addressing the recent question of confinement and its extension.



- ⇒ Glassy Dynamics and Glass Transition in Nanometric Thin Layers of Polystyrene M. Tress, M. Erber, E.U. Mapesa, H. Huth, J. Müller, A. Serghei, C. Schick, K.-J. Eichhorn, B. Voit, F. Kremer / Macromolecules (2010) 43 9937
- ⇒ Partial Deuteration Probing Structural Changes in Supercontracted Spider Silk R. Ene, P. Papadopoulos, F. Kremer / Polymer (2010) 51 4784
- ⇒ Correlation between Polarity Parameters and Dielectric Properties of [Na][TOTO] a Sodium Ionic Liquid
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- ⇒ Glassy Dynamics and Glass Transition in Thin Polymer Layers of PMMA Deposited on Different Substrates M. Erber, M. Tress, E.U. Mapesa, A. Serghei, K.-J. Eichhorn, B. Voit, F. Kremer / Macromolecules (2010) 43 7729
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From single molecule dynamics to slow glassy relaxation of networks and living cells

Prof. Dr. Klaus Kroy

Dipl.-Phys. Jens Glaser, Dipl.-Phys. Sebastian Sturm, Dipl.-Phys. Lars Wolff

We investigate the statics and dynamics of polymer materials with applications ranging from the rheology of living cells and crosslinked polymer networks to the nonlinear force response of single biopolymers. On a single-polymer level, nonequilibrium stress propagation produces nontrivial dynamics in the millisecond regime that is now investigated experimentally in collaboration with partners at the Cavendish Laboratory. On a more macroscopic level, the static and dynamic heterogeneities of pure, entangled polymer solutions have been rendered accessible by

a systematic extension of the meanfield tube model of semiflexible polymers to an effective liquid state theory of entanglement segments (segment fluid model). Experimental results obtained in cooperation with our partners in Jülich show excellent agreement with theory. At the highest level of complexity, we trace back the dynamic force response of cells and reversibly cross-linked polymer networks to the interplay between single-polymer dynamics and crosslinker binding/unbinding kinetics. This is achieved in terms of the model of the inelastic glassy wormlike chain, a phenomenological extension of the standard wormlike chain model that accounts for structural rearrangements within cells and polymer networks in an effective way. Starting from a simple



Biocompatibility of Fe₇₀Pd₃₀ ferromagnetic shape memory alloys

Prof. Dr. Stefan G. Mayr

The aim of our research is to get a better understanding of magnetic shape memory alloys and to improve the synthesising process and properties to make them suitable for different kinds of applications. By applying an external magnetic field internal strains are induced and easy moveable martensitic twin variants can reorientate. Using molecular beam epitaxy (MBE) single crystalline $Fe_{70}Pd_{30}$ thin films can be synthesised making these materials also usable for biomedical micro-applications. Although induced strains in $Fe_{70}Pd_{30}$ by an external magnetic field are not as large as for other FSMAs like e.g. Ni_2MnGa , $Fe_{70}Pd_{30}$ has better mechanical properties. It is more ductile and does not tend to fracture formation. So it offers a high potential in various fields e.g. actuators, different kinds of sensors, valves and switches. Furthermore $Fe_{70}Pd_{30}$ is also showing good biocompatibility making it an interesting candidate as an actuator for medical purposes.

At the present state our work has focused on in vitro biocompatibility assessments of single crystalline Fe₇₀Pd₃₀ FSMA films grown on MgO (100) single crystal substrates. As the first step, a simulated body fluid (SBF) approach to mimic the nominal ion concentrations in human blood plasma, as proposed by Kokubo



Optical morphological features of mouse cells on Fe₇₀Pd₃₀ film surface *(left)* and plastic culture dish *(right)*

physical model of purely passive microscopic mechanisms, it predicts a broad range of experimentally observable macroscopic "emodelling effects" such as viscoelastic shakedown and fluidisation. A further major success of the inelastic GWLC model is the explanation of apparently contradictory experimental observations of stress stiffening and stress softening in cells. Experiments on reconstituted Actin/ HMM networks performed in collaboration with the Bausch lab in Munich confirm our theoretical predictions and suggest that the corresponding nonequilibrium response of living cells may be explained in terms of a relatively simple polymer physics model.



The task of predicting macroscopic properties of a polymer solution (essentially resembling a portion of spaghetti) from its molecular structure is known as the entanglement problem; our recent joint experimental and theoretical work revealed the detailed heterogeneous microstructure of biopolymer solutions (F-actin) akin to those found in animal cells and explained it by a systematic theory

⇒ Tube Width Fluctuations in F-Actin Solutions
J. Glaser, D. Chakraborty, K. Kroy, I. Lauter, M. Degawa, N. Kirchgeßner, B. Hoffmann, R. Merkel, M. Giesen / Phys. Rev. Lett. (2010) 105 037801

⇒ Inelastic Mechanics of Sticky Biopolymer Networks L. Wolff, P. Fernandez, K. Kroy / New J. Phys. (2010) 12 053024

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and Takadama, was employed at the IOM. The SEM images of the morphological changes on the surface of FePd films during SBF test showed that bonelike apatites with granular microstructure formed after soaking in SBF for 65 hours. These findings clearly indicate, that Fe₇₀Pd₃₀ film can, in fact, induce material aggregation from the SBF on its surface, which is very important for bone-bonding between the live tissues and implants. Moreover, the Ca/P ratio of 1.32 was determined from the EDX spectra. Fe and Pd concentrations within SBF before and after specimen removal were measured with inductively coupled plasma optical emission spectroscopy (ICP-OES). The Fe concentration clearly increased, indicating a higher reactivity of Fe in the Fe–Pd alloy while the concentration of Pd did not change during the test.

As the second step, viability cell tests were performed to investigate the interactions of NIH3T3 embryonic mouse fibroblast cells with the sample material. This work was conducted by Dr. Zink from the Soft Matter Physics Division of Universität Leipzig.

The figures present the optical morphological features of NIH 3T3 cells after 65 h growing on a 500 nm $Fe_{70}Pd_{30}$ film and staining with calcein acetoxymethylester (AM) and propidium iodide (PI). It turned out that cells adhered and proliferated on the surface of the film, some samples exhibited a lower cell density compared to the cells on the surface of the surrounding culture dish. Additionally, cells on the film were slightly smaller than cells on the culture dish. After staining with calcein AM and PI, cells on the film surface fluoresced in green. Only a few red cell cores were determined, whereas these cells also exhibited a strong green calcein signal and adhered to the film surface. This behavior indicates that these cells were not apoptotic but pathologically transformed. In contrast, only viable cells fluorescing in green were obtained in the surrounding culture dish without any red fluorescing cores.

These results suggest that $Fe_{70}Pd_{30}$ films are biocompatible with little restrictions. Therefore, *in vivo* mouse test are planed to further test the biocompatibility of $Fe_{70}Pd_{30}$ films. Additionally, film coatings will be employed to improve biocompatibility.

⇒ Biocompatibility of single crystalline Fe₇₀Pd₃₀ ferromagnetic shape memory films Y. Ma, M. Zink, S.G. Mayr / Appl. Phys. Lett. (2010) 96 213703

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Influence of the aliphatic chain length of imidazolium based ionic liquids on the surface structure

Prof. Dr. Harald Morgner

M.Sc. Chem. Tobias Hammer

We study the molecular surface structure of imidazolium based room temperature ionic liquids (RTIL) with two surface sensitive techniques. Angle resolved neutral impact collision ion scattering spectroscopy (ARNICISS) allows to determine elemental concentration depth profiles and to obtain information about the topography of the surface. Angle resolved X-ray photoelectron spectroscopy (ARXPS) can be used to study the chemical composition of the surface. One aspect of our work consits in the study of homologous series of the RTILs: the number of carbon atoms in the aliphatic chain of the imidazolium cation is varied. Due to this procedure it is possible to study the influence of the chain length on the composition of the surface and the strucutre of the surface near region. One example of our homologeous series of RTILS are 1-alkyl-3-methylimidazolium [C_RMIM] bis (trifluoromethylsulfonyl) imide $[Tf_2N]$, the alkyl-part (R) being varied between 1–12 carbon atoms. Due to the combination of our NICISS data with ARXPS data, we are able to develop a model of the surface structure of the different ILs. With this knowledge it is possible to adjust the hydrophobicity and polarisability of the interface for future applications. The influence of different anions, also with functional groups is one subject



of future research.

In another project *Influence of water onto the surface structure of 1-Hexyl-3-methylimidazolium Chloride*, we have investigated the influence of water on the surface structure of the ionic liquid (IL) 1-hexyl-3-methylimidazolium chloride with the vacuum based method NICISS (Neutral Impact Collision Ion Scattering Spectroscopy) up to a depth of 60 Å.

For both, the pure IL and the binary mixtures with water, the outermost surface layer is exclusively composed of carbon species (alkyl chain of the IL cation). We have found that the presence of water in the IL induces a shift of the chloride anions into a greater depth, while the depth distribution of the cation is almost unaffected. Based on the fact that during three hours of measurement under vacuum conditions, the mole fraction of water has decreased more slowly than expected, e.g. from 0.50 to >0.44 or from 0.89 to >0.71, water seems to be stable in the bulk phase of the liquid sample and has no tendency to move towards the surface. At low water content, a slight enhancement of water right at the surface is followed by a subsurface layer with depleted water concentration. As the water content increases (coordi-



nation number greater 2), the depletion layer is vanished and water molecules are homogeneously distributed within the investigated surface region.

In the future, it is planned to study the surface structure of binary mixtures of ILs or inorganic salts with water. Dynamic effects shall be investigated as well.

⇒ Influence of the aliphatic chain length of imidazolium based ionic liquids on the surface structure T. Hammer, M.Reichelt, H. Morgner / Phys. Chem. Chem. Phys. (2010) 12 11070

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Physical synthesis of thin films and nanostructures far from the thermodynamic equilibrium

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

M.Sc. Phys. Chinmay Khare, Dr. Johanna Lutz, Dr. Marisa Mäder, Dipl.-Phys. Lena Neumann, M.Sc. Chem. Eng. Erik Thelander, Dipl.-Phys. Hendrik Zachmann

The research was focused on the formation of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium. Preferentially ion and laser beam techniques are used. These methods influence the nucleation and growth as well as the structural, optical and electrical properties of growing films as a consequence of atomic rearrangement 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 deposition. Such heavily doped Si/Ge-nano-columns are predicted to have novel transport





Scanning tunnelling microscope image of a GaN film deposited on a 6H-SiC(0001) substrate exhibiting a terrace-step structure which is evidence for a two-dimensional growth mode High-resolution cross-section electron micrograph of an ultrathin GaN film grown on a 6H-SiC(0001) substrate showing a transition from hexagonal to cubic GaN polytype growth



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. An example of a grown gallium nitride layers shows the figure. 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.

- ⇒ Magnetic Tubular Nanostructures Based on Glancing-Angle Deposited Templates and Atomic Layer Deposition
- O. Albrecht, R. Zierold, C. Patzig, J. Bachmann, C. Sturm, B. Rheinländer, M. Grundmann, D. Görlitz, B. Rauschenbach, K. Nielsch / phys. stat. sol. (b) (2010) **247** 1365
- ⇒ Gold Nanostructure Matrices by Diffraction Mask-Projection Laser Ablation: Extension to Previously Inaccessible Substrates
 - M. Mäder, S. Perlt, T. Höche, H. Hilmer, M. Grundmann, B. Rauschenbach / Nanotechnol. (2010) 21 175304
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- M. Mäder, T. Höche, J.W. Gerlach, S. Perlt, J. Dorfmüller, R. Vogelgesang, K. Kern, B. Rauschenbach / Nano Lett. (2010) **10** 47

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- ⇒ Mikro- und nanostrukturierte dünne Schichten durch Deposition unter streifendem Einfall
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- ⇒ Nanostructures by Diffraction Mask Projection Laser Ablation
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 Böhme, B. Rauschenbach / phys. stat. sol.
 (b) (2010) 247 1372
- ⇒ Periodically Arranged Si Nanostructures by Glancing Angle Deposition on Pattered Substrates

C. Patzig, C. Khare, B. Fuhrmann, H.S. Leipner, B. Rauschenbach / phys. stat. sol. (b) (2010) **247** 1322

⇒ Arbitrarily Shaped Si Nanostructures by Glancing Angle Ion Beam Sputter Deposition

C. Patzig, A. Miessler, T. Karabacak, B. Rauschenbach / phys. stat. sol. (b) (2010) **247** 1310

- ⇒ Enhancment of Stiffness of Vertically Standing Si Nanosprings by Energetic Ions R. Nagar, B.R. Mehata, J.P. Singh, C. Patzig, B. Rauschenbach, D. Kanjilal / J. Appl. Phys. (2010) 107 094315
- ⇒ Influence of Substrate Temperature on Glancing Angle Deposited Ag Nanorods C. Khare, C. Patzig, J.W. Gerlach, B. Rauschenbach / J. Vac. Sci. Technol. A (2010) 28 1002
- $\Rightarrow The Impact of Sodium on Ion-Beam In$ $duced in Cu(In,Ga)Se_2 Absorber Films$

H. Zachmann, S. Puttnins, F. Daume, A. Rahm, K. Otte / Proc. 25th European Photovolt. Solar Energy Conf. and Exhibition (2010) 3382

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NanoBioenaineerina – novel nano- and micro-technoloaical aspects of multi-electrode arrays in Life Sciences

NanoBioengineering – novel nanoand micro-technological aspects of multi-electrode arrays in Life Sciences

Prof. Dr. Andrea A. Robitzki

Dipl.-Biochem. Marco Glaß, Dipl.-Biochem. Sina Haas, Dipl.-Biochem. Dana Krinke, Dipl.-Biochem. Anja Steude

The topics of the research in nano-micro-technology are addressing (i) characterising smooth muscle cell and cardiomyocyte based microrrays, (ii) investigating visco-elasticity of smooth and cardiac muscle cells via atomic force microscopy, and (iii) understanding neurodegenerative processes and neural cancer cells using bio-electronic based impedance spectroscopy. Thus Anja Steude established an electrochemical immuno-based biosensor for catching single neural cancer cells. Such a microarray consisting of platinum counter and gold measurement electrodes and a pinholder with Ag/AgCl reference electrodes is used for voltammetric and impedimetric analyses. Dana Krinke strengthened her research topics in investigating the progress of neurodegeneration in 3D in vitro neuroblastoma spheres. Hyperphosphorylation of the microtubule associated protein Tau could be simulated via mutagenesis and applying ocadaic acid and was impedimatrically monitored. Sina Haas and Marco Glass could demonstrate an impedimetric detection of viable synthetic and contractile smooth muscle cell phenotypes *in vitro* on a novel interdigital electrode array.



Interdigital electrode array consisting of indium tin oxide semiconductive material (compatible to an ansi 96-well format) for an impedimatric analysis of neurodegenerative processes in viable brain slices and human neuroblastoma cells SH-SY5Y; immuno-histochemical stain of neurofilament L (green) and nuclei (red) using confocal laser scanning microscopy (right)



- ⇒ Real-Time Monitoring of Relaxation and Contractility of Smooth Muscle Cellson a Novel Biohybrid Chip S. Haas, H.-G. Jahnke, M. Glass, R. Azendorf, S. Schmidt, A.A. Robitzki / Lab-On-Chip (2010) 10 2965
- ⇒ A Novel Organotypic Tauopathy Model on a New Microcavity Chip for Bioelectronic Label-Free and Real Time Monitoring
 - D. Krinke, H.-G. Jahnke, T.G.A. Mack, A. Hirche, F. Striggow, A.A. Robitzki / Biosens. Bioelectron. (2010) **26** 162

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ESF-NFG Trägergebundene Katalyse für innovative Bio-, Nano- und Umwelttechnologie

ESF-Nachwuchsforschergruppe "Trägergebundene Katalyse für innovative Bio-, Nano- und Umwelttechnologie"

Prof. Dr. Evamarie Hey-Hawkins

Dipl.-Biochem. Verena Ahrens, M.Sc. Chem. Martin Brehm, M.Sc. Chem. Matthias Golecki, Dr. Mike Hildebrand, M.Sc. Chem. Jörg Lincke, M.Sc. Chem. Martyna Madalska, M.Sc. Chem. Klara Rusevova, M.Sc. Chem. Markus Streitberger, M.Sc. Chem. Patrick With

The ESF-Nachwuchsforschergruppe addresses current problems and promising solutions in catalysis in an interdisciplinary approach with a special focus on the design of suitable supports for catalysts as well as the environment of the catalytically active site.

Immobilisation of active catalysts allows the best of homogeneous or enzymatic and heterogeneous catalysis to be combined. Thus, catalytically active metal complexes are encapsulated in cage molecules, such as derivatised β -cyclodextrins. The constrained, chiral cage environment is also expected to influence the catalytic performance (Matthias Golecki). Ionic liquids are worldwide the target of scientific interest due to their unusual properties and their use as reaction media, e.g. for immobilising molecular catalysts or nanoparticles. In this respect, chiral phosphorusbased functionalised ionic liquids promise to have enormous synthetic potential in catalytic applications (Mike Hildebrand). The results of ab initio molecular dynamics calculations on ionic liquids in the gas phase and mixtures with water in different proportions provide new information on the composition, structure and understanding of the interaction between water and ionic liquids (Martin Brehm).

Enzymes as biocatalysts are becoming increasingly important in many areas. The specific immobilisation of (modified) enzymes on different substrates and their catalytic activity are studied (Verena Ahrens).

Tailor-made reactions are enabled by using suitable ligand systems in catalytic processes. The ligands used are based on ferrocene, and their immobilisation on an electrode surface allows the development of (electrically) switchable catalysts (Martyna Madalska).

In three-dimensional coordination polymers, properties (adsorption of gases and



catalytic activity) and pore size are adjustable depending on the building blocks (Jörg Lincke). Similarly, polymeric materials can be used as carriers for organometallic catalysts as well as catalytically active nanoparticles. Here, the main focus is on transition metal phospholane complexes (Markus Streitberger).

Catalysis plays a major role in prevention and control of environmental pollution. As one approach for preparing appropriate catalysts, catalytically active metal nanoparticles can be generated and deposited on porous supports via ferrocene which was incorporated in a renewable raw material (olive stones) using supercritical CO_2 . The resulting iron-containing activated carbons are now employed in catalytic reactions for gas emission control (Patrick With). Another fundamental problem is the purification of contaminated water. Here, environmentally friendly iron catalysts on the basis of nanoscale magnetite (Fe₃O₄) and perovskite minerals are developed. They are being investigated for the removal of organic pollutants from aqeuous solutions (Klara Rusevova).

ESF-Nachwuchsforschergruppe "Funktionale multiskalige Strukturen"

Prof. Dr. Marius Grundmann

M.Sc. Ana A. Ballestar Balbas, Dipl.-Phys. Christof P. Dietrich, Dipl.-Phys. René Feder, Dipl.-Phys. Nils Neubauer, Dipl.-Phys. Marko Stölzel, M.Sc. Erik Thelander, Dr. Holger von Wenckstern

The research topics of the young researchers group "Multiskalige funktionale Strukturen" include synthesis and characterisation of micro- and nanocolumns, nanospirals and nanosheets or -flakes. Besides shape, the material composition determines the field of application comprising light emitters, polarisation filters, sensors and building blocks of ballistic and spin electronics, respectively.

For example, a sputter-enhanced glancing angle deposition process allows precise control of the habitus of Ag-nanostructures and with that their surface plasmon resonance significantly. Arrays of shape-optimised Ag-nanostructures, depicted in Fig. a), are deployable as biosensor monitoring water quality.

Graphite sheets are investigated electrically requiring an elaborate contacting procedure. A four-point contacting of a multigraphene sample is depicted in Fig. b). In order to conclude on ballistic charge carrier transport in graphene, which represents a milestone within the young researchers group, it is additionally necessary to constrict the current transport path geometrically. By varying the extension of the constriction it was possible to determine fundamental physical parameters such as the free carrier's mean free path.

A comparatively simple carbothermal chemical vapour transport process was used to grow transparent semiconducting ZnO micro- and nanostructures. Besides the investigation of low-field transport properties their optical properties are highly interesting. Photon confinement was confirmed in hexagonal ZnO mircocolumns by the observation of so-called whispering gallery modes (WGM). Again, the geometry particularly the diameter determines the energy of the WGM eigenmodes of the microwires. This was arrestingly demonstrated within a bending experiment (Fig. c) and optical spectroscopy accomplished at 10 K. While the energy of excitonic recombination lines shifted in dependence on strain, the WGM resonances remained unaffected which is shown in Fig. d).







Energy (eV)

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Secondary electron micros copy (SEM) image of a) Ag-Chevrons deposited on silicon. b) electrically contacted graphite lamella on SiN_x substrate: c) optical microscopic image of a bent ZnO microwire, inset: SEM image of bent ZnO microwire: d) area scan of low temperature near-bandedge recombination of bent ZnO microwire; the centre of the wire is set as zero for the position axis; the black. dashed lines frame the energy range in which WGMs appear, which are in contrast to excitonic contributions not affected by strain

Experiences

BuildMoNa's third year – an associated principal investigator's view

Prof. Dr. Roger Gläser



BuildMoNa has, after its third year, become a scientific institution. Both doctoral candidates and principal investigators know each other and have made significant progress towards opening their eyes and minds for an inter- and transdisciplinary approach to the natural sciences at our University. The scientific community within BuildMoNa has developed into a common body of mutual research interests and interwoven activities.

As an associated principal investigator, one might expect a somewhat outside view. In fact, however, the intense exchange with both doctoral candidates and the other principal investigators from all of BuildMoNa's disciplines – and the great integrative efforts of the BuildMoNa Office – made my first years within BuildMoNa an experience that indeed allows me a perspective from within.

Certainly, the fact that most of the positions of our doctoral candidates have to be funded by sources outside BuildMoNa, is one side, but the numerous opportunities for participation in the broad programme for scientific training and transferable skills, the yearly doctoral candidates' workshops or the grants for mini-projects or travel to conferences are the other side. My feeling is that the doctoral candidates are proud of being a part of BuildMoNa, although not all of them appreciate being exposed as the special excellence within the group.

Most importantly, BuildMoNa has supported us in becoming more visible. First of all, within our University: BuildMoNa holds a firm place in the Research Academy Leipzig, the overall frame for graduate research training at our University. Even more, it is strongly connected to the Top-Level Research Areas of our University. As we know already, BuildMoNa will be the only proposal of our University within the second round of the German Excellence Initiative. It, therefore, may even serve as a "leitmotif" for shaping the future of the profile of research training in natural sciences of our University.

Secondly, BuildMoNa makes us visible on the international level: we can invite and collaborate with internationally renowned scientists at our BuildMoNa workshops and symposia (although our university administration does not always support the reimbursement of travel grants easily). This ensures the highest level of scientific training on the one hand and of international input and feed-back on our activities on the other.

Wishing us all success for the future of BuildMoNa, not least for its extension within the second round of the German Excellence Initiative, but also as a continuously living platform of scientific exchange and growth,

Prof. Dr. Roger Gläser

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

Dipl.-Phys. Martin Lange



BuildMoNa is in its 4th year and has developed as an established, efficient part of the educational system in the field of natural sciences in Leipzig. Due to the graduate school and its possibilities many excellent students had the opportunity to proceed with their studies in Leipzig and additionally, outstanding students from Germany and abroad could be attracted – enriching BuildMoNa. Within the three years, the experience in organising the graduate school itself and the scientific and method modules and workshops has increased – but I see also a danger of some routines. Therefore, to my opinion, it is important to have a critical look on BuildMoNa – to look for things that could be improved and things that are already working fine. This was continuously carried out by the responsible persons in BuildMoNa with the aim to further strengthen our graduate school.

In addition to their own research, the training programme is a major topic for the doctoral candidates in BuildMoNa. In general the modules are well organised – they start with some lectures on basics and finally also discuss cutting-edge re-

sults. This sensitises doctoral candidates with a different scientific background to selected issues of other scientific disciplines and typical approaches how to solve them. In my opinion, however, there are some things that could be further improved, especially concerning the organisation of the examinations. Although I notice a clear progress, sometimes the requirements are still too ambitious and therefore discourage some students from other fields of study.

In addition to the modules, BuildMoNa promotes the development of the doctoral candidates by a transferable skills training programme, financial support for the participation in conferences and regular workshops and symposia. The BuildMoNa mini-projects that are offered by the graduate school are a great opportunity for both doctoral candidates and master students. The mini-projects are proposed by doctoral candidates and, given a successful application, carried out by outstanding master students. Thereby, the doctoral candidates gain practical leadership experience. Additionally, excellent students get to know BuildMoNa and benefit from the financial support of the graduate school.

Last but not least, the reconciliation of work and family life is an important issue for young scientists. To support BuildMoNa parents, the graduate school offers flexible childcare. Furthermore, childcare on a regular basis is offered in cooperation with the Research Academy Leipzig.

Altogether, I am convinced of the concept of BuildMoNa as it promotes the personal development of the doctoral candidates by stimulating a broader knowledge in natural sciences and helping in the acquisition of transferable skills. What convinces me additionally is the open-mindedness of BuildMoNa towards new ideas that can further improve the graduate school.

M. Lange

Dipl.-Phys. Martin Lange

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			Мог	nth (M	arch	to Fel	oruar	y)		_	_			
	Туре	Min. CP	М	А	м	J	J	А	S	0	Ν	D	J	F
				sum	mer	term					wi	nter	term	
Research work	R	-												
Scientific and methods modules	R/E	10	Μ	м	м	м	м			м	Μ	Μ	Μ	Μ
Workshop for doctoral candidates	R								W					
Scientific symposium	R/E		SY											
Literature seminars	R/E			S		S		S		S		S		S
Guest lectures/colloquia	E	5	L	L	L	L	L	L	L	L	L	L	L	L
Tutoring	R/E			Т	Т	Т	Т			Т	Т	Т	Т	
Research stays abroad	E		fle	exible	durin	g the	whol	e yea	r (1 v	veek	up to	a fev	/ mon	iths)
Summer/winter schools	E													
Industrial training	E													
Active participation in conferences/workshops	R/E			flex	ible c	luring	the v	whole	year	(1 up	o to a	few	days)	
Transferable (generic) skills	R/E	5		S	S	S	S			S	S	S	S	
					м		м				м		м	

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: (Bio)hybrid systems (2009-M09)

2 / 3 February 2010,

oral exam, 2 credit points, yearly recurrence with modification, 22 participants

Understanding the principle of biohybrid systems consisting of various nano-structured bioelectronical microarrays and viable cell and tissue models. The focus was the generation and characterisation of biomimetic interfaces and the biological component. Microfluidic and biosensoric monitoring systems were demonstrated for understanding how (bio)hybrid systems could be used for screening of active pharmaceutical ingredients.

Responsible Scientist:

Prof. Dr. A. Robitzki

Lecturers:

Dr. A. Schober, TU Ilmenau, Germany; Dr. R. Kurz, Universität Leipzig, Germany; Dr. H.-G. Jahnke, Universität Leipzig, Germany; Dr. D. Kloß, Universität Leipzig, Germany; Dr. R. Schulz, TRM, Germany; T. Mack, KeyNeurotek AG Magdeburg, Germany

Contents:

- \Rightarrow Development of planary and 3D microcavity-arrays with various substrates and conductive materials on the basis of up to date processing technologies
- ⇒ Biophysical techniques to characterise cells using impedance spectroscopy and electrophysiology on biosensors
- ⇒ Cell and tissue models on multielectrode-microarrays e.g. Morbus Alzheimer on a chip, Tumour-chip, cardiomyocyte-based array and new stem cell biochip
- ⇒ Microfluidic assays and bioreactors for eukaryotic cells technical design, development, fabrication and validation

Methods:

- ⇒ Processing techniques to develop and fabricate nano-structured 2D and 3D micro-electrode-arrays including characterisation of material surface topology
- ⇒ High resolution microscopic techniques (Multiphoton Laser Scanning-Microscopy with STED modus)
- ⇒ Monitoring and imaging of biological models via bioelectronical and optical monitoring

Nano-manipulations: Spectroscopy on the nanometric scale (2010-M01)

30 September / 1 October 2010,

written exam, 2 credit points, yearly recurrence with modification, 16 participants

Spectroscopies localised at the nanometric lenghtscales or aiming to measure interactions at similar separations have gained strong impact in modern Nano(bio) physics and materials science. The module gave an introduction into these modern techniques and the physical principles behind it.

Responsible Scientist:

Prof. Dr. F. Kremer

Lecturers:

Prof. Dr. F. Kremer, Universität Leipzig, Germany; Dr. R. Seidel, Biotechnology Centre TU Dresden, Germany; P. Papadopoulos, Universität Leipzig, Germany; Prof. Dr. U. Keyser, University of Cambridge, UK; E. Petrov, Universität Leipzig, Germany

Contents:

- \Rightarrow Absorption spectroscopy from 10⁻³ Hz to the IR
- ⇒ Broadband Dielectric Spectroscopy (BDS) using nanostructured electrodes
- ⇒ Time-resolved FTIR spectroscopy, IR transition moment orientational analysis
- \Rightarrow Fluorescence spectroscopy and related techniques (FCS and FRET)
- \Rightarrow Force spectroscopy using magnetic tweezers

Methods:

- ⇒ Broadband Dielectric Spectroscopy (BDS)
- \Rightarrow Fourier-Transform InfraRed Spectroscopy (FTIR)
- \Rightarrow Fluorescence Spectroscopy including FRET and FCS
- \Rightarrow Force Spectroscopies using optical and magnetic tweezers

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From molecules to materials: Magnetic nanoparticles (2010-M02)

28 / 29 October 2010,

written exam, 2 credit points, yearly recurrence with modification, 28 participants

Link molecular sciences and materials science. Understand how nano-sized materials with optimised magnetic properties are obtained from molecules or molecular precursors. Understand the properties and applications of these magnetic nanoparticles.

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Responsible Scientists:

Prof. Dr. P. Esquinazi, Prof. Dr. B. Kersting

Lecturers:

Prof. Dr. B. Kersting, Universität Leipzig, Germany; Prof. Dr. A. Powell, Karlsruhe, Germany; Prof. Dr. M. Julve, Valencia, Spain; Dr. B. N. Mbenkum, MPI Stuttgart, Germany; Prof. Dr. W. Kleemann, Universität Duisburg-Essen, Germany; Prof. Dr. P. Esquinazi, Universität Leipzig, Germany; Prof. Dr. G. Papaefthymiou-Davis, PA, USA; Dr. N. TK Thanh, London, UK

Contents:

- \Rightarrow Basic principles of molecular magnetism
- ⇒ High-spin polynuclear carboxylate complexes and molecular magnets with VII and VIII group 3d-metals
- \Rightarrow Assembly of core-shell magnetic structures
- \Rightarrow Synthesis of nanoparticular magnetic materials
- \Rightarrow Characterisation of nanoparticular magnetic materials
- \Rightarrow Supermagnetism
- \Rightarrow Electrical transport in magnetic nanostructures
- \Rightarrow Biomedical applications of magnetic nanoparticles

Methods:

- \Rightarrow Templated synthesis
- \Rightarrow Immobilisation techniques
- \Rightarrow Handling and characterisation of magnetic nanoparticles
- \Rightarrow SQUID-Magnetometry

Theory: Probability in physics (2010-M03)

10 / 11 November 2010,

written exam, 2 credit points, yearly recurrence with modification, 15 participants

The aim is to illustrate, using elementary examples, the role of probability theory as the inductive logic behind statistical physics, quantum physics and information theory. The concepts of entropy and dissipation were elucidated.

Responsible Scientists:

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

Lecturers:

Prof. Dr. H. Wagner, LMU Munich, Germany; Dr. R. Blythe, University of Edinburgh, United Kingdom

Contents:

- \Rightarrow Bayesian probability theory
- ⇒ The constitutive role of probability in quantum mechanics and statistical physics
- ⇒ Information-theoretic measure of irreversibility
- \Rightarrow Notions of entropy
- \Rightarrow Nonequilibrium work theorems
- ⇒ Entropy production in nonequilibrium steady-states

Methods:

⇒ Methods and concepts dealing with incomplete data, inductive inference, information theory, logics, analytical and numerical techniques

From biomolecules to cells: Ligands, receptors and signal transduction (2010-M04)

12 / 13 July 2010,

written exam, 2 credit points, yearly recurrence with modification, 32 participants

Understanding the signaling of cells to manipulate them and use them as smallest biosensor. Combinations of cell biochemistry with bioelectronics and nano-biotechnological applications were deepened. Understanding how the cellular machinery changes when extracellular signals are applied, and how these changes can be monitored.

Responsible Scientist:

Prof. Dr. A.G. Beck-Sickinger

Lecturers:

Prof. Dr. A.-G. Beck-Sickinger, Universität Leipzig, Germany; Prof. Dr. M. Haack, DiFe Potsdam, Germany; Dr. J. Stichel, Universität Leipzig, Germany; Dr. D. Lindner, Charité Berlin, Germany; M. Cöster, Universität Leipzig, Germany

Contents:

- ⇒ Introduction in basics of signal transduction, basics of hormone signals and their cellular responses, chemical nature of hormones
- ⇒ Methods to create artificial cells, to modulate cellular systems and to obtain read-out systems for signal transduction
- ⇒ High through-put methods to screen for biological activity: agonists, inverse agonists, antagonists, and modulators of biological activity
- ⇒ Eukaryotic systems to study protein-protein interaction, identification of novel interaction partners, primary cells and yeast systems
- \Rightarrow Application of the methods to toxic compounds, environmental and nutrition

Methods:

- ⇒ Techniques to characterise cells including different microscopic techniques, fluorescence read out, reporter gene assays and biochemical pathway analysis
- \Rightarrow Transfection studies to create artificial cells with different activities

Smart molecules: Biomolecules (2010-M05)

6 / 7 May 2010,

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

This module aimed at linking molecular sciences, as well as topics from solid-state chemistry and physics, homogeneous, heterogeneous and bio-catalysis.

Responsible Scientists:

Prof. Dr. A.G. Beck-Sickinger, Prof. Dr. E. Hey-Hawkins

Lecturers:

Prof. Dr. E. Hey-Hawkins, Universität Leipzig, Germany; Prof. Dr. A.G. Beck-Sickinger, Universität Leipzig, Germany; Prof. Dr. H.-J. Pietzsch, Forschungszentrum Dresden-Rossendorf, Germany; Prof. Dr. U. Schatzschneider, Ruhr-Universität Bochum, Germany; Prof. Dr. A.-M. Caminade, CNRS, Toulouse, France; Dr. R. Paschke, Biozentrum der Martin-Luther-Universität Halle-Wittenberg and BioSolutions Halle GmbH, Germany; Dr. G. Kaluderovic, Martin-Luther-Universität Halle-Wittenberg, Germany

Contents:

⇒ Specific synthesis, modification and understanding of the changes in the (electronic) structure of molecules that are precursors for materials with optimised catalytic activity and adjustable magnetic, electronic, and optical properties

- ⇒ Small molecules: organometallic and transition metal complexes, building blocks for metal-organic frameworks (MOFs), immobilisation of catalysts (on solid or in liquid supports), electronic structure of active units
- ⇒ Designing and synthesising smart molecules that contain biological and chemical segments, strategies to introduce metals into biomolecules by selectively introduced chelators, monitoring structural changes
- ⇒ Clusters and polynuclear compounds: links between mononuclear complexes and the corresponding solid-state phase, homo- and heterometallic systems, metallated container molecules, supramolecular chemistry
- \Rightarrow Supramolecular chemistry, self-assembly (concepts, strategies)

Methods:

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

Magnetic resonance: Fundamentals and applications (2010-M06)

12 / 14 / 15 September 2010,

written exam, 2 credit points, yearly recurrence with modification, 15 participants

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

Responsible Scientists:

Prof. Dr. S. Berger, Prof. Dr. J. Haase

Lecturers:

Prof. Dr. S. Berger, Universität Leipzig, Germany; Prof. Dr. J. Haase, Universität Leipzig, Germany

Contents:

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

Methods:

- \Rightarrow High-resolution methods for liquids
- \Rightarrow Nuclear double-, triple- resonance
- \Rightarrow Higher dimensional NMR methods
- \Rightarrow Pulsed fields
- \Rightarrow EPR
- \Rightarrow ENDOR

Complex nano-structures: Nanostructure formation, ferroic properties and optical confinement (2010-M07)

15 / 16 March 2010,

oral exam, 2 credit points, yearly recurrence with modification, 21 participants

Deepen the understanding of nanostructures' physical properties and their relation to shape and geometry as well as energy transfer mechanism. Properties of coupled nanosystems.

Responsible Scientists:

Prof. Dr. M. Grundmann, Prof. Dr. B. Rauschenbach

Lecturers:

Prof. Dr. M. Grundmann, Universität Leipzig, Germany; Prof. Dr. K. Gosh, University of Missouri, USA; Dr. J. Zúñiga-Pérez, CNRS, CREA, Valbonne, France; Prof. Dr. B. Rauschenbach, IOM, Germany; Prof. Dr. S. G. Mayr, IOM, Germany; Dr. F. Frost, IOM, Germany; Dr. K. Zimmer, IOM, Germany

Contents:

- \Rightarrow Functional nanostructures for advanced and novel applications
- ⇒ Fundamentals of confinement of charges and photons, light-matter interaction, coupled states, ferroic materials and their nanoscopic properties

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Methods:

 \Rightarrow Nanostructure fabrication and characterisation

Synthesis: Synthesis of thin films and nanostructures (2010-M08)

6 / 7 October 2010,

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

Deepen the understanding of epitaxial growth, growth of two-, one- and zero-dimensional films and heterostructures, synthesis of new materials via molecular precursors, ion beam methods, alloy formation, understanding and application of the different methods to prepare complex systems.

Responsible Scientists:

Prof. Dr. B. Rauschenbach, Prof. Dr. M. Grundmann, Prof. Dr. S. G. Mayr

Lecturers:

Dr. M. Lorenz, Universität Leipzig, Germany; Dr. A. Rahm, Solarion, Germany; Prof. Dr. K. Nielsch, University of Hamburg, Germany; Prof. Dr. L. Chang, Centre of Nanoscience, Wuhan, China; Dr. V. Mosneaga, University of Göttingen, Germany; Prof. Dr. S. G. Mayr, IOM, Germany

Contents:

- ⇒ Understanding the physical and chemical aspects of epitaxial processes for layered and nanostructured materials
- \Rightarrow Examples from industrial processes, device relevant layered structures

Methods:

⇒ Introducing the synthetic tools for materials, thin films and nanostructures, especially to prepare complex materials, e.g. chemical deposition techniques (MOCVD), physical deposition techniques (MBE, PLD, IBAD, etc.), preparation and characterisation of thin films

Multifunctional scaffolds: From colloids to amyloids, biomimetic scaffolds and nano-machines (2010-M10)

30 March / 1 April 2010,

written exam, 2 credit points, yearly recurrence with modification, 21 participants The module aims 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

Lecturers:

Prof. Dr. K. Kroy, Universität Leipzig, Germany; Prof. Dr. E. del Gado, ETH Zürich, CH; Dr. M. Claessens, Univ. of Twente, NL; Dr. A. Parmeggiani, Univ. Montpellier, France; Dr. A. Vilfan, Stefan Inst. Lubljana, Slovenia; Dr. S. Diez, MPI Dresden, Germany; Dr. O. Lieleig, Harvard University, USA; Dr. T. Gisler, Universität Konstanz, Germany; Dr. P. Kollmannsberger, MPI Golm, Germany

Contents:

- ⇒ The module introduces the participants to physical, chemical and biological perspectives onto various multifunctional scaffolds as well as to modern experimental techniques
- ⇒ Topics comprise general soft matter background, statistical physics and simulation approaches, protein assembly and aggregation, the complex interactions in aqueous media, biopolymers and biopolymer networks, molecular motors, artificial nano-actuators, biomimetic structures, cytoskeleton and extra-cellular matrix

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Methods:

- \Rightarrow Single molecule imaging/tracking
- \Rightarrow Advanced microscopy and scattering techniques
- \Rightarrow Quantitative 3d-nano-scale measurements
- \Rightarrow Micro-rheology
- \Rightarrow Biochemistry
- \Rightarrow Statistical mechanics
- \Rightarrow Modeling
- \Rightarrow Computer simulations

Scientific minisymposium

Physics of cancer

25 / 26 October 2010

The first BuildMoNa Minisymposium was organised by the Soft Matter Physics Group of Prof. J. Käs.

The investigation of changes in physical, i.e. material, properties of cells during progression of cancer is an emerging field in physics redefining medical physics, which has been predominately a service to clinicians (imaging, radiation, etc.) and now redefines itself based on material science. During malignant transformation of cells changes in their cytoskeleton, e.g. down regulation of actin and up regulation of intermediate filaments such as vimentin, occur. This leads to significant changes in tumour cells' viscoelastic properties, which are prerequisites for high cell proliferation and tumour invasion. Additionally, the expression of adhesion receptors such as E-cadherins decreases which changes cell motility due to less binding sites with adjacent cells and alters surface tensions that stabilise compartment boundaries between different cell types. The for tumour cells typical high proliferation, invasiveness, and metastasis are greatly hindered without these changes in a cell's material properties. Thus, the knowledge of these physical properties provides a powerful tool to determine the aggressiveness of a tumour and ultimately these findings may result in new therapies that stop the progression of cancer. These results illustrate that materials science can shed new light on tumour progression. The minisymposium "Physics of cancer" aimed towards bringing together the most important investigators in this field. Speakers of the minisymposium were:

- ⇒ Prof. Dr. med. Peter Friedl, Radboud University Nijmegen *Physical limits of cell migration*
- \Rightarrow Prof. Dr. Ramsey Foty, UMDNJ
- Physical models of malignant invasion
- ⇒ Prof. Dr. Jacques Prost, Institut Curie & KITP Constructing tools for describing tissue dynamics
- ⇒ Prof. Dr. Harald Herrmann, DKFZ Intermediate filaments in development and disease: Mediators of a cell typespecific switch in cell elasticity
- ⇒ Prof. Dr. Ben Fabry, University of Erlangen-Nürnberg Forces and migration of cancer cells in a 3-dimensional environment

- ⇒ Prof. Dr. rer. nat. Dr. med. Michael Höckel, Universität Leipzig Ontogenetic anatomy and the compartment theory of tumour permeation
- ⇒ Prof. Dr. Robert Austin, Princeton University The goldilocks principle and rapid evolution of resistance
- ⇒ Prof. Dr. Roland Eils, Bioquant, University of Heidelberg High-throughput mechanical cellular phenotyping by combined optical stretching and computational modeling

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- ⇒ Prof. Dr. Francoise Brochard-Wyart, UPMC Wetting transition of living drops
- ⇒ Prof. Dr. Josef Käs, Universität Leipzig Are biomechanical changes necessary for tumour progression?

Transferable skills workshops

Academic instruction for junior university teachers: Against boring teaching!

Gunda Mohr, Golin Wissenschaftsmanagement,

2/3 June 2010, 16 participants

The interesting and effective design of teaching sessions is one of the core tasks of university teachers. However, the conditions of everyday life in higher education often act against that:

Overcrowded lecture theatres, passive students and the immense time pressure make the implementation of good seminar planning more difficult.

Through utilisation of stimulating methods it is possible to improve one's own teaching significantly and to motivate students in large as well as in small teaching groups. On the basis of effective planning it is possible, even with limited expenditure of time, to teach good sessions which benefit both the teachers and the taught.

This two to three day workshop conveyed tested methods for the structured planning and implementation of teaching sessions.

Scientific writing and publishing research, part I

Dr. Dorothea Sommerfeldt

17/18 June 2010, 12 participants

This workshop aimed at building and enhancing English speaking and writing skills. Accordingly this course was held entirely in English. It ran through a morning session of practical English writing skills (common pitfalls, grammar, punctuation, abbreviations) and explained how to achieve good writing (accuracy, brevity, clarity and style). It helped in gaining practice and confidence in actually organising oneself and getting first words onto paper, using pieces of own writing (redraft and work on the abstract as an example). It demonstrated the process of publication, targeting writing for a specific journal, addressing the cover letter.

Project management for young scientists: Taking off as project pilot

Dr. Simon Golin, Golin Wissenschaftsmanagement,

29 June 2010, 17 participants

New, time limited and complex – such are the tasks generally undertaken as projects. A work environment without project work is almost unimaginable nowadays. And this is not only true for the non-academic sector: Even the doctorate is a project!

Proven project management tools pave the way for the professional development and planning of projects, for competent guiding of their implementation and for their successful completion. With the help of these tools even difficult steps in the project journey can be safely navigated.

During the workshop the participants familiarised themselves with the most important project management methods and instruments.

Conversation and networking: Reaching your goal through successful communication

Dr. Simon Golin, Golin Wissenschaftsmanagement,

30 June 2010, 21 participants

Success is based to a large extent on successful communication. Goal- and audience-oriented communication is necessary in almost all professional contexts such as making arrangements, or "talking shop" with colleagues or the quick and targeted contacting of experts, potential employers or funders. It is, therefore, helpful to be able to fall back on tried and tested strategies.

With a few basic communication strategies and negotiation techniques it is possible to explain complex issues in a context-specific way, to convince and motivate others, to make new contacts and win supporters and so reach the goals set.

In this workshop participants engaged with their own personal communication strategies and behavioural patterns. Exercises were designed to familiarise participants with established negotiation techniques and to develop communication skills.

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Advanced presentation skills

Prof. Dr. Roger Gläser, Universität Leipzig,

27 September / 4 / 5 October 2010 within the BuildMoNa 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 graduate students. 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 had basic experience in giving oral presentations, e.g. from the workshop "Erfolgreich Präsentieren", and should have had a fair knowledge of the English language.

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

Peter James Witchalls, Golin Wissenschaftsmanagement,

26 November 2010, 11 participants

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

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

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

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Nils Metzler-Nolte	Ruhr-Universität Bochum	Metal bioconjugates with peptide nucleic acids (PNA) – Solid phase synthesis, bio- sensors and biomedical applications	20 April 2010	Faculty of Biosciences, Pharmacy and Psychology
Prof. Dr. Klaus Ensslin	ETH Zürich, Switzerland	Electrons in quantum dots – One by one	11 May 2010	Faculty of Physics and Earth Sciences
Prof. Dr. Yuval Gefen	Department of Condensed Matter Physics, Weizmann Institute of Sci- ence, Rehovot, Israel	How to measure fractional statistics	12 October 2010	Faculty of Physics and Earth Sciences
Prof. Dr. Abdel Hadi Kassiba	Université du Main, Le Mans, France	Functional nanomaterials based on silicon carbide – Electronic and optical features	4 November 2010	Faculty of Physics and Earth Sciences



Events

3rd Scientific symposium

The third scientific symposium of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-Objects" (BuildMoNa) was held on 29 and 30 March 2010 at the Faculty of Physics and Earth Sciences. Interdisciplinary topics from the current research on the development and investigation of new materials were presented. Renowned invited scientists gave talks on current topics of BuildMoNa. During the poster session, as one part of the symposium, doctoral students were able to present their scientific topics and discuss these with the international guests, thereby receiving plenty of input for their ongoing work at the Graduate School BuildMoNa.

International guests were:

⇒ Prof. Dr. Robert S. Averback, University of Illinois at Urbana-Champaign, USA

Mesoscopic self-organisation in driven alloys: Effects of severe plastic deformation and particle irradiation

- ⇒ Prof. Dr. Kartik Ghosh, Missouri State University Springfield, USA Magnetoelectric effect in multiferroic perovskite oxides
- ⇒ Dr. Jesús Zúñiga Perez, CNRS-CRHEA, Valbonne, France Semiconductor nanostructures: Can they become basic building blocks for "lab-on-a-chip" applications?
- ⇒ Prof. Dr. Oliver Zerbe, Universität Zürich, Switzerland Structural studies of ligands and fragments of the human Y receptors
- ⇒ Prof. Dr. Sergio I. Molina, Universidad de Cádiz, Spain Advanced high resolutions electron microscopy of semiconductor nanostructures
- ⇒ Prof. Dr. Hauke Harms, Helmholtz Centre for Environmental Research, Leipzig, Germany Interaction of nanoparticles with microorganisms



Participants of the 3rd scientific symposium







3rd Workshop for doctoral candidates

30 doctoral candidates presented their scientific results with short talks at the 3rd BuildMoNa Workshop on 4 and 5 October 2010 in Wittenberg. About 100 Build-MoNa participants followed the lectures in the Martin Luther conference room, the conference venue of the Luther-Hotel Wittenberg. Presentations covered the whole research profile of the graduate school: Development of novel materials from appropriate building blocks, such as nano-objects, tailor-made molecules and polymers as well as peptides and proteins. Mechanisms of material formation from building blocks, e.g. by self-organisation, were also included.

For the 10 participants of the Transferable Skills Workshop "Advanced Presentation Skills" 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 the three best presentations given by the 30 doctoral candidates.

The first prize was awarded to Jochen Lach for his presentation "Magnetic exchange interactions of polynuclear nickel(II) complexes", the second to Carolin Wagner for her presentation "The interaction of tau-peptides and monoclonal antibodies – Dynamic force spectroscopy on single contacts" and the third to Erik Thelander for "Pulsed picoseconds laser deposition of lanthanum aluminate" and Christof Peter Dietrich for "Optical resonances in ZnO nanowires".



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Participants of the 3rd Workshop for doctoral candidates



Winners of the presentation awards at the 3rd Workshop: Erik Thelander (1.), Christof Peter Dietrich (c.) and Jochen Lach (r.)



3rd Annual reception

On 8 December 2010, BuildMoNa celebrated its third anniversary. The reception was opened by welcoming addresses of the speaker of the graduate school Professor Evamarie Hey-Hawnins and Mr Jörg Geiger from the Saxon Ministry for Science and the Arts (SMWK). Professor Klaus Kern (Max Planck Institute of Solid State Research, Stuttgart) gave a lecture on "Current at the nanoscale". In the talk, recent results on probing directly the nanocontact between single atoms and molecules as well as a metal electrode using scanning probe microscopy and spectroscopy were presented.

At this event, the BuildMoNa Awards were presented to doctoral candidates in recognition of their outstanding scientific achievements.

Lars Wolff (Institute for Theoretical Physics) received the first prize for the publications *Inelastic mechanics of sticky biopolymer networks* (Lars Wolff, Pablo Fernandez, Klaus Kroy / New Journal of Physics (2010) **12** 053024) and *Mean, variance, and autocorrelation of subthreshold potential fluctuations driven by filtered conductance shot noise* (Lars Wolff, Benjamin Lindner / Neural Computation (2010) **22** 94).

Carolin Limburg (Institute of Inorganic Chemistry) received the second prize for her research achievements and the subsequent publications *Synthesis of racemic aminoalkylferrocenyldichlorophosphanes and -dialkylphosphonites and their conversion to primary phosphanes* (Carolin Limburg, Peter Lönnecke, Santiago Gómez-Ruiz, Evamarie Hey-Hawkins / Organometallics (2010) **29** 5427) and *A sodium ferrocenyl-phosphanide polymer based on racemic primary aminoalkyl(bisphosphanyl)ferrocene* (Carolin Limburg, Santiago Gómez-Ruiz, Evamarie Hey-Hawkins / Dalton Transactions (2010) **39** 7217).

By awarding the third prize for the research work of Alexander Lajn on the whole route from the research on metal-oxide-contacts to the fabrication of electronic devices was honoured, and, in addition, the publication *Transparent rectifying contacts for visible-blind ultraviolet photo diodes based on ZnO* (Alexander Lajn, Matthias Schmidt, Holger von Wenckstern, Marius Grundmann / Journal of Electronic Materials (2011) doi:10.1007/s11664-010-1395-x) and the patent *Transparente gleichrichtende Metall-Metalloxid-Halbleiterkontaktstruktur und Verfahren zu seiner Herstellung und Verwendung* (Heiko Frenzel, Alexander Lajn, Holger von Wenckstern, Marius Grundmann, Deutsche Patentanmeldung Nr. 10 2009 030 045.7-33, granted August 2010).

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Congratulations again to the winners!



Prof. Dr. Klaus Kern during his lecture at the annual reception

The winners of the BuildMoNa Awards with their supervisors (from left to right): Dipl-Phys. Lars Wolff, Prof. Dr. Klaus Kroy, Prof. Dr. Evamarie Hey-Hawkins, Dr. Carolin Limburg, Prof. Dr. Marius Grundmann, Dipl.-Phys. Alexander Lajn



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 the doctoral 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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