

Graduate School Building with Molecules and Nano-objects



Cover image:

- ⇒ Left: Computed polarisation in terms of the Stokes vector for a cavity photon mode of an anisotropic microcavity depending on the in-plane momentum in the entire hemisphere. An optically uniaxial cavity medium with positive birefringence is assumed. The optic axis is aligned in the cavity plane and vertical in the plot. Colour represents the S_3 component (circular polarisation), arrows depict the projection of the Stokes vector in the S_1 - S_2 plane (linear polarisation). The positions of exceptional points (pure circular polarisation) are marked by the white dots.
- ⇒ Right: The image shows a 100 x 100 µm section of electron irradiated collagen (concentration: 2 mg/ml, dose: 50 kGy) obtained by confocal laser-scanning microscopy.
- ⇒ Bottom: Dinuclear nickel complexes supported by macrocyclic hexaaza-dithiophenolate ligands form a unique class of stable thiolate-halogen CT complexes (Hal = Br or I), in which short S-Hal bonds are always correlated to long Hal-Hal bonds and vice versa. The donating ability of the bridging thiolate functions was found to be similar to those of thioether or thiones as suggested by X-ray crystallographic analysis and accompanying DFT calculations.



Annual Report 2016

Founded as DFG Graduate School 185 in 2007

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

Preface Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins

The Graduate School BuildMoNa focuses on interdisciplinary education of young scientists based on excellent research. The materials research concept is based on a "bottom-up" approach. Progressive building blocks, such as nano-objects, smart molecules, polymeric scaffolds, peptides and active proteins, will be combined — preferentially by self-organisation — to create fundamentally new classes of materials that are inspired by active, adaptive living matter, and which are environmentally friendly, highly efficient, low-cost devices serving multifunctional purposes for a steadily more diversified modern



society. The paradigm shift from uniform bulk materials towards nanostructured multifunctional materials that emerge from combinations of smart molecules, proteins and nano-objects is essential for future knowledge transfer from fundamental to applied sciences.

Since the establishment of the Graduate School in 2007, the number of doctoral candidates has continuously grown. At the end of 2016, 53 doctoral candidates have been enrolled as members of BuildMoNa. Additionally, 127 young scientists have already finished their doctoral studies. In 2016, 5 doctoral candidates were funded by a DAAD-GSSP scholarship, and 67 doctoral candidates were funded by third-party grants.

The Graduate School provides a well-structured training programme including multi-disciplinary scientific training and a transferable skills programme in cooperation with the Research Academy Leipzig. The scientific training programme consists of introductory modules to bridge interdisciplinary gaps, thematic modules and advanced modules linked to ongoing research and technological applications. Each year, one of the advanced modules is organised as an international minisymposium. In 2016, the minisymposium "Physics of Cancer" was organised by the research group of Prof. Josef Käs and brought together researchers from pioneering groups worldwide that are concerned with the investigation of the physical mechanisms underlying cancer progression. Science-related events included the third Annual BuildMoNa Conference, which especially provided a platform for interdisciplinary exchange and discussion within the Graduate School.

Although the funding by the DFG within the German Excellence Initiative expired in October 2014, BuildMoNa will for now be continued with financial support from other sources as a class at the Research Academy Leipzig until October 2017.

Prof. Dr. Evamorie Hey-Hawkins

Organisation and management



SPOKESPERSONS OF THE DOCTORAL CANDIDATES

Faculty of Biosciences, Pharmacy and Psychology M.Sc. Chem. Jan-Patrick Fischer Faculty of Chemistry and Mineralogy Dipl.-Ing. Felix Link M.Sc. Chem. Antonio Buzharevski Faculty of Physics and Earth Sciences M.Sc. Phys. Peter Schlupp M.Sc. Phys. Martin Glaser Leibniz Institute of Surface Modification M.Sc. Phys. Alina Bischoff Institute of Medical Physics and Biophysics Dipl.-Phys. Martin Göse Helmholtz Centre for Environmental Research M.Sc. Chem. Yuting Guo

The Graduate School BuildMoNa is a class of the *Research Academy Leipzig* within the Graduate Centre Mathematics / Computer Science and Natural Sciences, its director being Prof. Dr. M. Droste. BuildMoNa is represented within the Research Academy by Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins as Research Academy Board member and by Peter Schlupp as representative of the doctoral candidates.

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

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

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

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

The BuildMoNa Office consists of one professional scientific manager (half-time position) and one multilingual secretary (part-time position), who support the Steering Committee. They coordinate the doctoral training activities and ensure information and communication between participating scientists, doctoral candidates, visiting researchers, and collaboration partners (non-university and industrial). The Office has regular business hours, especially for requests from applicants or doctoral candidates.

Doctoral candidates

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Anup Kumar Adhikari	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Synthesis and reactivity of phospho- rus-rich compounds
M.Sc. Chem. Angela Aleksovska	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Photoactive metal-organic-frame- works - synthesis and applications
M.Sc. Phys. Alina Bischoff	Prof. Dr. S. Mayr / Prof. Dr. M. Grundmann	Mechanical characterisation and training of ferromagnetic iron- palladium shape memory alloy thin films
M.Sc. Chem. Eng. Paul Cosmin Boar	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Phosphorus-based metallacycles for applications in catalysis
M.Ed. Math./Phys. Johannes Bock	Prof. Dr. W. Janke / Prof. Dr. F. Cichos	Computer simulations of semiflexi- ble polymers in disordered media
DiplPhys. Jakob Tómas Bullerjahn	Prof. Dr. K. Kroy / Prof. Dr. B. Abel	How a polymer breaks a bond
M.Sc. Chem. Antonio Buzharevski	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Synthesis, characterisation and evaluation of biologically active carborane derivatives of nonste- roidal anti-inflammatory drugs (NSAIDs) that are known COX in- hibitors to improve COX-2 selectiv- ity and reduce side effects
M.Sc. Chem. Peter Coburger	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	1,2-Dicarba-closo-dodecabo- rane(12) as scaffold for the develop- ment of new ligands with application in homogeneous catalysis
M.Sc. Chem. Milos Erak	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. T. Pompe	Synthesis of difficult and long pep- tide sequences, modifications and activity testing
M.Sc. Phys. Gianmaria Falasco	Prof. Dr. K. Kroy / Prof. Dr. F. Cichos	Non-equilibrium dynamics of heated and self-propelled nanoparticles
M.Sc. Chem. Jan-Patrick Fischer	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	Chemical modification and charac- terisation of therapeuticaly relevant peptide hormones
M.Sc. Phys. Nataliya Georgieva	Prof. Dr. J. Haase / Prof. Dr. B. Rosenow	Magnetic resonance of topological insulators

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Chem. Anika Gladytz	Prof. Dr. B. Abel / Prof. Dr. A.G. Beck-Sickinger	Nanospectroscopy near chemical and biological interfaces
M.Sc. Phys. Martin Glaser	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	Investigation of actin structures
M.Sc. Chem. Florian Glasneck	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	Novel calix[4]arene derivatives and their complexation behaviour towards f-elements
M.Sc. Phys. Tom Golde	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	Actin related contractile structures
M.Sc. Chem. Marta Gozzi	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Nido-carbaborate complexes as cytotoxic agents
M.Sc. Chem. Toni Grell	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Preparation of phosphorus-rich metal phosphides on the basis of oligophosphanide complexes
M.Sc. Chem. Yuting Guo	Prof. Dr. H. Harms / Prof. Dr. FD. Kopinke	Nanoparticle interactions with mi- croorganisms on the molecular level
DiplPhys. Tina Händler	Prof. Dr. J. Käs / Prof. Dr. A. Robitzki	Principles of mechanosensitivity and durotaxis in mammalian cells
M.Sc. Phys. André Heber	Prof. Dr. F. Cichos / Prof. Dr. M. Grundmann	Spatially resolved investigations of thermal transport in micro- and nanostructures
M.Sc. Chem. Reinhard Hoy	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Phospholane-based coordination cages for application in homoge- neous catalysis
M.Sc. Chem. Astrid Jäschke	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	Synthetic approaches towards novel calix[4]arene based f-metal recep- tors
DiplMath. Roger John	Prof. Dr. J. Meijer / Prof. Dr. B. Rosenow	Coupling ¹³ C-superlattices to single nitrogen vacancy centres in diamond
M.Sc. Chem. Ulrike Junghans	Prof. Dr. R. Gläser / Prof. Dr. H. Krautscheid	Heterogeneously catalysed liquid phase oxidation of hydrocarbons over metal-organic frameworks
M.Sc. Phys. Robert Karsthof	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	Transparent photovoltaic cells
M.Sc. Phys. Max Kneiss	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	Optical properties and lateral trans- port in $Mg_x Zn_{(1-x)}O$ quantum well nanostructures: a new approach for diluted magnetic semiconducters

Title and Name	First / Second Supervisor	Working title of doctoral thesis
DiplPhys. Jonas Kohlrautz	Prof. Dr. J. Haase / Prof. Dr. P. Esquinazi	Magnetic resonance under extreme conditions
DiplPhys. Andrea Kramer	Prof. Dr. K. Kroy / Prof. Dr. J. Käs	How temperature affects cell me- chanics
M.Sc. Chem. Robert Kuhnert	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Carbaboranes as phenyl mimetics in biologically active substances
DiplPhys. Anja Landgraf	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	Magneto-mechanical characterisa- tion and training of single crystal- line FePd films for the purpose of designing a thin film membrane pump
DiplPhys. Fritz Lehnert	Prof. Dr. S. Mayr / Prof. Dr. B. Rauschenbach	Ion-aided synthesis and investiga- tion of nanoporous materials
M.Sc. Phys. Susann Liedtke	Prof. Dr. B. Rauschenbach / Prof. Dr. J. Meijer	Sculptered metal films
DiplIng. Felix Link	Prof. Dr. R. Gläser / Prof. Dr. FD. Kopinke	Diesel exhaust catalyst deactivation by biofuel-originated poisons and hydrothermal treatment
M.Sc. Phys. Jürgen Lippoldt	Prof. Dr. J. Käs / Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	Stochastic analysis of plasma membrane fluctuations of neuronal growth cones
DiplPhys. Martin Marenz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	Development of a coarse-graining procedure for polymer adsorption
M.Sc. Chem. Georgia Mhanna	Prof. Dr. R. Gläser / Prof. Dr. A.G. Beck-Sickinger	Hexagonal mesoporous silicates for immobilisation of multi-enzyme conjugates
M.Sc. Phys. Tom Michalsky	Prof. Dr. M. Grundmann / Prof. Dr. F. Cichos	Light-matter interaction in systems of reduced dimensionality
M.Sc. Phys. Erik Morawetz	Prof. Dr. J. Käs / Prof. Dr. S. Mayr	Optical deformability and tumour aggressiveness
DiplPhys. Andreas Müller	Prof. Dr. T. Pompe / Prof. Dr. A.G. Beck-Sickinger	Peptide friction in cell adhesion
M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Metal-organic frameworks with chiral binaphthalene-based linkers
M.Sc. Chem. John Popp	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. B. Kersting	Redox-switchable catalysis with P-stereogenic dendritic ferrocenyl phosphine complexes
M.Sc. Mater. Sci. Eng. Rafaella Lima de Meneses Precker	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. D. Huster	<i>MOFs as drug carriers for cancer</i> therapy

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Marcus Purfürst	Prof. Dr. R. Gläser / Prof. Dr. M. Grundmann	Influence of soot loading on the catalytic behaviour of diesel particulate filters – experiment and modelling
M.Sc. Phys. Paul Räcke	Prof. Dr. J. Meijer / Prof. Dr. M. Grundmann	High precision fabrication of quan- tum sensor arrays via ion implanta- tion
M.Sc. Phys. Steffen Richter	Prof. Dr. M. Grundmann / Prof. Dr. J. Meijer	Spin polarisation investigations on exciton-polaritons and their condensates
M.Sc. Phys. Stefanie Riedel	Prof. Dr. S. Mayr / Prof. Dr. A. Käs	Radiation assisted modification of gelatin and collagen for biomedical applications
M.Sc. Biotechnology Chiara Ruggirello	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	Targeted tumor therapy by cell spe- cific receptor internalisation
M.Sc. Chem. Stefan Saretz	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Carbaboranes for medical applica- tions
M.Sc. Phys. Philipp Schierz	Prof. Dr. W. Janke / Prof. Dr. F. Kremer	Investigation of polymer aggrega- tion by computer simulations
M.Sc. Phys. Peter Schlupp	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	Growth and optimisation of amor- phous p- and n-type oxide semi- conductors for electronic device applications
M.Sc. Chem. Benedikt Schwarze	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. A.G. Beck-Sickinger	Metal carborate complexes with bioactive ligands as organometallic anticancer agents
M.Sc. Phys. Daniel Thomas Splith	Prof. Dr. M. Grundmann / Prof. Dr. S. Mayr	Investigation and optimisation of β -Ga ₂ O ₃ thin films and their applica- tion for electronic devices
M.Sc. Chem. Axel Straube	Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins / Prof. Dr. R. Gläser	Multi-ferrocene-based phosphorus ligands for homogeneous catalysis
M.Sc. Phys. Xinxing Sun	Prof. Dr. B. Rauschenbach / Prof. Dr. S. Mayr	Phase change materials
DiplPhys. Martin Thunert	Prof. Dr. M. Grundmann / Prof. Dr. B. Rosenow	Bose-Einstein-condensation and superfluids of exciton-polaritons in ZnO-based microresonators
M.Sc. Chem. Steve Ullmann	Prof. Dr. B. Kersting / Prof. Dr. H. Krautscheid	Extraction of rare earths by means of preorganised calixarene

Title and Name	First / Second Supervisor	Working title of doctoral thesis
M.Sc. Phys. Marcel Wille	Prof. Dr. M. Grundmann / Prof. Dr. H. Krautscheid	Whispering gallery modes: influence of the resonator shape on lasing properties
B.Sc. Eng. Emilia Wisotzki	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	Interaction of nanoparticles and polymers with biological matter for mechanical coupling
M.Sc. Biochem. Dennis Worm	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. mult. E. Hey-Hawkins	Synthesis and biochemical evalua- tion of carbaborane-modified pep- tide ligands
M.Sc. Nanosc. Muhammad Ayman Zaheer	Prof. Dr. R. Gläser / Prof. Dr. Kopinke	Studying of diffusion in reacting catalytic systems by means of NMR spectroscopic methods
DiplMath. Heinrich-Gregor Zirnstein	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundman	Topological aspects of dirac fermi- ons in condensed matter systems

Alumni 2016

Title and Name	First / Second Supervisor	Title of doctoral thesis
Dr. rer. nat. Uta Allenstein	Prof. Dr. S. Mayr / Prof. Dr. J. Käs	Dynamic mechanical cell manipu- lation and characterisation using magnetostrain
Dr. rer. nat. Michael Bonholzer	Prof. Dr. M. Grundmann / Prof. Dr. B. Kersting	Magneto-tunnel junctions with oxidic contacts
Dr. rer. nat. Annemarie Finzel	Prof. Dr. B. Rauschenbach / Prof. Dr. B. Abel	Ion-beam assisted deposition of gallium nitride films
Dr. rer. nat. Niklas Fricke	Prof. Dr. W. Janke / Prof. Dr. K. Kroy	Polymer conformations in disor- dered environments
Dr. rer. nat. Martin-Patrick Göse	Prof. Dr. D. Huster / Prof. Dr. T. Pompe	Surface functionalisation of layer- by-layer coated colloidal microcar- riers for specific cell uptake
Dr. rer. nat. Alexander Janot	Prof. Dr. B. Rosenow / Prof. Dr. M. Grundmann	Quantum condensates-coherence, fluctuations and disorder
Dr. rer. nat. Cathleen Jendrny	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	Design and development of peptides for therapeutic application
Dr. rer. nat. Karolin Kobalz	Prof. Dr. H. Krautscheid / Prof. Dr. B. Kersting	Bis(carboxyphenyl)-1,2,4-Triazole als Linker für poröse Koordina- tionsnetzwerke: Synthese, Charakte- risierung und Adsorptionsuntersu- chungen
Dr. rer. nat. Andy Schmied	Prof. Dr. Dr. h.c. E. Hey-Hawkins / Prof. Dr. R. Gläser	Phosphorus-based nano-frames
Dr. rer. nat. Ria Anne-Rose Schönauer	Prof. Dr. A.G. Beck-Sickinger/ Prof. Dr. Dr. h.c. E. Hey-Hawkins	Chemical modification of peptide analogues

Statistics



ORIGIN OF DOCTORAL CANDIDATES:



Biophysical and macromolecular chemistry

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

Research Topics

The Abel group at the IOM and the Universität Leipzig works in the fields of biophysical chemistry and macromolecular chemistry, as well as smart functional materials and surfaces. Structure and dynamics are investigated with the long-term goal of obtaining fundamental knowledge about light-matter and particle-matter interaction and about new smart functional materials. Another goal is also to develop new molecular and analytical probes for fundamental research and to develop advanced materials and analytical devices for industry and industrial applications.

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



Together with A. Beck-Sickinger's group and A. Robitzki's group we also study and develop biofunctionalised surfaces, i.e., proteins/peptides and biomolecules such as enzymes immobilised and bound to oxidic and metal surfaces for biocompatible interfaces and biomolecule assays as well as electronic devices. Peptide based multifunctional molecules are employed as anchors for cells near inorganic interfaces. Molecular adsorption and structure formation are investigated via a number of novel imaging and spectroscopic techniques (A. Gladytz). Another big research focus of the Abel group at BuildMoNa at present is time-resolved dynamics and structure of chemical and biological molecular systems at water interfaces (T. Gladytz). The analytical tools here are mainly ultrafast laser systems. With J. Meijer and P. Esquinazi we are currently pushing instrument development towards nanoscale (magnetic) imaging at surfaces based upon cryo-AFM/CFM sensors.



 Molecular dynamics simulation (A. Gladytz / H. J. Risselada) of peptide aggregation and structure formation near gold nanoparticles.

- ⇒ Multifunctional Coating Improves Cell Adhesion on Titanium by using Cooperatively Acting Peptides
 M. Pagel, R. Hassert, T. John, K. Braun, M. Wießler, B. Abel, A.G. Beck-Sickinger / Angew. Chem. Int. Ed. (2016) 55 4826
- ⇒ A Detailed Analysis of the Morphology of Fibrils of Selectively Mutated Amyloid beta (1-40)
 J. Adler, M. Baumann, B. Voigt, H.A. Scheidt, D. Bhowmik, T. Häupl, B. Abel, P.K. Madhu, J. Balbach, S. Maiti, D. Huster / ChemPhysChem (2016) 17 2744
- ⇒ Peptides@mica: from Affinity to Adhesion Mechanism
 A. Gladytz, T. John, T. Gladytz, R. Hassert, M. Pagel, H.J. Risselada, S. Naumov, A.G. Beck-Sickinger, B. Abel / Phys. Chem. Chem. Phys. (2016) 18 23516
- ⇒ Gold-Induced Fibril Growth: The Mechanism of Surface-Facilitated Amyloid Aggregation
 A. Gladytz, B. Abel, H.J. Risselada / Angew. Chem. Int. Ed. (2016) 55 11242
- ⇒ Peptide-Mediated Specific Immobilisation of Catalytically Active Cytochrome P450 BM3 Variant S. Zernia, F. Ott, K. Bellmann-Sickert, R. Frank, M. Klenner, H.-G. Jahnke, A. Prager, B. Abel, A. Robitzki, A.G. Beck-Sickinger / Bioconjugate Chem. (2016) 27 1090

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Chemical modification of peptides and proteins

Prof. Dr. Annette G. Beck-Sickinger

M.Sc. Chem. Milos Erak, M.Sc. Chem. Jan-Patrick Fischer, Dipl.-Pharm. Cathleen Jendrny, M.Sc. Biotechnol. Chiara Ruggirello, Dipl.-Biol. Ria Anne-Rose Schönauer, M.Sc. Biochem. Dennis Worm

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

In 2016, Ria Annerose Schönauer and Cathleen Jendrny successfully finished their PhD theses in the field of chemical modification of peptides. Ria succeeded in the chemical stabilisation of adrenomedullin, a peptide involved in vasodilation,



which is very promising for the treatment of acute lung diseases. She developed a suitable synthesis strategy that allowed the site specific introduction of modifications like fatty acids, methyl groups or lactams. Furthermore, she developed cell based signalling assays in order to evaluate the activity of all modified variants of adrenomedullin. In addition, she thoroughly evaluated the metabolic stability of the compounds in blood plasma as well as in liver homogenates. Based on these data she could develop a super-stable adrenomedullin variant by combining several modifications in one peptide. Additionally, she investigated the fate of the peptide after receptor binding and found that both peptide and receptor internalise and are degraded in liposomes rather than recycle back to the membrane.

Cathleen Jendrny studied the interaction between the serin protease kallikrein 7 (KLK7) and vaspin. Her goal was to develop peptidic mimetics of vaspin that are able to inhibit KLK7 as well as peptidic inhibitor of the vaspin-KLK7 interaction. She successfully synthesised peptidic inhibitors of KLK7 by introducing sequences out of the vaspin and other inhibitory proteins reactive center loop into the sunflower trypsin inhibitor scaffold. With these peptides she did thorough enzyme kinetic studies on KLK7 as well as other kallikreins and found valuable data on the activity and selectivity of these peptides. In addition, she could elucidate the binding site of a peptide that binds to a serin protease inhibitory protein called Protein Z dependent protease inhibitor (ZPI). This may perspectively help to generate im-



Introduction of several modifications into adrenomedullin led to a 13-fold stabilisation of the peptide against proteolytic degradation in human blood plasma (R. Schönauer et al. / J. Med. Chem. (2015) 12 5695).

proved inhibitors of this interaction.

The field of chemical modification of peptides and proteins is pursued successfully. Jan-Patrick Fischer further explores the field of adrenomedullin and its interaction with its receptor system. He aims to stabilise different structural elements of the molecule and to evaluate their impact on the selectivity of these peptides. Dennis Worm synthesises and evaluates carbaboranylated neuropeptide Y derivatives that eventually will serve as therapeutics within a boron neutron capture therapy regimen. Milos Erak develops a synthesis strategy for the generation of single-chain relaxin-2, a peptide that is involved in relaxation of the cervix uteri during labor. In October 2016, Chiara Ruggirello joined the group as a DAAD-funded student and will work on peptides coupled to nanoparticles.

In addition to current members, several papers of former BuildMoNa-members have been published, including Verena Ahrens, Lars Baumann, Sylvia Els-Heindl, Mareen Pagel and David Böhme. Work achieved during their PhD project were delayed in publication owing to collaborators.

- ⇒ Development of Potent and Metabolically Stable APJ Ligands with High Therapeutic Potential C. Juhl, S. Els-Heindl, R. Schönauer, G. Redlich, E. Haaf, F. Wunder, B. Riedl, N. Burkhardt, A.G. Beck-Sickinger, D. Bierer / ChemMedChem (2016) 11 2378
- ⇒ The Structural Investigation of Glycosaminoglycan Binding to CXCL12 Displays Distinct Interaction Sites N. Panitz, S. Theisgen, S. A. Samsonov, J.-P. Gehrcke, L. Baumann, K. Bellmann-Sickert, S. Köhling, M.T. Pisabarro, J. Rademann, D. Huster, A.G. Beck-Sickinger / Glycobiology (2016) 26 1209
- ⇒ Peptides@mica: From Affinity to Adhesion Mechanism
 A. Gladytz, T. John, T. Gladytz, R. Hassert, M. Pagel, H.J. Risselada, S. Naumov, A.G. Beck-Sickinger, B. Abel / Phys. Chem. Chem. Phys. (2016) 18 23516
- ⇒ Adrenomedullin 2.0: Adjusting Key Levers for Metabolic Stability
 R. Schönauer, S. Els-Heindl, J.-P. Fischer, J. Köbberling, B. Riedl, A.G. Beck-Sickinger / J. Med. Chem. (2016) 12 5695
- ⇒ On-Resin Diels-Alder Reaction with Inverse Electron Demand: An Efficient Ligation Method for Complex Peptides with a Varying Spacer to Optimise Cell Adhesion
 M. Pagel, R. Meier, K. Braun, M. Wiessler, A.G. Beck-Sickinger / Org. Biomol. Chem. (2016) 14 4809
- ⇒ Double Methotrexate-Modified Neuropeptide Y Analogues Express Increased Toxicity and Overcome Drug Resistance in Breast Cancer Cells
 D. Böhme, J. Krieghoff, A.G. Beck-Sickinger / J. Med. Chem. (2016) 59 3409
- Multifunctional Coating Improves Cell Adhesion on Titanium by Using Cooperatively Acting Peptides
 M. Pagel, R. Hassert, T. John, K. Braun, M. Wiessler, A.G. Beck-Sickinger / Angew. Chem. Int. Ed. (2016) 55
 4826
- ⇒ Charge-Compensated Metallacarborane Building Blocks for Conjugation with Peptides
 R. Frank, V.M. Ahrens, S. Boehnke, A.G. Beck-Sickinger, E. Hey-Hawkins / ChemBioChem (2016) 17 308
- ⇒ Inhibition of Kallikrein-Related Peptidases 7 and 5 by Grafting Serpin Reactive Center Loop Sequences onto Sunflower Trypsin Inhibitor-1 (SFTI-1)
 C. Jendrny, A.G. Beck-Sickinger / ChemBioChem (2016) 17 719

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Programmed self-organisation of artificial micro-swimmers

Prof. Dr. Frank Cichos

M.Sc. Phys. André Heber

Self-organisation is the generation of order out of local interactions in non-equilibrium. It is deeply connected to all fields of science from physics, chemistry to biology where functional living structures self-assemble and constantly evolve all based on physical interactions. The emergence of collective animal behaviour, of society or language are the results of self-organisation processes as well though they involve abstract interactions arising from sensory inputs, information processing, storage and feedback resulting in collective behaviours as found for example in crowds of people, flocks of birds, schools of fish or swarms of bacteria. This type of virtual interaction has so far not been considered in experiments on microscale active particles.

In new experiments, we introduce such information-based interactions to the behaviour of self-thermophoretic micro-swimmers. A real-time feedback of other swimmer positions controls the swimming direction and speed (see figure top part). The emerging structures reveal frustrated geometries due to confinement to two di-



mensions (see figure bottom part). Clusters of 4 swimmers reveal not the 3-dimensional tetrahedral structure but rather a flat structure with two isomers. Larger clusters even reveal the bond length between the swimmer "atoms", which are smaller than the adjusted bond length in the feedback loop.

All clusters diffuse like passive clusters of colloids but possess internal dynamical degrees of freedom that are determined by the feedback to the active particles. As the information processing in the feedback loops can be designed almost arbitrarily new perspectives for self-organisation studies involving machine learning and swarm intelligence arise. These experiments have been conducted in collaboration with the group of Prof. Yang at the Chemistry Department of Princeton University.



— The figure shows the definitions for the feedback rules for a self-organisation of artificial microswimmers. If the distance between two swimmers is smaller than req, the swimmers are propelled away from each other, otherwise towards each other (top two pictures). The lower images display example realisations of the self-organised swimmer molecule structures together with the corresponding simulated structures (lower pictures).

⇒ Thermophoretic Trapping and Manipulation of Single Molecules M. Braun, T. Thalheim, K. Günther, M. Mertig, F. Cichos / Proc. SPIE (2016) 9922 99220Z

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Research Topics

Programmed self-organisation of artificial micro-swimmers

Nano-scale investigations on innovative catalytic systems

Prof. Dr. Roger Gläser

M.Sc. Chem. Ulrike Junghans, Dipl.-Ing. Felix Link, M.Sc. Chem. Georgia Mhanna, M.Sc. Phys. Marcus Purfürst, M.Sc. Nanosc. Muhammad Ayman Zaheer

Innovative nanostructured catalysts with defined porosity on the nanometer scale and tunable active components continue to play a key role for the solution of current challenges in heterogeneous catalysis such as fluctuating reaction conditions, catalyst stability and mass transfer. Following the principle approaches of the graduate school, the research in our group is focused on the design of novel materials and their use as catalysts and catalyst supports. In this respect, we investigate the potential of innovative solid support systems, i.e., hierarchical hexagonal mesoporous silicates (HMS) for the selective immobilisation of multi-enzyme conjugates applied in cofactor regeneration or in cascade reactions. Two mesopores systems with different pore widths are introduced into the HMS to enable the immobilisation of enzymes with different sizes (see figure). Another research project deals with the partial oxi-



dation of hydrocarbons on microporous metal-organic frameworks containing transition metals under continuous-flow conditions in the liquid phase. Catalyst stability and deactivation due to poison deposits present in trace amounts are investigated for catalysts for the selective catalytic reduction of nitrogen oxides. Mass transfer and diffusion are major challenges when using solid porous catalysts. In this field, we study the influence of soot deposited on catalytically coated diesel particle filters on the mass transfer of reactants to the catalytic layer. Molecular transport processes on the nano-scale, i.e., the progress of mixing and composition during the course of catalytic reactions in multi-component partially miscible liquid mixtures are addressed using in-situ and in-operando investigations. These include the utilisation of xenon gas, which acts as an atomic nanosensor solvated in the reacting mixture with multinuclear NMR spectroscopy.



Tailoring the porosity of HMS for the immobilisation of enzymes with different sizes by addition of small mesopores into a material with large mesopores via pseudomorphic transformation using alkyltrimethylammonium hydroxides (C_nTAOH) and alkyltrimethyl-ammonium bromides C_nTABrt.

- ⇒ Bis(carboxyphenyl)-1,2,4-triazole Based Metal-Organic Frameworks: Impact of Metal Ion Substitution on Adsorption Performance
 - K. Kobalz, M. Kobalz, J. Möllmer, U. Junghans, M. Lange, J. Bergmann, S. Dietrich, M. Wecks, R. Gläser, H. Krautscheid / Inorg. Chem. (2016) **55**(14) 6938
- ⇒ Dimethyl Carbonate Synthesis from Carbon Dioxide by Ceria-Zirconia Catalysts Prepared Using Templating Method: Characterisation, Parametric Optimisation and Chemical Equilibrium Modeling
 P. Kumar, P. With, V.C. Srivastava, K. Shukla, R. Gläser, I.M. Mishra / RSC Advances (2016) 6 110235

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Don't mourn the losses – they give you an exceptional point!

Prof. Dr. Marius Grundmann

M.Sc. Phys. Michael Bonholzer, M.Sc. Phys. Robert Karsthof, M.Sc. Phys. Max Kneiss, M.Sc. Phys. Tom Michalsky, M.Sc. Phys. Steffen Richter, M.Sc. Phys. Peter Schlupp, M.Sc. Phys. Daniel Thomas Splith, Dipl.-Phys. Martin Thunert, M.Sc. Phys. Marcel Wille

Typically dissipation is an unwanted phenomenon, leading to loss of motion, waste heat and the like. BuildMoNa student Steffen Richter has now predicted a stunning consequence of dissipative processes in a microcavity – the emergence of circularly polarised states without the presence of magnetic ions, magnetic fields or spin-orbit coupling, the usual ingredients of spintronics. At the heart of the new microcavity physics lies the century-old optics of biaxial anisotropic crystals, translated into a modern metamaterial featuring two tailored optic directions. But let's unroll this one by one.

It was W. Voigt in 1902 [W. Voigt: *Beiträge zur Aufklärung der Eigenschaften pleochroitischer Kristalle /* Ann. Phys. (1902) **314** 367] who understood what happens to the optic axes in the absorption regime of biaxial crystals (which can be from the orthorhombic, monoclinic and triclinic crystal systems). The two optic axes of a biaxial crystal in the transparency regime split into a total of four singular



optic axes in the absorption regime. This regime is characterised by a symmetric dielectric tensor with imaginary components; thus at the core of the electrodynamic problem stands a non-Hermitian tensor, similar to recent investigations of non-Hermitian Hamiltonians. At such singular axis, the index of refraction is the same for all polarisations, now extending to the real *and* imaginary part of the index of refraction, i.e. speed of light and extinction coefficient. However, besides this degeneracy of the index of refraction the particularity is that only a *single eigenvector* exists and the singular axis is either left- or right-circularly polarised, representing a chiral state. Such singularity is also termed *exceptional point* from the theory of degeneracies of complex matrices.

The loss of time symmetry is due to the absorption process itself. The energy dependence of the dielectric tensor of such biaxial bulk crystal and the spectral and angular position of the exceptional points have been investigated by us [C. Sturm, M. Grundmann: *Singular Optical Axes in Biaxial Crystals and Analysis of Their Spectral Dispersion Effects in* β -Ga₂O₃/Phys. Rev. A (2016) **93** 053839] for monoclinic gallia (β -Ga₂O₃). However, bulk crystals offer little degrees of freedom for tailoring the properties of exceptional points regarding their energy and angular positions. For this purpose we have turned our interest towards anisotropic microcavities [S. Richter, T. Michalsky, C. Sturm, B. Rosenow, M. Grundmann, R. Schmidt-Grund: *Exceptional Points in Anisotropic Planar Microcavities* / Phys.



(a-h) Theoretical calculation of the modes in an anisotropic micro-cavity with five-period (N=5) DBR's. (a,b) In-plane dispersion of the mode energies, and (c) the difference of mode energies AE. (d,e) In-plane dispersion of the mode broadening, and (f) the difference in mode broadening Ay. The optic axis of the cavity material is along the y-direction. Panels (g,h) depict the Stokes vector component S₃ of these two modes. The exceptional points are at S₃⁻⁼±1. (i) The variation of position of the exceptional points in reciprocal space as a function of the number N of layer pairs in the DBR's between N=0 and 15. Rev. A (2017) **95** 023836; J. Zúñiga-Pérez, L. Kappei, C. Deparis, F. Reveret, M. Grundmann, E. de Prado, O. Jamadi, J. Leymarie, S. Chenot, M. Leroux: *Homoepitaxial Nonpolar (10-10) ZnO/ZnMgO Heterostructures: From Single Layers to Monolithic Bragg Reflectors and Optical Microcavities /* Appl. Phys. Lett. (2016) **108** 251904]. In such system, one optic direction is given by the mirror axis providing a cylindrical symmetry. The second optic direction is given by the c-axis of the wurtzite (hexagonal, optically uniaxial) cavity material that is oriented perpendicular or at least inclined with respect to the mirror direction. Thus an effectively orthorhombic or monoclinic optical metamaterial is present. In our theory, the Maxwell equations are solved using a matrix approach fully considering polarisation properties [S. Richter, T. Michalsky, L. Fricke, C. Sturm, H. Franke, M. Grundmann, R. Schmidt-Grund: *Maxwell Consideration of Polaritonic Quasi-Particle Hamiltonians in Multi-Level Systems /* Appl. Phys. Lett. (2015) **107** 231104].

The prediction made by Steffen Richer is that, given proper cavity thickness, the photon loss from the cavity alone (typically accounted for through mode broadening γ and a complex mode energy E+i γ) is enough to evoke exceptional points (see figure page 27) [S. Richter, T. Michalsky, C. Sturm, B. Rosenow, M. Grundmann, R. Schmidt-Grund: *Exceptional Points in Anisotropic Planar Microcavities* / Phys. Rev. A (2017) **95** 023836]. This publication, jointly with BuildMoNa PIs Profs. Grundmann and Rosenow, means that the generally elliptically polarised eigenmodes are circularly polarised in certain directions and for certain energies. Now it remains to verify these exciting predictions with artificial photonic



(a) Scattering geometry for transmission experiments on an m-plane anisotropic ZnO/(Mg,Zn)O microcavity (optic axis of cavity material "c-axis" is perpendicular to the growth direction). (b) Stokes vector components of the cavity mode dispersion. The finite values of S3 (circularly polarised light has S3= \pm 1) indicate elliptical polarisation states; for Bragg band modes |S3| is about 0.15, for the cavity modes 0.05-0.07. This result indicates already partially coalesced eigenstates.

Research Topics

layered structures. For the first anisotropic cavities, obtained in cooperation with CNRS-CRHEA in Valbonne, based on non-polar epitaxy of ZnO/(Mg,Zn)O Bragg mirrors and cavity, BuildMoNa students Steffen Richter and Tom Michalsky have found that the eigenmodes are indeed elliptically polarised (see figure page 28) [M. Grundmann, C. Sturm, C. Kranert, S. Richter, R. Schmidt-Grund, C. Deparis, J. Zúñiga-Pérez: *Optically Anisotropic Media: New Approaches to the Dielectric Function, Singular Optical Axes, Microcavity Modes and Raman Scattering Intensities* / Phys. Status Solidi RRL (2016) **11** 1600295]. Further optimisation of the cavity geometry and material quality will hopefully lead to the experimental realisation of fully circularly polarised states.

Related work to the role of absorption and spatially inhomogeneous absorption and gain in nanostructures such as tetrapods and nanowires has been published by BuildMoNa students Marcel Wille and Tom Michalsky [M. Wille, T. Michalsky, E. Krüger, M. Grundmann, R. Schmidt-Grund: *Absorptive Lasing Mode Suppression in ZnO Nano- and Microcavities* / Appl. Phys. Lett. (2016) **109** 061102; M. Wille, C. Sturm, T. Michalsky, R. Röder, C. Ronning, R. Schmidt-Grund, M. Grundmann: *Carrier Density Driven Material Dynamics of Lasing ZnO Nanowires* / Nanotechnol. (2016) **27** 225702]. For the first time a critical analysis has been performed of optically pumped lasing in nanostructures taking into account in theory the spatially inhomogeneous excitation and the related carrier dynamics and the effect of time-dependent carrier density on the index of refraction in various parts of the structures.

- ⇒ Singular Optical Axes in Biaxial Crystals and Analysis of Their Spectral Dispersion Effects in β-Ga₂O₃
 C. Sturm, M. Grundmann / Phys. Rev. A (2016) 93 053839
- ⇒ Exceptional Points in Anisotropic Planar Microcavities S. Richter, T. Michalsky, C. Sturm, B. Rosenow, M. Grundmann, R. Schmidt-Grund / Phys. Rev. A (2017) 95 023836
- ⇒ Homoepitaxial Nonpolar (10-10) ZnO/ZnMgO Heterostructures: From Single Layers to Monolithic Bragg Reflectors and Optical Microcavities

J. Zúñiga-Pérez, L. Kappei, C. Deparis, F. Reveret, M. Grundmann, E. de Prado, O. Jamadi, J. Leymarie, S. Chenot, M. Leroux / Appl. Phys. Lett. (2016) **108** 251904

- Optically Anisotropic Media: New Approaches to the Dielectric Function, Singular Optical Axes, Microcavity Modes and Raman Scattering Intensities
 M. Grundmann, C. Sturm, C. Kranert, S. Richter, R. Schmidt-Grund, C. Deparis, J. Zúñiga-Pérez / Phys. Status Solidi RRL (2016) 11 1600295
- ⇒ Absorptive Lasing Mode Suppression in ZnO Nano- and Microcavities
 M. Wille, T. Michalsky, E. Krüger, M. Grundmann, R. Schmidt-Grund / Appl. Phys. Lett. (2016) 109 061102
- ⇒ Carrier Density Driven Material Dynamics of Lasing ZnO Nanowires
 M. Wille, C. Sturm, T. Michalsky, R. Röder, C. Ronning, R. Schmidt-Grund, M. Grundmann / Nanotechnol. (2016) 27 225702

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Nuclear magnetic resonance of modern materials

Prof. Dr. Jürgen Haase

M.Sc. Phys. Nataliya Georgieva, Dipl.-Phys. Jonas Kohlrautz

Our group applies Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance for materials science with focus on high-temperature-superconductors, topological insulators, and porous materials. The efforts in materials research are accompanied by the development of new methods such as high-pressure NMR and NMR at the highest fields.

One topic supported by BuildMoNa was the investigation of the model 3D topological insulator Bi_2Se_3 . This class of materials is of great current interest as it represents a new electronic state of matter with dissipationless conducting surface states and an insulating bulk band gap. Crystals with different bulk doping levels and surface-to-volume ratios were studied leading to a first identification and characterisation of signals from distinct lattice sites. Furthermore, a magnetic coupling caused by interband excitations of bulk electrons was discovered, demanding a reinterpretation of published literature data [Phys. Rev. B (2016) **93** 195120].

In a collaboration with the Dresden High Magnetic Field Laboratory, we estab-





(a) Magnetisation of SrCu₂(BO₃)₂ for B||c at 2.1 K (data from Matsuda et al.). Arrows mark prior NMR work in DC fields. (b) Structure of the magnetic superlattice in the 1/3 plateau (after Takigawa et al.) with three different ¹¹B sites (red numbers). (c) ¹¹B NMR spectrum at about 54 Tesla and 2 K. Details and further references in [J. Magn. Reson. (2016) **271** 51].

lished and applied NMR in pulsed magnets that give access to the highest fields for research. Articles detailing shift and relaxation measurements [J. Magn. Reson. (2016) **263** 1], as well as the detection of a field-induced electronic spin superstructure in the spin-dimer system $SrCu_2(BO_3)_2$ using reconstructed broad frequency spectra [J. Magn. Reson. (2016) **271** 52] were published. These efforts required different approaches compared with conventional NMR experiments due to the inherent time-dependence of the external magnetic field and our work pushed the state of the art considerably.

Firstly, in case of the shift measurement, signal averaging across multiple field pulses was demonstrated. Secondly, an adiabatic inversion with subsequent small angle read-out pulses showed the feasibility of single field pulse T_1 measurements. Finally, the inherent time-dependence was not only overcome, but used for a field-stepped acquisition of a 9 MHz broad spectrum with a single field pulse instead of time-consuming field-stepped spin-echo measurements as in previous attempts by others.

- \Rightarrow ⁷⁷Se Nuclear Magnetic Resonance of Topological Insulator Bi_2Se_3
- N.M. Georgieva, D. Rybicki, R. Guehne, G.V.M. Williams, S.V. Chong, K. Kadowaki, I. Garate, J. Haase / Phys. Rev. B (2016) **93** 195120
- ⇒ NMR Shift and Relaxation Measurements in Pulsed High-Field Magnets up to 58 T
 J. Kohlrautz, S. Reichardt, E.L. Green, H. Kühne, J. Wosnitza, J. Haase / J. Magn. Reson. (2016) 263 1
- \Rightarrow Field-Stepped Broadband NMR in Pulsed Magnets and Application to $SrCu_2(BO_3)_2$ at 54 T

J. Kohlrautz, J. Haase, E.L. Green, Z.T. Zhang, J. Wosnitza, T. Herrmannsdörfer, H.A. Dabkowska, B.D. Gaulin, R. Stern, H. Kühne / J. Magn. Reson. (2016) **271** 52

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

Smart phosphorus- or carbaboranecontaining molecules and transitionmetal complexes as building blocks in catalysis, materials science and medicinal chemistry

Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins

M.Sc. Chem. Anup Kumar Adhikari, M.Sc. Chem. Angela Aleksovska, M.Sc. Chem. Eng. Paul Cosmin Boar, M.Sc. Chem. Antonio Buzharevski, M.Sc. Chem. Peter Coburger, M.Sc. Chem Marta Gozzi, M.Sc. Chem. Toni Grell, M.Sc. Chem. Reinhard Hoy, M.Sc. Chem. Robert Kuhnert, M.Sc. Chem. Juan Antonio Navarro Garcia-Cervignon, M.Sc. Chem. John Popp, M.Sc. Mater. Sci. Eng. Rafaella Lima de Meneses Precker, M.Sc. Chem. Stefan Saretz, M.Sc. Chem. Benedikt Schwarze, Dr. Andy Schmied, M.Sc. Chem Axel Straube

The Hey-Hawkins group focuses on smart molecular precursors for novel materials (binary metal phosphides, polymers, hybrid materials), catalysis (bio-inspired and switchable catalysts) and biosciences (carbaborane clusters and antitumour drugs). *Smart Catalysts: Phosphorus-based ligands* play an important role in homogeneous catalysis. We design functionalised phosphine ligands containing suitable groups



(ferrocene - see figure, aromatics, heterocycles, etc.) to modify their donor-acceptor properties in situ (i.e., electrochemically, UV-Vis spectroscopically, by modifying the temperature or the pH, etc.) and to develop in this way "switchable" phosphines for catalytic applications (J. Popp). A new approach includes C_3 -symmetric ligands (A. Straube) and carbaborane-based (P. Coburger) phosphine ligands.



Hydrophosphination reactions with transition metal ferrocenylphosphine complexes – a convenient method for the modification of phosphine.

Another approach focuses on the use of selective phosphorus-based macrocycles or nano-frames (P. C. Boar, R. Hoy, A. Schmied), and containers, or cavities (functionalised (S)-BINOL as linkers) in metal-organic frameworks (MOFs) with welldefined structure and porosity (J. A. Navarro). These compounds can be used as receptors for catalytically active transition metals, generating molecular nanosized reactors that should allow specific interactions of the cavity with substrates during a catalytic process. Variation of the coordinated metal atom or the size of the cavity will influence the selectivity in catalytic processes.

From Molecules to Novel Materials:

Molecular Building Blocks: Our approach to new functional materials starts from suitable inorganic or organometallic molecular precursors which incorporate diverse functionalities, such as catalytically active metal complexes or nanoparticles, chirality (for non-linear optical properties or asymmetric catalysis), redox-active metal complexes (for switchable magnetic or catalytic properties), or molecular assemblies as templates for organic-inorganic frameworks (polymers, MOFs). Selected examples of *functionalised building blocks* for organometallic or phosphorus-based polymers are: strained inorganic phosphorus-based rings (T. Grell, P. Coburger), alkylene- and arylene-bridged bis-phospholanes (P. C. Boar, R. Hoy, A. Schmied) or (planar-chiral) ferrocene derivatives (A. Straube) and bis-, tri- and tetrakis-carboxylates of conjugated aromatic systems as ligands in optically active coordination polymers or MOFs (A. Aleksovska; see figure).

Molecular Precursors: Binary metal phosphides MP_x often exhibit interesting optical, electronic and magnetic properties and thus have a wide range of applications, such as corrosion resistors, catalysts, semiconductors, electrode materials in lithi-

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



Depending on the direction of light polarisation, crystals of the highly stable metal-organic framework, $[{Fe_3(ACTBA)_2}X \cdot 6DEF]_n$ (X = monoanion), based on trinuclear iron(III) secondary building units (left) connected by tetracarboxyles with an anthracene core (ACTBA), exhibit anisotropic optical properties with birefringence $\Delta n = 0.3$ ($\lambda = 590$ nm) (right).

um-ion batteries, etc. We have developed an approach to this class of compounds starting with volatile phosphorus-rich metal complexes (A. K. Adhikari, T. Grell) as molecular precursors.

Inorganic Building Blocks in Medicinal Chemistry: Carbaboranes are highly hydrophobic and extremely stable icosahedral carbon-containing boron clusters. The cage framework of these clusters can easily be modified with a variety of substituents, both at the carbon and at the boron atoms and can either be used as pharmacophoric entities in cyclooxygenase (COX) (S. Saretz, A. Buzharevski) or lipoxygenase inhibitors (R. Kuhnert) or for boron neutron capture therapy as conjugates with tu-



Novel cobalt bis(dicarbollide) derivatives conjugated to the Y₁ receptor-selective derivative of neuropeptide Y, [F⁷,P³⁴]-NPY, show selective internalisation and are, therefore, promising candidates as boron-delivering agents for boron neutron capture therapy (BNCT).

mour-targeting entities (see figure), such as a Y_1 receptor-selective neuropeptide Y (NPY) derivative (S. Saretz, R. Kuhnert).

Chemotherapy using platinum-based anti-tumour agents, such as cisplatin, is often associated with strong side effects and is further limited by resistance of tumour cells. Specific MOFs with large cavities are, therefore, being studied for targeted drug delivery (R. Precker). Furthermore, to increase the efficacy of tumour treatment, metal complexes are conjugated with bioactive molecules that are efficient tumour-targeting entities (e.g. tamoxifen (B. Schwarze)). A new approach utilises the *nido* cluster (carbollide, $[C_2B_9H_{11}]^{2-}$ (which is isolobal to cyclopentadienide) as ligand in metal complexes that exhibit anticancer properties (M. Gozzi, B. Schwarze).

- ⇒ Nido-Dicarbaborate Induces Potent and Selective Inhibition of Cyclooxygenase-2
 W. Neumann, S. Xu, M.B. Sárosi, M.S. Scholz, B.C. Crews, K. Ghebreselasie, S. Banerjee, L.J. Marnett, E. Hey-Hawkins / ChemMedChem (2016) 11 175, Special Issue: Drug Discovery for Autoimmune & Inflammatory Disorders, front cover
- ⇒ P-chiral 1-Phosphanorbornenes: From Asymmetric Phospha-Diels-Alder Reactions Towards Ligand Design and Functionalisation
 T. Möller, P. Wonneberger, M.B. Sárosi, P. Coburger, E. Hey-Hawkins / Dalton Trans. (2016) 45 1904, invited

1. Moller, P. Wonneberger, M.B. Sarosi, P. Coburger, E. Hey-Hawkins / Dalton Trans. (2016) **45** 1904, invited contribution to special issue "Phosphorus Chemistry: Discoveries and Advances", back cover

- ⇒ Hydrophosphination Reactions with Transition Metal Ferrocenylphosphine Complexes J.R.F. Pritzwald-Stegmann, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2016) 45 2208, invited contribution to special issue "Phosphorus Chemistry: Discoveries and Advances"
- ⇒ Formation of a Carbene–Phosphinidene Adduct by N-Heterocyclic Carbene-Induced P–P Bond Cleavage in Sodium Tetramesityltetraphosphanediide

A.K. Adhikari, T. Grell, P. Lönnecke, E. Hey-Hawkins / Eur. J. Inorg. Chem. (2016) 620, invited contribution to special issue "Low Coordinate Phosphorus Compounds", back cover

- ⇒ Charge-Compensated Metallacarborane Building Blocks for Conjugation with Peptides
 R. Frank, V.M. Ahrens, S. Boehnke, A.G. Beck-Sickinger, E. Hey-Hawkins / ChemBioChem (2016) 17 308, back cover
- ⇒ Unique Anisotropic Optical Properties of a Highly Stable Metal-Organic Framework Based on Trinuclear Iron(III) Secondary Building Units Linked by Tetracarboxylic Linkers with an Anthracene Core
 A.V. Vinogradov, V.A. Milichko, H. Zaake-Hertling, A. Aleksovska, S. Gruschinski, S. Schmorl, B. Kersting,
 E.M. Zolnhofer, J. Sutter, K. Meyer, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2016) 45 7244, inside front cover
- \Rightarrow Selective Formation of Silver(I) Bis-phospholane Macrocycles and Further Evidence that Gold(I) is Smaller than Silver(I)
 - M. Streitberger, A. Schmied, R. Hoy, E. Hey-Hawkins / Dalton Trans. (2016) 45 11644, inside front cover
- ⇒ Antiproliferative Activity of Ruthenium(II) Arene Complexes with Mono- and Bidentate Pyridine-Based Ligands

S. Richter, S. Singh, D. Draca, A. Kate, A. Kumbhar, A.S. Kumbhar, D. Maksimovic-Ivanic, S. Mijatovic, P. Lönnecke, E. Hey-Hawkins / Dalton Trans. (2016) **45** 13114, invited contribution to Dalton Transactions themed issue: Metallodrugs: Activation, Targeting and Delivery Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawk

⇒ Unusual Reactivity of Sodium Tetramesityltetraphosphanediide Towards Cyclohexyl Isocyanide A. Adhikari, M.B. Sárosi, T. Grell, P. Lönnecke, E. Hey-Hawkins / Chem. Eur. J. (2016) 22 15664 Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins Institute of Inorganic Chemistry http://research.uni-leipzig.de/hh/ E-mail: hey@uni-leipzig.de Phone: +49 341 97-36151 Fax: +49 341 97-39319

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

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

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

This research project focuses on the development of new drug delivery systems to exhibit a targeted transport and time controlled release as well as which are able to transport multiple active agents safely and in a defined dosage in just one carrier system.

The Layer-by-Layer technique (LbL), based on modular assembly of polymers on a spherical micrometer-sized template, supports the development of such multifunctional carriers. In this context, we put emphasis on the assembly, characterisation and application of a supported lipid bilayer (SLB) as surface modification of the carrier. Such an SLB not only mimics the cell surface and enhances biocompatibility, but can be further equipped with specific antibody in a very defined way. While previous investigations involved assembly and characterisation, we now focused on the antibody functionalisation of the SLB.

Using the optimal layer composition to provide a tightly packed lipid layer, POPS/POPC in 1:1 molar ratio and a low amount of functional lipid PE-PEG-Biotin



(0.5mol%), biotinylated specific antibody was attached to the surface via streptavidin. Figures a and b now show the interaction of these carriers with 3T3 and Vero cells, respectively, while using the respective specific antibody. Interaction rate increases significantly compared to non-functionalised and non-specific controls. Also different assembly strategies of specific antibody, such as a direct coating onto the polymer surface or using a random (porous) underlying lipid layer, are less successful in cell application.

CLSM images of defined cell-carrier interaction time frames gave a first insight into the intracellular processing of lipid-antibody functionalised LbL microcarriers (figure c). Red fluorescent SLB shows carrier localisation in endolysosome and is nearly intact 1h after uptake. After 24h the lipid bilayer starts to dis-assemble, and carriers are partially found released into cytoplasm. During this process, both cell lines possess different kinetics.



a) Flow cytrometric investigations of specific antibody-functionalised microcarriers equipped with a POPS/POPC + 0.5 mol % PE-PEGbiotin lipid bilayer (striped bars) interacting with (a) 3T3 (AB-CXCR4) and (b) Vero (AB-CD155) cells. As controls, nonspecific antibody (ABCCR5) was used compared to basis SLB with and without streptavidin (filled bars). In (c), CLSM investigations of specific antibody-functionalised SLB microcarriers after interaction with 3T3 (1-2, AB-CXCR4) and Vero cells (3-4, AB-CD155) are shown. Before AB attachment, POPS/POPC + 0.5 mol % PE-PEG-biotin were assembled to the carrier polymer surface. Microcarriers are additionally labeled with PE-RITC as lipid bilayer constituent (red). Lysosomes / endolysosomes are visualised by LysoTracker-green (green) and cell membranes are stained with WGA-AF350 (blue). The individual images have a size of 52µm × 52µm.

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- ⇒ Oberflächenfunktionalisierung von Layer-by-Layer-beschichteten kolloidalen SiO₂-Mikropartikeln für eine spezifische Aufnahme durch Zellen M. Göse / PhD-Thesis (2016)

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Monte Carlo and molecular dynamics simulations of structure formation processes

Prof. Dr. Wolfhard Janke

M.Ed. Math./Phys. Johannes Bock, Dipl.-Phys. Niklas Fricke, Dipl.-Phys. Martin Marenz, M.Sc. Phys. Philipp Schierz

The BuildMoNa funded research activities of the computationally oriented theoretical physics group focuses on several interrelated subprojects. In most projects, the employed methodology relies mainly on sophisticated Monte Carlo computer simulations based on generalised ensemble methods such as multicanonical and parallel-tempering (sometimes also called replica-exchange) techniques, chain-growth algorithms with population control, (thermostated) Molecular Dynamics methods, and exact enumeration techniques. These methods are adapted and tailored by us to the problems at hand and constantly further improved in order to cope with the



complexity of the considered problems:

(i) Johannes Zierenberg uses multicanonical methods to investigate the analogy of condensation phenomena for particle systems with the aggregation process in ensembles of polymers, considering both lattice and off-lattice formulations. Special emphasis is laid on the distinguishing differences between flexible and semiflexible macromolecules. In the latter case he found very interesting twisted bundle-like structures for large bending stiffness and low temperatures, which prompted many further analyses.

(ii) Martin Marenz develops with the help of a few of his fellow PhD students a tool box ("framework") for multi-scale Monte Carlo computer simulations of meso-scopic and atomistic models of polymers in confined geometries such as a spherical cage or in interaction with a solid substrate. By generalising our previous studies of a generic bead-stick model of flexible polymers to the case of semiflexible polymers governed by bending stiffness, he discovered with a combination of parallel-tempering and multicanonical simulations for the unconstrained bulk system novel thermodynamically stable phases of knotted polymers of different topology. The next steps include studies of the adsorption propensity to substrates and the corresponding structure formation processes under confinement.

(iii) Niklas Fricke extended our recently proposed novel renormalisation group inspired exact enumeration method for self-avoiding random walks on a percolation cluster, modeling polymers in disordered environments with fractal properties, to up to seven space dimensions. The gain of efficiency implied by the reduction from exponential to polynomial complexity is enormous: enumerating all conformations



Sub-aggregation transitions for M = 2, 4, and 8 semiflexible polymers with stiffness parameter $\kappa = 6$ for decreasing temperature *T*.

of a 10000-step self-avoiding walk (typically about 10^{1550} on a two-dimensional cluster) would take over 10^{1500} ages of the universe using the standard enumeration method – our new procedure does it in about twenty minutes. As a main physical result he found that established asymptotic scaling predictions need to be corrected. In April 2016 he has successfully defended his PhD thesis on this topic.

(iv) Johannes Bock focuses on the intriguing properties of semiflexible polymers and proteins in quenched, disordered environments ("crowded cell problem") and thereby continues the work of a previous BuildMoNa-PhD student (Sebastian Schoebl) by extending it to the three-dimensional case subject to additional confinement constraints. One goal is to investigate to what extent the disorder can be effectively described by a "renormalised" bending stiffness of the macromolecules.

(v) Philipp Schierz aimed at efficient computer simulations of polymer systems. To this end he investigated the advantages of computations performed on powerful graphics cards (GPUs) over the use of standard CPUs and carefully compared the performances of Molecular Dynamics (MD) and Monte Carlo (MC) implementations for this class of problems. In particular he considered the microcanonical ensemble and showed how conservation laws in MD can be properly treated and related to each other and to MC by reweighting techniques. This turns out to be very important for small systems at the nanoscale. Subsequently he investigated Monte Carlo computer simulations in the so-called "real" microcanonical ensemble which, with a few further developments, promises to become a competitive alternative to generalised ensemble methods.

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- ⇒ First-Order Phase Transitions in the Real Microcanonical Ensemble P. Schierz, J. Zierenberg, W. Janke / Phys. Rev. E (2016) 94 021301
- ⇒ Dilute Semiflexible Polymers with Attraction: Collapse, Folding and Aggregation J. Zierenberg, M. Marenz, W. Janke / Polymers (2016) 8 333, invited review
- ⇒ Finite-Size Scaling of Lennard-Jones Droplet Formation at Fixed Density J. Zierenberg, W. Janke / J. Phys. Conf. Ser. (2016) 750 012017
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Mechanics and dynamics of semiflexible polymer structures

Prof. Dr. Josef Alfons Käs

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The mechanics of complex soft matter such as cells or tightly-entangled biopolymer networks as well as bundles cannot be understood in the classical physical frame of flexible polymers or rigid rods. Instead, the underlying filaments are semiflexible, with their finite bending stiffness leading to non-trivial bulk mechanical responses. We recently investigated two different structural arrangements of these polymers, networks and bundles.

To investigate bundles, we used the natural model actin and arranged the filaments via crowded environments. Modeling approaches and recent experimental data have shown that the arising depletion forces between rod-like particles display different signatures depending on the orientation of these particles. It has been shown that depletion-driven, axial attraction of two rods (in our case actin fila-



ments) yields a constant contractile force of 0.1 pN, which corresponds to a linear energy potential. We extended these pairwise interactions to a multi-filament level by investigating arising dynamics within actin bundles. Without any additional proteins such as crosslinkers or molecular motors, we found contractile forces in a biologically relevant regime of up to 3 pN. Generated forces due to bundle relaxation were not constant as in a two filament case, but decayed exponentially with a mean decay time of 3.4 s. These different dynamics are explained within the frame of a mathematical model (and supported by simulations) by taking pairwise interactions to a multi-filament scale [Schnauß et al. / Phy. Rev. Lett. (2016) **116** 108102].

Experimental studies of actin networks, however, are limited since the persistence length cannot be readily tuned. We experimentally investigated this parameter for the first time through bulk rheological and single-filament measurements of entangled networks formed by structurally tunable DNA nanotubes (see figure). This *de novo* model system enabled the validation of numerous characteristic proper-



n-helix tube (nHT) filament architecture. (a) Schematic of the assembly of a 4HT formed of four distinct 42-mers. Adjacent single-stranded DNA oligonucleotides share continuous complementary sections enabling the formation of a tube-like ring. The half-staggered motif of these rings with sticky ends on both sides promotes polymerisation-like axial growth. (b) Cross sections of all seven different nHTs employed in our study with according measured values for l_p and two exemplary fluorescence images (c),(d). [Schuldt et al. / Phy. Rev. Lett. (2016) **117** 197801].

ties inherent to semiflexible polymers and networks thereof, i.e. persistence length, inextensibility, reptation, and mesh size scaling. The scaling of the elastic plateau modulus with concentration is consistent with previous measurements and established theories. In contrast, we showed that the elastic plateau modulus scales linear with the persistence length, which drastically opposes the predominant theoretical predictions [Schuldt et al. / Phy. Rev. Lett. (2016) **117** 197801].

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Coordination compounds in supramolecular chemistry and materials chemistry

Prof. Dr. Berthold Kersting

M.Sc. Chem. Florian Glasneck, M.Sc. Chem. Astrid Jäschke, M.Sc. Chem. Steve Ullmann

Our research is focused on macrocyclic calixarene and thiophenolate-based ligands that are able to coordinate a range of d- and f-block metals. By introducing appropriate binding sites the selectivity of such host systems towards a specific group of guest ions can be modified. Ligating groups with high affinities towards hard lanthanide cations including P=O and C=O functionalities are used to obtain potent calix[4]arene-based receptors for rare earth metal separation via solvent extraction.

To satisfy the high coordination numbers of f-block metals tetrasubstituted derivatives of calix[4]arenes have been employed recently. Introducing dissimilar donor groups on the calix[4]arene scaffold opens up further possibilities for fine-tuning and modifying the binding pocket. Employing the synthesised ligands in titration and solvent extraction experiments yields valuable information about the affinity and selectivity of the compounds towards lanthanides is the basis for fur-





Synthesis of tetrasubstituted derivatives of calix[4]arenes

ther improvement of the ligand structures.

The coordination behaviour of a series of ligands $(H_2L^1 - L^4)$ towards Ln^{3+} cations is studied and the properties of the obtained complexes are examined in the light of selective solvent extraction. Solid state studies reveal a large diversity in the coordination behaviour over the course of the ligand series.

 H_2L^2 and H_2L^3 form dinuclear eight-fold coordinated complexes, respectively, of the composition $[Ln_2L^2_2(\eta^2-NO_3)_2(H_2O)_2]$ and $[Ln_2L^3_2(\mu-H_2O)](BPh_4)_2$. The Ln…Ln distances are ca. 7.8 Å for the complexes of H_2L^2 and 3.9 Å in the case of H_2L^3 com-



Molecular structures of $[Yb_2L^2_{,(\eta^2-NO_3)_2}(H_2O)_2]$, $[Gd_2L^3_{,(\mu+H_2O)}](BPh_4)_2$ and $[LaL^6(\eta^2-NO_3)_2]NO_3$ (from left to right).

plexes allowing for the antiferromagnetic coupling of the metal centres. In contrast, for L⁴ the formation of mononuclear 1:1 complexes of the form $[LnL^6(\eta^2-NO_3)_2]NO_3$ is observed where the metal centres exhibit a coordination number of ten.

Liquid-liquid-extraction experiments with H_2L^1 showed that calix[4]arene based ligands can act as potent extractants under acidic conditions. Quantitative extraction of Yb³⁺ into a chloroform phase was achieved at pH 5.5. Furthermore a selectivity towards smaller Ln³⁺ cations is observed.



Extraction diagram of $\mathbf{H}_{3}\mathbf{L}^{1}$ with Ln(NO₃)₃ (Ln = La, Yb). Organic phase: $[\mathbf{H}_{2}\mathbf{L}^{1}] = 10^{-2}$ M in CHCl₃: aqueous phase: $[Ln^{3+}] = 10^{-4}$ M in HNO₃/borate buffer; shaking time: 15 min; equilibration time: 30 min; T = 298(1) K. ICP-OES detection.

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Ring-opening polymerisation of $[Ag_3(triazol)_3]$ complexes

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Solid-state structural transformations in coordination compounds are an interesting phenomenon since changes in coordination number, coordination geometry and dimensionality of the structures are related to altered physical properties such as colour, luminescence behaviour, chirality, magnetism or catalytic activity. The cage-like silver complexes $[Ag_6(L)_6]\cdot 9H_2O$ (1) and $[Ag_6(L)_6(H_2O)_4]\cdot 4H_2O$ (2) (L⁻ = 2-(4H-1,2,4-triazol-4-yl)- ethanesulfonate) undergo solid-state structural transformations from cyclic triangular units to the one-dimensional polymeric complex $[Ag(L)]_n$ (3) via a ring-opening polymerisation process. This transformation involves opening of nine-membered Ag_3N_6 rings of $Ag_3(triazol)_3$ units via Ag–N bond breaking followed by rotation of the ligand and rearrangement of the Ag^+ coordination sphere by formation of new bonds. Thermogravimetric analysis in combination with single-crystal and powder X-ray diffraction methods reveals that the release of lattice water molecules initiates the transformation which starts already at room temperature after grinding of 1 and after separating 2 from its aqueous mother li-



queur, respectively. Driving force is the change in ligand conformation from gauche to trans.

Formation of compounds 1, 2, and $\{[Ag(L)]\cdot 1.5 H_2O\}_n$ (4) with the same Ag^+/L^- ratio but different crystal structures depends on the concentration and acidity of the reaction mixture; 3 crystallises directly from hot water.



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- ⇒ Bis(carboxyphenyl)-1,2,4-Triazole Based Metal-Organic Frameworks Impact of Metal Ion Substitution on Adsorption Performance

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 ⇒ Composition Space Analysis in the Development of Copper Molybdate Hybrids Decorated by a Bifunctional Pyrazoly//1,2,4-Triazole Ligand
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Non-isothermal Brownian motion and rapid force spectroscopy

Prof. Dr. Klaus Kroy

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We derive coarse-grained theories for the rupture of weak bonds in biomacromolecules. We have previously developed a rigorous theory of forcible bond rupture to facilitate the analysis of rupture events recorded in single-molecule simulations and experiments. We have now expanded this theory to so-called catch-slip bonds, which are characterised by rupture rates with a non-monotonic force dependence. They are thought to play an important role for the adhesion of cells, bacteria and platelets. We were able to analytically compute the mean lifetime and rupture-force distribution of a catch-slip bond for arbitrary forces and loading rates, covering the whole range of conditions found in experiments and all-atom simulations.

We also investigated the stochastic dynamics of particles suspended in solvents driven far out of equilibrium. We generalised the classical theory of Brownian dynamics to globally non-isothermal conditions, which resulted in a generalised Langevin equation with long-term memory for the particle's motion. In a combined numerical, experimental and theoretical study, we compared molecular dynamics simulations with experiments on hot Janus particles, performed in the group of Prof. Frank Cichos, to probe the validity of certain novel fluctuation relations.



The (reduced) free-energy landscape of a catch-slip bond is composed of two separated one-dimensional transition pathways from the bound to the unbound state. An applied force gets projected onto these reaction pathways, resulting in an effective tilt (red solid lines) that affects the landscape (green dashed line) along each reaction coordinate differently, depending on the force's specific direction.

These are very general theorems relating the fluctuating particle current of these self-propelled microswimmers to the associated entropy production. With the help of a minimal model for the swimmer dynamics, we further elucidated the underlying physics. Finally, we considered non-equilibrium solvents consisting of many of such active particles, and analysed their effects on the dynamics of interacting probe particles.

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New functional materials for biomedical applications and material physics at the nanoscale

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The work of our research group within the BuildMoNa Graduate School concentrates on the development of new functional materials for biomedical applications and material physics. Thereby, special focus was placed on modification of collagenous biopolymers by high energy electron irradiation as well as characterisation of biocompatible ferromagnetic shape memory alloy Fe₇Pd₃ and amorphous carbon materials.

Collagenous hydrogels represent promising biopolymers for a variety of biomedical applications. Within BuildMoNa, the potential of collagen modification using reagent-free crosslinking induced by electron irradiation was investigated.



Thereby, special focused was placed on mechanical and structural characterisation (see figure). We were able to show that structure and mechanics of the biopolymer collagen can be precisely tuned by high energy electrons for a variety of biomedical applications such as bio-coatings, tissue engineering or regenerative medicine.

The ferromagnetic shape memory alloy Fe_7Pd_3 , which is of particular scientific interest because of its biocompatibility, can feature reversible strains of several percent in an applied magnetic field. An essential prerequisite for both the occurrence and magnitude of these magnetic field induced strains is twin boundary mobility within the material. To investigate the behaviour of twin boundaries, an abrupt movement of these structures is locally induced by nanoindentation while concomitant acoustic emissions within samples are detected with an underlying piezoelectric acoustic sensor. With this approach, acoustic emissions were detected in a martensitic Fe_7Pd_3 bulk sample. The signals could be correlated to so called pop-in events in the force-depth curves of the nanoindentation measurements indicating twin boundary movement.

Within the investigation of ion beam induced surface changes of amorphous carbon materials two effects were studied. On the one hand, the ion beam induced



Three dimensional CLSM images of collagen samples (2 mg/ml) crosslinked by high energy electron irradiation: (left) 0 kGy, (middle) 50 kGy, (right) 100 kGy. Due to irradiation, the network becomes denser and the pore size decreases significantly. The scales are in µm.

synthesis of nanoporous carbon materials was investigated. On the other hand, ion beam induced material compaction and hardening was studied. The process could be correlated to the change of stress state in the material induced by the continued introduction of defect by the ion beam. Possible applications include abrasion wear resistance coatings. Nanoporous structures are of constant interest for research due to their manifold application areas, which include percolation and adsorption filters, heat exchangers, catalysts, membranes, prostheses, coatings, and drug delivery systems. In addition carbon is a promising bio-compatible material for biomedical applications.

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The L1 colour centre in diamond: statistics on its optical properties

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Dipl.-Math. Roger John, M.Sc. Phys. Paul Räcke

The L1 colour centre [New J. Phys. (2017) **19** 053008] that was found in two diamonds after yet unknown and still unreproducible treatment has been subjected to a large scale batch measurement to gather statistical knowledge about its optical properties. These measurements comprise spectral emission properties with potentially vibronic structure (see figure, a), excited state lifetimes, polarisation, blinking and saturation behaviour. The spectral emission of the measured L1 centres shows a high spread in their zero-phonon lines (ZPL) at \approx 583(22)nm (see figure, b), pointing at their most likely strain susceptible structure, noting that their diamond hosts were subjected to ion irradiation and plasma etching and that these centres were



measured closely beneath the surface of their hosts. The measured polarisation angles in the figure (d) also support this point due to their obvious broadening, which may prove the L1 centre useful as a diamond surface quality indicator. Additionally, the spectral emission also contains features at 15 THz and 49 THz (see figure, a) that may be attributed to the vibronic structure of the L1 centre but are still to be understood, though providing a characteristic property of these colour centres useful for further investigations. Finally, these diamonds also host the ST1 colour centre [S.-Y. Lee, M. Widmann, T. Rendler, M. W. Doherty, T. M. Babinec, S. Yang, M. Eyer, P. Siyushev, B. J. M. Hausmann, M. Loncar, Z. Bodrog, A. Gali: *Readout and Control of a Single Nuclear Spin with a Metastable Electron Spin Ancilla /* Nat. Nano. (2013) **8** 487] which shows significant differences compared to the L1 centres, one major being the <110> orientation of the optical dipole [SBDD XXI:





(a) Fluorescence spectrum of a characteristic L1 centre with 532 nm excitation showing a ZPL at 579.0 nm with a FWHM of 3.5 nm and potentially vibronic features at 640 nm corresponding to an energy offset of about 200 meV \approx 49 THz. (b) Distribution statistic of ZPLs with centre at 583(22) nm. (c) Several spectra of L1 centres with widely spread ZPL translated to ZPL at zero frequency to visualise the potential vibronics at 15 THz and 49 THz. (d) Distribution statistics of angles of the linearly polarised emission of the L1 centres showing strong peaks at \approx 45° and \approx 135° indicating a <111° orientation of the optical dipole. Note the strong peak at 50° due to sample drift while the linearly polarised excitation was rotated starting from this angle.

(a)

Hasselt Diamond Workshop (Hasselt, Belgium, 2016)] compared to <111> for the L1 centre (see figure, d). Still these two types of colour centres are found in close vicinity to each other in both samples, thus suggesting a connection between those regarding their creation and structure.

⇒ Bright Optical Centre in Diamond with Narrow, Highly Polarised and Nearly Phonon-Free Fluorescence at Room Temperature

R. John, J. Lehnert, M. Mensing, D. Spemann, S. Pezzagna, J. Meijer / New J. Phys. (2017) 19 053008

⇒ ST1 Colour Centre in Implanted and Plasma Treated Diamond R. John, J. Lehnert, M. Metsch, L. Rogers, S. Pezzagna, F. Jelezko, J. Meijer / SBDD XXI: Hasselt Diamond Workshop (Hasselt, Belgium, 2016)

Engineering biomimetic microenvironments for *in vitro* cell studies

Prof. Dr. Tilo Pompe Dipl.-Phys. Andreas Müller

The extracellular microenvironment controls many cellular processes including cell growth, differentiation and apoptosis. For better understanding of these regulating cues biomimetic systems are used for in-depth analysis in high-resolution *in vitro* studies. We design and construct material scaffolds to model important extracellular cues like stiffness, viscosity, spatial constraints and gradients of signalling molecules. Based on those biomimetic scaffolds we aim to reveal the detailed cell response to such extracellular signals including traction forces, single cell tracking, gene analysis.

Additionally, we apply polymer-based surface functionalisation strategies to develop new biosensors in various biotechnological applications.



Prof. Dr. Jan Meijer Institute for Experimental Physics II https://bloch.physgeo.uni-leipzig.de/nfp/ E-mail: jan.meijer@uni-leipzig.de Phone: +49 341 97-32701 Fax: +49 341 97-36939 A. Müller specifically investigates the impact of spatial constraints and matrix mechanics on cell behaviour. Micropatterned hydrogels are used to study traction force generation of laterally constricted cells. Actin cytoskeleton dynamics are observed in living cells with high temporal and lateral resolution. Correlating these measurements will expand the understanding of the tight coupling between matrix geometry and mechanics, cell morphology, and cellular function.

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Observation of traction forces and actin cytoskeleton dynamics. A) Time resolved measurement of traction force of laterally constrained cell (adhering to a fibronectin stripe-like pattern) reveals sites of focal adhesions (cyan, with purple circles) along with actin cytoskeleton morphology (red) observed with SiR-actin probes. B) Kymograph of actin stress fibres in the central region of such a cell reveals stress fibre dynamics. Scale, see (C). C) Quantification of inward movement of actin stress fibres.

Ion and laser beam induced thin films and nanostructures

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

M.Sc. Phys. Annemarie Finzel, M.Sc. Phys. Susann Liedtke, M.Sc. Phys. Xinxing Sun

The studies were focused on the fundamental processes at ion beam assisted deposition of ultra-thin films and nanostructures under conditions far away from the thermodynamic equilibrium.

For the synthesis of high-quality thin films, ion-beam assisted deposition (IBAD) is a frequently used technique providing precise control over several substantial film properties. An experimental setup was developed together with the Department Nanoscale Science of the Max-Planck-Institute for Solid State Research Stuttgart, that enables the separate control of ion mass and ion kinetic energy in the region of hyperthermal energies (few 1 eV – few 100 eV). This ion energy re-



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gion is of increasing interest not only for ion-assisted film growth but also for the wide field of preparative mass spectrometry. The setup consists of a constricted glow-discharge plasma beam source and a tailor-made, compact quadrupole system equipped with entry and exit ion optics. It could be demonstrated, that the separation of monoatomic and polyatomic nitrogen ions (N⁺ and N²⁺) is accomplished. For both ion species the kinetic energy can be controlled in the region of hyperthermal energies.

The feasibility for hyperthermal ion-beam assisted growth with mass and energy selected ions could be demonstrated by fabricating high-quality thin films of gallium nitride (GaN) deposited epitaxially on single-crystalline substrates at elevated temperatures.



Detail of the quadrupole mass filter, which was developed to deposit thin films with mass and energy selected ions.

- $\Rightarrow Real-Space Imaging of Atomic Arrangements and Vacancy Layers Ordering in Laser Crystallised Ge_2Sb_2Te_5$ Phase Change Thin Films
 A Latenda S Description II Prove X See M Eliterative D D and the latendary of the Control of Cont
 - A. Lotnyk, S. Bernütz, U. Ross, X. Sun, M. Ehrhardt, B. Rauschenbach / Acta Materialia (2016) 105 1
- ⇒ Microstructure Evalution in Pulsed Laser Deposited Epitaxial Ge-Sb-Te Chalcogenide Thin Films
 A. Lotnyk, U. Ross, S. Bernütz, E. Thelander, B. Rauschenbach / J. Alloys and Compounds (2016) 676 582
- ⇒ Crystallisation of Ge₂Sb₂Te₅ Thin Films by Nano- and Femtosecond Single Laser Pulse Irradiation
 X. Sun, M. Ehrhardt, A. Lotnyk, E. Thelander, J.W. Gerlach, U. Decker, B. Rauschenbach / Science Reports
 (2016) 6 28246
- ⇒ Local Atomic Arrangements and Lattice Distortions in Layered Ge-Sb-Te Crystal Structures
 A. Lotnyk, U. Ross, S. Bernütz, E. Thelander, B. Rauschenbach / Scientific Rep. (2016) 6 26724
- ⇒ Epitaxial Ge₂Sb₂Te₅ Films on Si(111) prepared by Pulsed Laser Deposition
 I. Hilmi, E. Thelander, P. Schumacher, J.W. Gerlach,
 B. Rauschenbach / Thin Solid Films (2016) 619 81

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

Topological quantum phases: Symmetries and charge response of topological insulators

Prof. Dr. Bernd Rosenow

Dipl.-Phys. Alexander Janot, Dipl.-Math. Heinrich-Gregor Zirnstein

Research in the group focuses on mesoscopic systems. These physical systems are so small that the quantum nature of individual particles in the system becomes relevant, but still large enough such that statistical averaging is possible. One exciting example where both the quantum nature and the collective motion of particles play a fundamental role are so-called topological quantum phases. These are novel phases of matter which seem ordinary when looking only at a small part of the system (locally), but which, due to quantum effects, are decidedly non-trivial when looking at the system as a whole (globally).

Topological insulators are an example of a topological quantum phase. There, the non-triviality manifests in the following way: a sample of such a material is



insulating in the bulk, but due to quantum effects, perfectly conducting surface states emerge at the sample boundary. Moreover, these surface states are robust against small perturbations like disorder, though the robustness may need mild additional requirements, for example time-reversal symmetry. Concrete examples of time-reversal symmetric topological insulators that exist as 3D bulk materials are Bi_2Se_3 and Bi_2Te_3 .

In this project, we have studied the symmetries of the electromagnetic response of surface states of time-reversal (TR) symmetric topological insulators more closely. One of their hallmark responses is the topological magnetoelectric effect, where a magnetic field induces an electric charge and vice-versa. So far, a variant of this effect has attracted much attention where time-reversal is, however, broken explicitly. Thus, we face the puzzling situation where these surface states are protected by TR-symmetry, yet their hallmark effect requires explicit TR-breaking. We have resolved this conundrum and presented a topological magnetoelectric effect that is explicitly time-reversal-symmetric.

In particular, we have shown that threading a thin magnetic flux tube of one flux



Spherical topological insulator threaded by a thin magnetic flux tube with flux Φ and subject to an electric field \mathbf{E}_i in vertical direction. Insertion of one flux quantum induces a charge $\Delta Q = e^2$. (a) Geometry. (b) Analytical result for the charge difference in the top hemisphere, $\Delta Q(\Phi)$, in the thin flux tube limit for an external electric field \mathbf{E}_x , giving rise to a potential difference $U = -2R\mathbf{E}z$ between top and bottom, with $eU = 0.2v_F/R$. Here, R denotes the radius of the sphere and v_F is the Fermi velocity of the surface states.

quantum through the material and applying a uniform electric field will induce a half-integer charge $\Delta Q = e/2 \cdot \text{sgn}(E_z)$ on the surface of the topological insulator if the system has mesoscopic size. This is illustrated in the figure. A key point of this effect is that the sign of this induced charge does not depend on the direction of magnetic field, only on the direction of the electric field. This is the defining char-

acteristic of a time-reversal symmetric charge response.

The effect can be understood in terms of the surface states of the topological insulator. Threading the flux tube through the material will lead to two electronic states, which are located at the two places where the flux tube meets the surface. Without electric field, these states will hybridise and a superposition of these states with equal weight in either place will be occupied. In the presence of a small electric field, one state will be occupied, while the other one will be emptied. This corresponds to a transfer of charge e/2. The validity of this argument depends on how well these two particular states can be separated from the other electronic states on the surface. By a combination of analytic and numerical arguments, we have shown that there are two energy scales: The energy splitting of the two states, which vanishes with decreasing flux tube size, and the energy of the other states, which is determined by the system size, but independent of the (relative) flux tube size. By choosing the electric potential in between these two energy scales, it is possible to single out the response of these two states. In the limit of a vanishing flux tube size, this leads to the half-integer charge as described. For a finite flux tube size, which is experimentally more relevant, we have shown numerically that the effect still yields an appreciable charge response. This means that the effect could be observed experimentally, though realising the proposed setup is likely challenging.

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Experiences

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

Prof. Dr. Ralf Seidel

I got to know the Graduate School BuildMoNa long before I joined the University Leipzig two years ago. I was twice giving a lecture during a BuildMoNa teaching module. Already at that time I admired that PhD students from different disciplines among them physics, chemistry and biochemistry come together, learn together and exchange knowledge and ideas. When joining BuildMoNa last year and experiencing my first BuildMoNa conference, I was impressed by the top level science and the quality of the talks given by the student members. Furthermore, BuildMoNa unites members from a large number of different nations. Thus, looking at BuildMoNa as a "newcomer", the graduate school is truly successful, highly interdisciplinary and international. The student members get here a great opportunity to look outside their research group and their specialist area. This setting is truly unique within Leipzig and should in my opinion be taken as a prototype example for the foundation of other graduate schools.

Despite its success BuildMoNa is now in a transition period and will have to change in the coming months and years. This is due to the funding that will be only provided by the university in the future, new rules for graduate schools demanded by the administration and at least in physics due to the omission of the examination prior the PhD defense that reduced for some students the benefits of the school. I am fully convinced that BuildMoNa will successfully master this transition period, since the past and present BuildMoNa leadership has always succeeded in navigating through all the challenges in the BuildMoNa history. Nonetheless, I want to take the opportunity to encourage the PhD students of the school to actively contribute to this transition and take over even more initiative and responsibility in shaping BuildMoNa. In my opinion BuildMoNa could be a home for all aspects of a PhD student career including the research and the PhD student training but importantly also the social life including the social support and exchange during problems that may arise during a PhD work. To make BuildMoNa to such a place, a more "bottom-up" organisation will be necessary, maybe in form of a student-organised BuildMoNa conference or an annual student retreat etc.

In that sense I am curious how BuildMoNa will reshape itself in the next one to two years while continuing the successful education of young scientists in preparing them for their future careers in industry and academia.

Ray Sicht

Prof. Dr. Ralf Seidel

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

M.Sc. Phys. Peter Schlupp

The Graduate School BuildMoNa offers a structured program to doctoral candidates coming from physics, chemistry, biology and biochemistry. This means that the doctoral candidates get an interdisciplinary education during their time within the Graduate School. This interdisciplinary education consists of three parts: scientific modules, transferable skills modules and the participation in international conferences. In the scientific modules basic knowledge as well as latest research topics are offered. The Principal Investigators (PI) organise these modules in a broad variety of styles: lectures, lab tours, experiments but also symposia or international conferences. The transferable skills modules are offered mainly by the Research Academy Leipzig (RAL). This is the parent organisation wherein all graduate schools and classes of the University of Leipzig are organised. Unfortunately, this is also the reason why the courses do not always suit the scientific background of the doctoral candidates. However, scientific writing or presentation workshops provide beneficial skills not only for an academic career. Suggestions from the doctoral candidates for workshop topics are possible but the implementation is quite slow. Participation of the doctoral candidates is especially possible and desired within the Annual BuildMoNa Conference which takes place once a year in Leipzig. International guest speakers, who can be suggested by the doctoral candidates, are invited by the speaker of the doctoral candidates to this interdisciplinary event. All session chairs are members of BuildMoNa. Each doctoral candidate should contribute at least one talk in his or her time in the Graduate School. Every year, the best three talks as well as the best three papers published in the last year are awarded with prizes. A poster session is organised in the evening giving the students the opportunity to discuss their topics with their PIs.

Every year the graduate school also organises a barbecue where all PIs and doctoral candidates are invited. This is always a good possibility for getting in contact with each other.

Altogether, there are many chances for the doctoral candidates to participate in different fields of the Graduate School. They can learn many important skills for their later career in both, scientific and non-scientific fields. After BuildMoNa has run for the 9th year, there is a kind of routine in the organisation and execution of all parts. It is planned to stabilise the school with this structure within the RAL. If this succeeds, there would be a stable funding in the next years.

M.Sc. Phys. Peter Schlupp

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 and a half 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 and HIGRADE (at the Helmholtz Centre for Environmental Research) including transferable skills and scientific activities.

TRAINING CONCEPT

Training activity			Month (March to February)											
	Туре	Min. CP	Μ	A	м	J	J	А	S	0	Ν	D	J	F
			summer term				winter ter			term				
Research work	R	-												
Scientific and methods modules	R/E	10	Μ	м	м	м	Μ			м	м	м	м	Μ
Annual BuildMoNa Conference	R		С											
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		flexible during the whole year (1 week up to a few months)					ths)						
Summer/winter schools	E													
Industrial training	E													
Active participation in conferences/workshops	R/E		flexible during the whole year (1 up to a few days)											
Transferable (generic)	R/E	5		S	S	S	S			S	S	S	S	
					м		м				М		м	

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

Scientific and methods modules

Basic concepts in molecular spectroscopy (2016-B4)

16 / 17 June 2016,

written exam, 2 credit points, yearly recurrence, 12 participants

This module introduced the basic concepts in molecular spectroscopy, i.e. infrared (IR), (surface enhanced) Raman- with imaging options and broadband dielectric spectroscopy (BDS), nuclear magnetic resonance spectroscopy, optical microscopy, superresolution microscopy and single molecule fluorescence detection.

Responsible Scientists/Lecturers:

Prof. Dr. Bernd Abel, Prof. Dr. Daniel Huster, Prof. Dr. Friedrich Kremer

Contents:

- \Rightarrow Quantum mechanical foundation of infrared spectroscopy
- \Rightarrow Experimental principles of Fourier transform infrared spectroscopy
- \Rightarrow Principle of broadband dielectric spectroscopy
- \Rightarrow Modern applications of broadband dielectric spectroscopy
- ⇒ Discussion of the chemical shift Hamiltonian with isotropic and anisotropic parts in NMR spectroscopy
- \Rightarrow Influence of sample orientation and molecular dynamics on the NMR signals
- \Rightarrow Magic angle spinning
- ⇒ Requirements for single molecule fluorescence detection at low and room temperature
- \Rightarrow Optical microscopy
- \Rightarrow Schemes as well as microscopic detection beyond the diffraction limit

Basic concepts in electrochemistry (2016-B5)

21 / 22 March 2016,

written exam, 2 credit points, 20 participants

This module introduced the basics in electrochemical methods, i.e. cyclic voltammetry, polarography, potentiometry. The doctoral candidates were given an overview of applications within the fields of analytics, biocatalysis, (bio)electrosynthesis, and the development of electrochemical energy storages and fuel cells.

Responsible Scientists:

Prof. Dr. Dr. h.c. mult. Evamarie Hey-Hawkins, Dr. Andy Schmied

Lecturers:

Dr. Falk Harnisch, UFZ Leipzig, Germany; Dr. Alexander Hildebrandt, TU Chemnitz, Germany; Dr. Jürgen Mattusch, UFZ Leipzig, Germany; Prof. Dr. Christina Roth, FU Berlin, Germany

Contents:

- ⇒ Basics in electrochemical methods, electrode processes, structure of interfacial region, types of electrochemical electrodes
- ⇒ Electroanalytical methods: i.e. potentiometry, polarography, cyclic voltammetry, square wave voltammetry
- ⇒ Cyclic voltammetry as an indispensable tool in materials development, battery tests in fuel cells, electrochemical impedance spectroscopy
- ⇒ Study of activity and degradation phenomena, spectroelectrochemistry combining spectroscopy and electrochemistry
- \Rightarrow Cell design
- ⇒ X-ray absorption spectroscopy to unravel reaction mechanisms during real operation
- ⇒ Applications: characterisation of multivalent systems, sensors, biosensors, bioelectrocatalysis, bioelectrochemical reactors

From molecules to materials – Artificial molecules and solid

state crystals (2016-T4)

19 / 20 September 2016,

poster presentation, 2 credit points, bi-yearly recurrence with modification, 6 participantss

This module linked molecular sciences and materials science, teached how materials with optimised catalytic activity and adjustable magnetic, electronic, or optical properties are obtained from molecules, and provided an understanding of the properties and applications of these materials.

Responsible Scientists:

Prof. Dr. Pablo Esquinazi, Prof. Dr. Jan Meijer

Lecturers:

Prof. Dr. Christoph Becher, Saarland University, Saarbrücken, Germany; Prof. Dr. Fedor Jelezko, Ulm University, Germany; Dr. Paolo Olivero, University of Torino, Italy; Dr. Sébastien Pezzagna, Universität Leipzig, Germany; Dr. Jose Luis Barzola Quiquia, Universität Leipzig, Germany; Prof. Dr. Jan M. van Ruitenbeek, Leiden University, Netherlands; Prof. Dr. Ralf Seidel, Universität Leipzig, Germany; Dr. Daniel Spemann, Leibniz Institute of Surface Modification, Leipzig, Germany

Contents:

- ⇒ Materials from "hard" (synthetic molecules, crystalline nanostructures, quantumelectronic structures) building blocks and/or "soft" (polymers, biomolecules, MOFs, metal-binding peptides, thin films) building blocks
- ⇒ Supramolecular arrangements (proteins and peptides together with modifications to improve the material qualities [pegylation, lipidation, glycosylation])
- ⇒ Properties of these materials (magnetic, electronic, and optical properties, electronic, photonic, and magnetoresistive devices, superconductivity)
- ⇒ Applications (catalysis [immobilised catalysts, MOFs], gas separation or gas storage [MOFs], sensors in electronics and photonics, quantum information technology [spintronics], energy conversion [including solar energy])
- ⇒ Theory (structure and interfaces within systems containing complex nanoaggregates)
- \Rightarrow Atomistic particle transport through MOFs

Methods:

- \Rightarrow Immobilisation techniques
- ⇒ Deposition (chemical vapour deposition [CVD, PECVD, MOVPE], physical deposition [PLD], atomic layer deposition [ALD])
- \Rightarrow Surface analysis (MIES)
- \Rightarrow Device characterisation (e.g. *I*⁻ *V*, *C*⁻ *V*, S-Parameter)

⇒ Modelling (mesoscale simulations, classical molecular dynamics simulations, multi-scalar approach, QM/MM simulations, advanced Monte Carlo techniques)

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From biomolecules to cells (2016-T5)

19 / 20 July 2016,

written exam, 2 credit points, bi-yearly recurrence with modification, 18 participants

The module provided tools and concepts from biophysics, biochemistry, molecular and cell biology, nanophotonics, and theory that are helpful for understanding, measuring, and manipulating live biological cells and their motility and transport properties, as well as self-propelled microorganisms from a bottom-up perspective, i.e. on a mechanistic molecular basis. The emphasis was on innovative interdisciplinary concepts and methods, and established and emerging physical measurement techniques.

Responsible Scientists:

Prof. Dr. Klaus Kroy

Lecturers:

Dr. Karen Alim, MPI Göttingen, Germany; Prof. Dr. Carsten Beta, Uni Potsdam, Germany; Dr. Benjamin Friedrich, MPI Dresden, Germany; Prof. Dr. Sarah Köster, University of Göttingen, Germany; Dr. Frank Vollmer, MPI Erlangen, Germany; Dr. Vasily Zaburdaev, MPI Dresden, Germany

Contents:

- \Rightarrow Structure and constituents of the cytoskeleton
- \Rightarrow Slime molds
- ⇒ Fungi
- \Rightarrow Selfassembly, cell mechanics, molecular interactions
- \Rightarrow Intermediate filaments
- \Rightarrow Established and novel biophysical measurement techniques
- ⇒ Motility of microorganisms, organelles employed to achieve self-propulsion (flagella, cilia)
- \Rightarrow Random walks in biology
- ⇒ Stochastic models used to quantify the motion of cells and of particles inside cells
- \Rightarrow Bacteria and eukaryotic cells performing chemotaxis
- \Rightarrow Cell motility beyond random walks

1 Participants of the module From molecules to materials – Artificial molecules and solid state crystals.

Methods:

- ⇒ Biophysical tools and methods: small angle x-ray scattering, light scattering, microfluidics, microscopy, x-ray imaging, optical tweezers, nanophotonic detection
- ⇒ Theoretical and numerical methods: random walks, Langevin equations, correlation functions, trajectory analysis, nonlinear dynamics, low-Reynolds-number hydrodynamics, Monte Carlo simulations

Hybrid systems – Metamaterials (2016-T6)

29 / 30 September 2016,

poster presentation, 2 credit points, bi-yearly recurrence with modification, 9 participants

The module teached the principles of and modern developments in metamaterials.

Responsible Scientists:

Prof. Dr. Frank Cichos, Prof. Dr. Marius Grundmann

Lecturers:

Prof. Dr. Mikhail Belkin, The University of Texas at Austin, United States; Prof. Dr. Kurt Bosch, Humboldt-Universität zu Berlin, Germany; Prof. Dr. Rudolf Bratschitsch, Universität Münster, Germany; Dr. Patrice Genevet, CRHEA, Valbonne, France; Dr. Geoffroy Lerosey, Institut Langevin, ESPCI Paris Tech and CNRS, France; Prof. Dr. Markus Lippitz, Universität Bayreuth, Germany; Prof. Dr. Thomas Pertsch, Friedrich-Schiller-Universität Jena, Germany; Dr. Sergey Sadofev, Humboldt-Universität zu Berlin, Germany

Contents:

- ⇒ Metamaterials are artificial materials with specific optical properties, typically evoked with sub-wavelength structures (periodic or non-periodic) in order to manage the dielectric function in particular ways such as negative index of refraction
- ⇒ While structural features are easy to fabricate for the micro-wave regime, structural features acting in the visible spectral range are typically $\lambda/4$ (about 100 nm) with even higher precision (few nm) require nano-fabrication tools

Methods:

- \Rightarrow Theoretical calculations of Maxwell's equations in the sub-wavelength regime
- \Rightarrow Calculation of effective dielectric functions
- \Rightarrow Nanofabrication of structures
- \Rightarrow Ion beam fabrication
- \Rightarrow Lithography-based processing

Participants of the module Hybrid systems – Metamaterials.

Smart and active assemblies: Advanced fluorescence techniques (2016-A1)

23 / 24 November 2016,

poster presentation, 2 credit points, bi-yearly recurrence with modification, 11 participants This module for physicists, chemists and biochemists focused on an in depth explanation of recently emerged advanced fluorescence and microscopy techniques including the development of smart fluorescence based sensors. Beyond introducing these techniques, their application in a broad variety of current cutting-edge scientific problems was demonstrated.

Responsible Scientists/Lecturers:

Prof. Dr. Ralf Seidel

Lecturers:

Dr. Kirsten Bacia, Martin-Luther-University, Halle, Germany; Dr. Christian Bökel, Technical University Dresden, Germany; Prof. Dr. Thomas Kiefhaber, Technical University of Munich, Germany; Prof. Dr. Andreas Lutter, Kiel University, Germany; Prof. Dr. Michael Schlierf, B Cube Center for Molecular Bioengineering, Dresden, Germany; Dr. Sandra Orthaus, PicoQuant, Berlin, Germany

Contents:

- ⇒ Fluorescence (phenomenon, fluorescence lifetime, Fluorescence-Resonance-Energy-Transfer FRET, fluorescence anisotropy)
- ⇒ Fluorescence spectroscopy (time-resolved spectroscopy, Triplet-Triplet-Quenching)
- ⇒ Fluorescence microscopy (confocal and wide-field microscopy, superresolution microscopy)
- ⇒ Fluorescence-(Cross-)Correlation-Spectroscopy (Diffusion of molecules, interaction between molecules)
- \Rightarrow Time-resolved single-molecule spectroscopy, confocal and wide-field FRET
- ⇒ Investigations of biological macromolecules/machines using fluorescence techniques, labeling of proteins with fluorescence markers (e.g. using non-natural amino acid incorporation)
- \Rightarrow Fluorescence sensors for in vivo applications based on fluorescent proteins

Methods:

- \Rightarrow Time resolved, fluorescence spectroscopy
- \Rightarrow Confocal and wide-field microscopy
- \Rightarrow Time-resolved fluorescence microscopy
- \Rightarrow Multi-colour detection
- \Rightarrow Correlation spectroscopy
- \Rightarrow Protein labeling

Scientific minisymposium

Physics of cancer (2016-A2)

04 October - 06 October 2016

The seventh BuildMoNa Minisymposium was organised by the research group of Prof. Dr. J. Käs. It brought together researchers from the worldwide pioneering groups that are concerned with the investigation of the physical mechanisms underlying cancer progression. The speakers were:

- ⇒ E. Barnhill, Charité Berlin, Germany, Investigating Heterogeneity of Tumour Mechanical Properties with Super-Resolution Multifrequency Magnetic Resonance Elastography
- ⇒ H. Clausen-Schaumann, University of Applied Sciences Munich, Germany, Cancer Metastasis in Bone: Investigating the Role of Cancer Cell Interaction

with Bone Matrix Proteins and Mesenchymal Stem Cells on the Single Cell Level

- ⇒ F. Cleri, Lille University I, France, Insights about the Role of Single- and Double-Strand Breaks in Cancer Radiotherapy
- ⇒ P. M. Davidson, Institut Curie, Paris, France, *LINC-ing the Nucleus, the Cytoskeleton and Cancer*
- ⇒ H.-G. Döbereiner, University of Bremen, Germany, *Dynamics of Circular* Dorsal Ruffles and their Role in Cancer
- ⇒ D. Allen Ehrlicher, McGill University, Montréal, Canada, Cytoskeleton Mechanics and Forces in Cancer
- ⇒ R. Eils, German Cancer Research Center, Heidelberg, Germany, Phenotyping Single Cell Derived Microtissues by Time-Resolved Imaging and Molecular Sequencings
- ⇒ B. Fabry, Friedrich-Alexander University of Erlangen-Nuremberg, Germany, Novel Methods to Study Cancer Cell Migration and Invasion
- ⇒ K. Franze, University of Cambridge, United Kingdom, *The Mechanical* Control of CNS Development and Disease
- ⇒ P. Friedl, The University of Texas, Houston, United States, *Mechanics of Cancer Cell Invasion in Vivo*
- ⇒ D. Goncalves-Schmidt, Leibniz-Institut for Polymer Research Dresden, Germany, Death by Gold: Targeting Invasive Glioblastoma Cells by Peptide -Functionalised Gold Nanorods
- ⇒ C.-M. Horejs, Karolinska Institutet, Solna, Sweden, Basement Membrane Fragments Contribute to the Regulation of the Epithelial-to-Mesenchymal Transition
- ⇒ P. Janmey, University of Pennsylvania, United States, *Effect of Hyaluronic* Acid on Mechanoresponse of Cancer Cells
- ⇒ J. A. Käs, Universität Leipzig, Germany, Why Do Rigid Tumors Contain Soft Cancer Cells?
- ⇒ S. Köster, Georg August University Göttingen, Germany, Cytoskeletal Intermediate Filaments - from Self-Assembly to Cell Mechanics
- ⇒ W. Losert, University of Maryland, United States, *Measuring and Modeling* Collective Cell Migration
- ⇒ C. Mark, Friedrich-Alexander University Erlangen-Nuremberg, Germany, Change Matters: A Time-Varying Parameter Model for Cell Migration
- ⇒ L. J. McCawley, Vanderbilt-Ingram Cancer Center, Nashville, United States, Physical Dynamics of Cancer Response to Chemotherapy in 3D Microenvironments: A Platform to Examine Complex Physical and Chemical Microenvironments
- ⇒ J. J. Min, Chonnam National University Medical School, Republic of Korea, Bacteria Associated Cancer Theranostics: When Bacteria Meet Cancer
- \Rightarrow H. Mohammadi, The Francis Crick Institute, London, United Kingdom,

Fiber Slippage in Collagen Matrices Enables Long-range Transmission of Mechanical Signals Between Local Cells

- ⇒ D. Niederwieser, University Hospital Leipzig, Germany, *Gene Therapy* Coming of Age
- ⇒ T. Pflüger, NanoTemper Technologies GmbH, Munich, Germany, Novel Tools for Discovery, Development and QC of Therapeutic (Bio)Molecules
- ⇒ M. Quaisser, TA Instruments AG, Eschborn, Germany, TA Instruments High Performance Thermal and Rheological Characterisation
- ⇒ J. Rädler, Ludwig Maximilians University of Munich, Germany, *Micro-Structured Surfaces for Assessment of Migratory Phenotypes*
- ⇒ J. Schnauß, Universität Leipzig, Germany, Programming the Mechanical Properties of Bionic Networks
- ⇒ R. Seidel, Universität Leipzig, Germany, *Membrane Targeting DNA* Nanostructures
- ⇒ F. Simmel, Technical University Munich, Germany, Condensing DNA into Nanostructures
- ⇒ D. M. Smith, Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany, *Bottom-up Engineering of Nanoscale Devices to Program Biological Materials*
- ⇒ D. Stamov, JPK Instruments AG, Berlin, Multiparametric Imaging of Collagen I Self-Assembly, and Cytoskeleton Reorganisation in Living Cells
- ⇒ M. Szardenings, Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany, Cell Binding Peptides from Statistical Analysis of Random Peptide Phage Display Libraries
- ⇒ K. Tanner, National Cancer Institute, Bethesda, United States, *Probing the Physical Properties of the Microenvironment Niche*
- ⇒ A. Teixeira, Karolinska Institutet, Solna, Sweden, Spatial Signalling at the Membrane
- ⇒ R. Wells, University of Pennsylvania, United States, *Liver Mechanics and Hepatocellular Carcinoma*
- ⇒ D. Weihs, Technion-Israel Institute of Technology, Haifa, Israel, Mechanobiology, Migration and Coordinated Cell-Remodeling in Invading Breast-Cancer Cells
- ⇒ S. Zahler, Ludwig Maximilian University of Munich, Germany, *Mechanical* Aspects of Angiogenesis
- ⇒ T. Zech, University of Liverpool, United Kingdom, Matrix Adhesion Sites Drive 3D Cancer Cell Migration through Direct Force Coupling to the Nucleus
- ⇒ M. Zink, Universität Leipzig, Germany, Employing Nanostructured Scaffolds for Long-Term Adult Tissue Culture and Investigation of Tissue Mechanics at the Nanoscale

Invited speakers of the scientific minisymposium

Transferable skills workshops

Presentation workshop

Dr. Frank Lorenz, Rhetoric Excellence,

03 / 17 March 2016 in combination with the Annual BuildMoNa Conference, 10 participants

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

Colloquia

Invited Speaker	Institution	Title	Date	Place
Prof. Dr. Toby Bell	Monash University, Melbourne, Australia	Super-resolution localisation micros- copy: Resolving fluorescence from single molecules in time and space	15 June 2016	Faculty of Chemistry and Mineralogy
Prof. Dr. Marjan Randjelovic	University of Niš, Serbia	Xonotlite and wollastonite as bioceramic materials: Process parameters for their electrophoretic deposition on stainless steel substrate	15 November 2016	Faculty of Chemistry and Mineralogy
Prof. Dr. Aleksandra Zarubica	University of Niš, Serbia	Spider silk-based materials: Perspective(s) in regenerative and biomedicine	15 November 2016	Faculty of Chemistry and Mineralogy
Prof. Dr. Rudolf Pietschnig	Universität Kassel, Germany	Henkel mit Funktion - Phosphorreiche [3] Ferrocenophane	23 November 2016	Faculty of Chemistry and Mineralogy

Annual BuildMoNa Conference

The fourth annual conference of the Graduate School "Leipzig School of Natural Sciences – Building with Molecules and Nano-objects" (BuildMoNa) was held on 14 and 15 March 2016 at the Faculty of Chemistry and Mineralogy. The following renowned guest speakers gave talks on current topics of BuildMoNa:

- ⇒ Prof. Dr. Thomas Høeg-Jensen, Novo Nordisk and University of Copenhagen: Design of Insulin Degludec and Co-Formulations with Insulin Aspart and Liraglutid
- ⇒ Prof. Dr. Gianaurelio Cuniberti, TU Dresden: Reinventing Computing or: Molecular Electronics is Dead, Long Live Molecular Electronics!
- ⇒ Prof. Dr. Ingrid Mertig, Martin-Luther Universität Halle-Wittenberg: Transversal Transport Coefficients and Topological Properties

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

Participants of the Annual BuildMoNa Conference

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

Mareen Pagel (Institute of Biochemistry) received the first prize for her work on the development of multifunctional coating that displays two cell binding peptides, published in:

Multifunctional Coating Improves Cell Adhesion on Titanium by Cooperatively Acting Peptides

M. Pagel, R. Hassert, T. John, K. Braun, M. Wiessler, B. Abel, A. G. Beck-Sickinger / Angew. Chem. Int. Ed. (2016) **55** 1

Marco Braun (Institute for Experimental Physics I) received the second prize for his work on the development of a single molecule trapping method, published in:

Single Molecules Trapped by Dynamic Inhomogeneous Temperature Fields M. Braun, A. P. Bregulla, K. Günther, M. Mertig, F. Cichos / Nano Letters (2015) **15** 5499 Uta Allenstein (Institute for Experimental Physics II, Leibniz Institute of Surface Modification (IOM)) was awarded the third prize for her experiments and calcula-

tions on biomimetic hydroxyapatite coatings on ferromagnetic shape-memory alloys, published in:

Coupling of Metals and Biominerals: Characterising the Interface Between Ferromagnetic Shape-Memory Alloys and Hydroxyapatite

U. Allenstein, S. Selle, M. Tadsen, C. Patzig, T. Höche, M. Zink, S. G. Mayr / ACS Applied Materials & Interfaces (2015) **7** 15331

and her new insights on contractile forces using a cantilever bending experiment, published in:

Contractile Cell Forces Deform Macroscopic Cantilevers and Quantify Biomaterial Performance

U. Allenstein, S. G. Mayr, M. Zink/ Soft Matter (2015) 11 5053

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

For the 10 participants of the Presentation Workshop by Dr. Frank Lorenz this was the opportunity to directly apply their newly acquired knowledge in that area. Their talks were filmed and critically discussed afterwards. At the end of the workshop a jury selected the three best presentations given by the doctoral candidates.

Winners of the BuildMoNa Awards 2016: Uta Allenstein, Marco Braun, Mareen Pagel (from right to left)

The first prize was awarded to Robert Kuhnert for his presentation "Carbaboranes as phenyl mimetics for the inhibition of lipoxygenases", the second to Antonio Buzharevski for his presentation "Carboranyl analogues of nonsteroidal antiinflammatory drugs (NSAIDs)" and the third to Marcel Wille for "Lasing dynamics in ZnO nanowires".

Winners of the presentation awards at the Annual BuildMoNa Conference together with the Speaker and Vice-speaker of the Graduate School: Marcel Wille, Prof. Dr. Marius Grundmann, Prof. Dr. Evamarie Hey-Hawkins, Robert Kuhnert, Antonio Buzharevski (from right to left)

Funding of doctoral candidates

www.buildmona.de