Graduate School BuildMoNa

Leipzig School of Natural Sciences - Building with Molecules and Nano-objects
Universität Leipzig

Research Topics

No.	Title	Description	Supervisor	Co-supervisor
136	Aggregation and self-assembly of peptides near inorganic interfaces and metal surfaces	Experimental and theoretical work on the aggregation and self-assembly of proteins and peptides near inorganic, semiconductor or metal interfaces. Peptides and/or peptide aggregates e.g. act as an anchors for cells at surfaces The goal is here to achieve biocompatibility at the interfaces (e.g., for implants, future cell-chips).	Abel	Beck-Sickinger
137	Development of novel singlet-oxygen sensitizer systems for tumor therapy	Novel molecular systems are developed and characterized that act as very efficient sensitizers for singlet oxygen to be used in photodynamic therapy. The work includes photophysical and photochemical characterization, synthesis, and efficiency studies.	Abel	Kremer
138	Chiral interaction and recognition	Chiral recognition is investigated from first principles theory and via time-resolved (excited state fluorescence) spectrocopy. Systems include ionic liquids, as well as smart biosystems.	Abel	Hey-Hawkins
97	Adhesive peptides to modulate surfaces	Peptides can be modified and used to bind to selective surfaces. This can be used to immobilize proteins, e. g. enzymes, or selectively attract cells. Aim of the project is to discover novel peptides, e. g. derived from biological systems to obtain new properties for biomaterials	Beck-Sickinger	Pompe
98	Selectively labelled biopolymers for tracing biomolecular movement	Many peptides or proteins target cells and influence the subcellular structures. By synthesizing selectively labelled chemokines we will address the internalisation on a subcellular level. Chemokines will be produced by native chemical ligation strategies and investigated by microscopy to enrol the mechanisms of internalisation networks in the cell.	Beck-Sickinger	Huster
99	Targeted tumor therapy approaches by cell specific receptor internalisation	Tumor cells frequently express selective receptors. By chemical modification of ligands that bind to tumor selective receptors, and subsequently are internalized, tumor cells will selectively be identified. Selective tumor targeting will be applied with cytotoxic compounds.	Beck-Sickinger	Hey-Hawkins

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100	Selfpropelled thermo-phoretic micro- and nanostructures	This research topic explores the laser-controlled self-propelled motion of asym-metrically shaped particles by thermophoretic forces. Individual particle dynamics as well as particle interaction and swarming behavior is studied.	Cichos	Kroy
101	Molecular motion in localized thermal fields	Gold nanoparticles are emplyed to generate localized temperature gradients to steer, trap and assemble individual molecules in solution.	Cichos	Kroy
102	Light emission in photonic crystals	The manipulation of light emission from single emitters and aggregates of emitters is studied in 3-dimensional photonic crystals by new types of spectrally resolved microscopy.	Cichos	Grundmann
103	Superconductivity at graphite/graphite interfaces	The phenomenon of superconductivity at interfaces in graphite, bismuth as well as in oxides has been observed in the last years. The aim of this thesis is its characterization in specially prepared multigraphene samples and the change produced after different kinds of treatment. Main aim is to trigger reproducible high temperature superconductivity.	Esquinazi	Haase
104	Ballistic transport in mesoscopic structures	When the mean free path and Fermi wavelength are of the order or larger than the sample size the wave nature of the electrons influence the electronic transport. Main aim of this thesis is the study of coherent ballistic transport in mesoscopic structures on multigraphene basis.	Esquinazi	Rosenow
105	Defect-induced magnetism in carbon and oxide nanostructures	Aim is the triggering of magnetic moments and their possible magnetic order via the introduction of vacancies and hydrogen in carbon as well as oxide nanotubes. The characterization will be done measuring the transport properties of individual nanotubes as a function of magnetic field and tempe-rature at different defect or hydrogen concentration. Main aim is to trigger smallest structures with permanent magnetic moment at room temperature.	Esquinazi	Kersting
106	Tailoring catalyst surfaces via task-specific ionic liquids	Thin films of ionic liquids (ILs) can be supported on the surfaces of porous solid catalysts to tailor their mode of action. Both porous polymers and inorganic molecular sieves will be functionalized using selected ILs. The goal is to achieve a specific interaction between the (task-specific) ionic liquid and the catalytically active sites on a molecular level. Active sites can be immobilized metal complexes, metal clusters or metal sites incorporated into the solid framework. The catalysts will be tested in selected redox conversions with industrial and environmental relevance.	Gläser	Kirchner

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107	Environmental catalysis on iron-containing molecular sieves	Iron-contiaining micro- and mesoporous materials possess a high potential as catalysts in environmental protection such as catalytic off-gas-treatment. The goal of this project is to investigate how a rational design of nanoscale structuring of iron-containing silicates with defined porosity can be applied to improve the performance of these catalysts, e.g. in the DeNOx reaction of industrially relevant process off-gases. Besides a thorough characterization by physico-chemical techniques and a systematic study of the catalytic properties by transient methods, also the influence of transport properties on different length scales will be studied.	Gläser	Kopinke
108	One-dimensional polariton superfluids	ZnO nano- and microwires are coated coaxially with dielectric "wrapped" Bragg mirrors such that strong coupling of light and matter is observed. The wave-guiding properties of the wires for the resulting polariton fluid shall be investigated.	Grundmann	Rosenow
109	Modeling of optical modes in deformed nanowire resonators	The optical modes, such as Fabry-Perot and whispering gallery modes, in hexagonal ZnO microwire resonators and resonators with coatings and heterostructures shall be modeled with respect to mode energies and dispersion and effects of deformed shape.	Grundmann	Cichos
110	Ultra-high field magnetic resonance of modern materials	Magnetic resonance techniques at the highest magnetic fields (up to 90 Tesla) in particular in pulsed magnets, will be developed and applied to various condensed matter systems to probe their behavior in extreme magnetic fields.	Haase	Gläser
111	Magnetic resonance of nano-structured quantum solids	Strong electronic correlations between electrons and with the lattice in modern materials such as high-temperature superconductors (the new Fe-based materials or cuprates), multiferroics, or topological insulators cause the complex physical properties of such systems. As a function of chemical composition, temperature, external fields, and pressure they will be investi-gated predominantly with magnetic resonance as a local probe with atomic scale resolution to elucidate their electronic properties, e.g. quantum-critical behavior.	Haase	Grundmann

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112	GigaPascal NMR	With pressures above 10 GPa one can alter the physical properties of many solids, however, NMR techniques that are very useful for the study of materials have not been available so far. We have developed a new technique to perform GPa NMR and will apply it to the study of various materials (high-temperature superconductors, multiferroics, complex metals, magnetic materials, topological insulators).	Haase	Rosenow
113	Interaction of microbial cells with nanoparticles	The steadily increasing use of nanoparticles in consumer products raises concerns about their mobility, lifetimes and whereabouts in terrestrial and aquatic environments. The subject (i) the colloidal stability of selected nanoparticles (to be addressed by model-assisted experiments), (ii) the sorption of nanoparticles to bacteria and uptake of nanoparticles into bacteria and (iii) the transfer of bacteria-associated nanoparticles into predator organisms (protists) and further up the foodchain.	Harms	Kopinke
114	Phages as nano-scale phylogenetic markers for environmental application	The high host cell specificity of phages can then be used to track and quantify their host cells within complex microbial communities by epifluorescence microscopy and flow cytometry. Fields of application are aquatic and terrestrial environments, technical installations (waste water treatment plants and biogas plants) and the human gut microflora. QDots and dyes markers will be used to fluorescently label phage particles.	Harms	Gläser
115	Carbaboranes as versatile inorganic building blocks in biologically active molecules	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. We are interested in substituted carbaboranes which can be used in medicine as suitable boron neutron capture therapy (BNCT) agents or as pharmacophores in which the carbaborane replaces the phenyl rings in drug candidates.	Hey-Hawkins	Beck-Sickinger or Käs

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116	Tailored phosphines and their application in catalysis	Phosphine-based ligands are designed in which the phosphanyl group is located inside a basket-, bucket- or tub-like cavity. Transition metal complexes thereof should allow selective transformation of molecules (regio-, stereo-, enantioselectivity) depending on the size and shape of the cavity, similar to the function of enzymes (bioinspired synthesis) or zeolites (heterogeneous catalysis). Furthermore, suitable phosphorus-based ligands such as (chiral) ferrocenylphosphines and related bimetallic catalysts (for tandem catalysis) will be immobilised on surfaces (e.g., graphite, gold, silica, etc.) or incorporated in polymers (via copolymerisation). A major target will be to manipulate or vary the properties by external stimuli (electrochemically, UV-vis, pH, etc.). The application of these immobilised molecular switches will be scrutinised with respect to changing the catalytic activity at will and shutting down or activating catalysts to trigger catalytic events.	Hey-Hawkins	Gläser
117	Hybrid materials: Inorganic polymers	Strained inorganic phosphorus-based rings will be employed in ring-opening polymerisation or copolymerisation reactions, or catalytic dehydrogenation of suitable precursors will be employed as an innovative route to novel inorganic/organometallic polymers that are more than just carbon-based polymer mimics. These polymers can function as scaffolds, e.g., for transition metals (homo- or heterometallic) with applications in catalysis or as novel materials with interesting magnetic (molecular magnets) and optical (non-linear optics) properties.	Hey-Hawkins	Abel or Kersting or Kremer
118	Investigation of the inter-action of biomolecules triggered by the domain structure of lipid membranes	Biomembranes are characterized by a well regulated domain structure. Such domains can also be prepared in artificial nanosystems as well, where the domain structure is modified by temperature changes. We have developed molecules that specifically partition into different domains, which allows to microscopically separate them. Goal of the project is to obtain control about the interaction of biomolecules on membrane surfaces by temperature variation. In particular, enzyme reactions will be the focus of the project.	Huster	Beck-Sickinger

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119	Modelling and computer simulations of molecular pattern recognition	In the focus of this project are general principles of the recognition of surface patterns by heteropolymers. Using a simple hydrophobic-polar lattice model for the heteropolymers as well as the patterned substrate, the pattern formation process shall be studied by means of multicanonical chain-growth simulations and exact enumeration studies. The main goal is to find a classification scheme of the interrelation between various surface patterns and the sequence of hydrophobic and polar monomers of the heteropolymers.	Janke	Grundmann
11	Quantum properties of Bose-Einstein condensates	The properties of Bose-Einstein condensates of interacting (quasi-)particles shall be described using quantum field theoretic methods (second quantization and path integrals) and evaluated by means of Monte Carlo computer simulations.	Janke	Grundmann
24	Modelling and computer simulations of adsorption specificity of synthetic peptides	A reasonable, computationally manageable, semiclassical model for the interaction between soft and solid materials on an atomic length scale shall be developed. For the simulations sophisticated generalized-ensemble Monte Carlo methods (multicanonical, parallel tempering, etc.) shall be implemented and run on the local compute cluster as well as, after the necessary adaptions, on powerful supercomputers.	Janke	Beck-Sickinger
87	Chemical oscillations in cell membranes	The regulative function of MARCKS proteins is based on a cyclic attachment and detachment to the cell membrane. We will investigate this aspect by means of mixed monolayers at the air-water interface. The interaction of PKC with MARCKS causes oscillating changes in lateral pressure, which will be detectable by pattern formation in the monolayer.	Käs	Abel
86	Biomimetic actin networks	The aim of the project is to establish a technique to form actin networks on cellular scales. Such a reproducible experiment for research on one of the major components of the cytoskeleton under physiological conditions would give new insides to cell mechanics and biology.	Käs	Beck-Sickinger
85	Role of intermediate filaments in tumor invasiveness	Optically induced forces will be used to study strain functions of cells under various stresses. Some deformations can be approached by viscoelastic models, but there are responses that need further investigation. This will lead to a better understanding of the contribution of the cytoskeletal elements to the mechanic integrity of cells.	Käs	Robitzki

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54	Inorganic materials based on coordination compounds: Clathrates	Novel coordination compounds of the type $[LM_2(L')][Anion]$, where L = macrocylic ligand and L' = coligand, that are suitable as host systems for the construction of clathrate structures will be studied. The host guest chemistry (i.e. sorption, storage and transport of small molecules such as halogens, CO_2, H_2, etc…) will be investagted as a function of the individual components of the host system.	Kersting	Krautscheid
13	Rational design of molecular based magnetic materials	This project deals with the synthesis, functionalization and characterization of molecular-based magnetic materials. Particular emphasis will be put on the development of magnetic molecules and their deposition onto surfaces. Issues that will be adressed are the targeted assembly of novel non-oxide based single-molecule magnets, their deposition and arrangement on solid surfaces, and thin film characterization by various techniques such as SQUID magnetometry and near-field techniques (STM, AFM).	Kersting	Esquinazi
57	Mixtures of ionic liquids	Ionic liquids (ILs) are salts with a melting temperature below 100 °C. Owing to their low vapor pressure and their tuneable properties, ILs have become a hot research area and so-called task specific ionic liquids were recently developed. One step further considers mixtures of ionic liquids. Molecular dynamics simulations should aid in understanding the properties of these hybrid systems.Questions such as “Can the IL-(mixture) be converted to a switchable, i.e. a smart solvent?” should be investigated.	Kirchner	Gläser
55	Investigation of crystal growth from molecular dynamics simulations and electronic structure calculations	Melting and crystal growth are still not very well understood on the molecular level. This theoretical chemistry project develops and applies methods for the investigation of crystal growth and melting, especially of ionic complexes from the group of Prof. Krautscheid. Methods from molecular dynamics simulations to the quantum cluster equilibrium should be employed.	Kirchner	Krautscheid
56	Impact of electronic structure on the solvent effects of smart molecules	This project investigates the importance of the accurate electronic structure description for solvent effect phenomena in large systems. For example questions as “Is the explicit relativistic treatment important for the description of relativistic elements interacting with bio-molecules in solution?” or: “How important is the accurate description of dispersion interactions in such systems?” should be tackled.	Kirchner	

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120	Catalysis in water with nano-materials	Nano-particles as reactants or catalysts are among the most promising new tools for in-situ cleaning of contaminated groundwater and aquifers. Special emphasis will be placed on nano-particles containing zero-valent iron (nZVI) as a reductant and Pd as a hydrodechlorination catalyst. Among others, the project aims at procedures to prepare nZVI on activated carbon or black carbon and to test these materials under environmental conditions. It is close to practical application.	Kopinke	Krautscheid
121	Spill over effects between nanoparticles in water	Nanoparticles such as Fe(0) or Pd(0) can generate reactive species on their surfaces, e.g. hydrogen atoms or electrons. These species can be transfered onto other particles, where chemical reactions may take place. This phenomenon is known from the gas phase chemistry as 'spill over'. However, little is known about spill over effects in condensed media such as water. The aim of the present topic is to find spill over effects with nanoparticles in water and to exploit them for water treatment processes. Preliminary results indicate spill over of H atoms between metal and carbon nanoparticles in aqueous suspension.	Kopinke	Gläser
122	Catalysis in water at interfaces and interphases	Heterogeneous catalysis is mostly controlled by surface reactions. The chemistry is effected by the properties of the fluid, e.g. water, which surrounds the catalyst surface. When changing the local reaction medium, e.g. by coating the catalyst surface with an organic microlayer, the reaction conditions are strongly effected. The catalytic reaction takes place at a new interface and in a new interphase. This opens tools for local enrichment of reactants, protection of the catalyst and changing reaction selectivities. The aim of the present topic is to exploit interphases on the nanoscale to improve nanocatalysts for water cleaning reactions.	Kopinke	Gläser
77	Novel precursors for photovoltaic materials	Novel precursors such as molecular chalcogenide clusters or polysilanes shall be studied for the fabrication of photovoltaic materials. Synthetic approaches are developed, the structural and thermal properties of the products are determined.	Krautscheid	Kersting
33	Porous coordination polymers	Synthetic approaches to novel coordinations polymers will be developed and combined with their structural characterization. Advanced magnetic resonance spectroscopy (NMR, EPR) will be employed to explore specific host guest interactions.	Krautscheid	Haase

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123	Broadband dielectric spectroscopy on the molecular dynamics in thin layers of block-co-polymers	Using novel nanostructured electrode-arrangements it is possible to measure the molecular dynamics in nanometer thick polymer layers in a broad temperature and frequency range. This enables one to unravel the dynamics in block-co-polymers deposited on a solid surface.	Kremer	Cichos
124	Forces of interaction bet-ween polymerbrushes as measured by Optical Tweezers	Optical Tweezers offer the unique advantage to measure directly the forces of interaction between polymerbrushes in surrounding media of varying ionic concentration and valence. By that the predictions of scaling theories can be checked.	Kremer	Cichos
125	Receptor-Ligand interactions as measured on the level of a single contact	Optical Tweezers enable one to carry out force spectroscopy on single receptor/ligand contacts. This offers a multitude of novel perspectives for Biochemistry, Biophysics and Bio-Nanotechnology.	Kremer	Kroy
126	How temperature affects cell mechanics	Internally and externally generated mechanical forces and deformations are increasingly realized to play a pivotal role for the development, differentiation, growth, and (mal-)functioning of living cells and tissues. Based on a recently developed mathematical model for the inelastic mechanics of cytoskeletal networks, the fundamental physical and biological role played by temperature shall be elucidated.	Kroy	Käs
127	Hot active nanoparticles	Laser-heated metal nanoparticles perform a special non-equilibrium form of Brownian motion, so-called “hot Brownian motion”. Anisotopic particles moreover undergo self-phoretic active motion if heated. The aim is to work out the appropriate coarse-grained mathematical framework to predict this motion. The research involves close collaboration with corresponding experiments.	Kroy	Cichos
128	How a polymer breaks a bond	Chemists know how chemical bonds break. However, if one of the binding partners is a polymer or a protein, the internal modes can affect the decay dynamics and renormalize the bond kinetics in a non-trivial way. This shall be worked out theoretically, in coordination with ongoing pertinent experimental studies.	Kroy	Kremer
90	Mechanical properities of metallic glasses	The mechanical properties of metallic glasses are characterized by a rather complex viscoelastic response. Although recently mechanical heterogeneities (soft „shear transformation zones“ vs. hard solid-like-regions) have been iden-tified, the underlying atomistic foundations are still poorly understood. The present project aims to employ classical molecular dynamics computer simulations to shead some light into these issues.	Mayr	

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129	Magnetic shape memory alloys for miniaturized actuators	The magnetic shape memory effect bears a high potential for new types of actuators in high–strain low–stress applications at constant temperature with frequencies up to several kHz. The present project focuses on the miniaturization of Ni-Mn-Ga based magnetic shape memory alloys towards the nanoscale via the thin film-route. Central challenges include MBE growth, mechanical, magnetic, structural and morphological optimization, as well as set up of an actuator prototype.	Mayr	Rauschenbach
134	Mathematical analysis of nucleation in shape memory alloys	Mathematical analysis of nucleation in shape memory alloys (cubic-to-tetragonal, cubic-to-ortorhombic), in particular nuclei of Martensitic phase near the sample edges/corners and for dimensionally reduced samples	Otto	Mayr
135	Mathematical analysis of models in epitaxial growth	Mathematical analysis (in particular numerical simulation) of models in epitaxial growth, e.\ g.\ Burton-Cabrera-Frank, modelling of the diverse effects of sputtering	Otto	Mayr
130	Novel Multielectrode-Multi-well-Arrays for multi-modal bioelectronic and photonic monitoring of stem cells	CAD and fabrication of various multiwell based mciroelectrode arrays based on glass and/or polymer substrates with various conductive and semi-conductive electrode materials. The main scientific apsect will be the proof of principle and proof of concept concerning the feasibility of multimodal biophysical measurements on viable stem cells. New microelectrode configurations and the research of cell-electrode interfaces available for impedance spectroscopy, field potential recording and optical analysis will be in the focus.	Robitzki	Pompe
131	Establishment and characterisation of viable solid tumours and metastases on new and optimised high dense microelectrode arrays	Design, fabrication and validation of 3D microeletrode arrays for catching/ selecting viable 3D and 2D solid tumour models and metastases for a real time and online bioelectronic monitoring. New high dense semi-conductive microelectrode arrays should be designed and developed for a parallel optical measurement and biompedance spectroscopy. Characterisation and optimisation of various nano-micro-electrode configurations with software and hardware adaption for data acquisition and data ware housing will be further scientific aspects.	Robitzki	Käs

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132	Coherence and dissipation in quantum condensates	Quantum particles with Bose-Einstein statistics condense into a collective quantum state at low temperatures. Examples are polaritons in micro-cavities and excitons in quantum Hall bilayer systems. Coherence of the condensate allows to observe macroscopic quantum phenomena. Understanding the effect of dissipation in such systems is important for a quantitative under-standing of their behavior.	Rosenow	Grundmann
133	Topological superconductivity	The interplay of superconductivity with strong spin orbit coupling can give rise to a new state of matter, so-called topological superconductors (TS). A TS is characterized by a gapped quasiparticle spectrum in the bulk of the material and unusual, topologically protected surface states, which give rise to a novel magnetic response, interesting tunnel spectra and unconventional interference phenomena	Rosenow	Haase