## **Graduate School BuildMoNa**

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

## **Research Topics**

No.	Title	Description	Supervisor	Co-Supervisor
1	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
2	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
3	Chiral interaction and recognition	Chiral recognition is investigated from first principles theory and via timeresolved (excited state fluorescence) spectrocopy. Systems include ionic liquids, as well as smart biosystems.	Abel	Hey-Hawkins
4	Role of nuclear quantum effects in hydrogen adsorption	Experimental and theoretical work on the role of nuclear quantum effects in hydrogen adsorption at confined metal sites studied using gas phase cluster model systems.	Asmis	Abel
5	Single nanoparticle action spectroscopy	Development and improvement of novel techniques for characterizing isolated single nanoparticles in the gas phase using action spectroscopy. A highly sensitive non-destructive mass spectrometer will be used to determine absorption cross sections by determining laser-induced changes in the mass-to-charge ratio.	Asmis	Cichos
6	Chiral differentiation of short-lived reaction intermediates	Cryogenic ion vibrational spectroscopy will be combined with microflow reactors for the isomer-specific on-the-fly analysis of short-lived reaction intermediates. The technique will then be extended to the selective detection of enantiomers using chiral differentiation.	Asmis	Abel
7		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

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8	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
9	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
10	Selfpropelled thermophoretic micro- and nanostructures	This research topic explores the laser-controlled self-propelled motion of asymmetrically shaped particles by thermophoretic forces. Individual particle dynamics as well as particle interaction and swarming behavior is studied.	Cichos	Kroy
11	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
12	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
13	Oxidic Monoliths with Hierarchically Structured Pore Systems for Advanced Heterogeneous Catalysis	The project is focused on the development of materials with hierarchically structured pore systems for the enhancement of diffusion-limited heterogeneously catalyzed conversions in the gas and liquid phase. Model systems will be alumina- and silica-based monoliths loaded with metals. The potential for rate and selectivity enhancement will be studied tow industrially important conversions: (i) SCR-DeNOx reaction with NH <sub>3</sub> as the reducing agent and (ii) conversion of carbon dioxide with renewable hydrogen to methane and alcohols.		Abel
14	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	

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15	Exceptional points in electrodynamical systems	Exceptional points are degeneracies of a complex parameter and occur in many physical systems. Possible applications are novel sensors and many questions remain about noise and quantum mechanics at these points. We design such points in electrodynamical systems such as (i) optical microcavities and (ii) integrated electronic circuits.	Grundmann	Rosenow
16	Combinatorial approach to functional thin films	Using special combinatorial methods of pulsed laser deposition we investigate multinary oxide semiconductor compounds for applications in photonics and electronics, ranging from amorphous materials to epitaxial superlatices.	Grundmann	von Wenckstern
17	Magnetic resonance of nano-structured quantum solids	Strong electronic correlations between electrons and with the lattice in modern materials such as high-temperature superconductors, 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 investigated predominantly with magnetic resonance as a local probe with atomic scale resolution to elucidate their electronic properties, e.g. quantum-critical behavior.	Haase	Grundmann
18	GigaPascal NMR	With pressures well into the GPa range one can alter the physical properties of many solids. We have developed new techniques that enable us to perform such GPa NMR and we will apply it to the study of various materials (high-temperature superconductors, multiferroics, complex metals, magnetic materials, topological insulators).	Haase	Rosenow
19	Carbaboranes as versatile inorganic building blocks in biologically active molecules	Carbaboranes are highly hydrophobic and extremely stable icosahedral carboncontaining 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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20	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
21	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
22	Investigation of the interaction 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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54	Environmental catalysis on Cu- containing zeolites	Selective catalytic reduction of $NO_x$ by $NH_3$ ( $NH_3$ -SCR-DeNO_x) is used as an efficient technology to eliminate $NO_x$ from diesel exhaust gases. Especially interesting seems to be a combination of $NH_3$ -SCR-DeNOx and the selective ammonia oxidation into nitrogen and water vapor ( $NH_3$ -SCO). Thus, residual $NH_3$ after the $NH_3$ -SCR-DeNO_x process is removed over ammonia slip catalysts. The Cu-containing zeolite-based catalysts will be investigated for their catalytic activity, selectivity and stability in $NH_3$ -SCO and $NH_3$ -SCR-DeNO_x. The present study is directed at understanding the mechanisms on powder and structured catalysts under dynamic conditions. (https://www.chemie.uni-leipzig.de/en/institute-of-chemical-technology/professorship-heterogeneous-catalysis/emission-reduction)	Jabłońska	
23	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.		Grundmann
24	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
25	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
26	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
27	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

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28	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	
29	Inorganic materials based on coordination compounds: Clathrates	Novel coordination compounds of the type [LM2(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, CO2, H2, etc) will be investagted as a function of the individual components of the host system.	Kersting	Krautscheid
30	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).		
31	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
32	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
33	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
34	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
35	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

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36	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	
37		Mixed-valence transition-metal chalcogenides with the additional benefit of dynamically disordered atoms represent a promising class of thermoelectric compounds. A broad range of diffraction, pectroscopic and TEM methods shall provide a reliable basis for advanced discussion. Cheap and non-toxic sulfides are an attractive starting point; however, anion substitution is expected to enhance thermoelectric properties. Oxidation states and chemical bonding in iron-containing compounds will be probed by Mößbauer spectroscopy, supplemented by EPR, XPS and susceptibility measurements	Oeckler	Krautscheid
38	Synthesis, characterization, phase transitions and structure-property relations of chalcogenides, including metastable ones		Oeckler	
39	Thermoelectric materials: crystal structure, nanostructures, heterostructuring, optimization of performance and stability		Oeckler	
40	Synchrotron methods: microcrystals, resonant scattering, diffuse scattering, diffraction tomography, XAS, also in situ and operando		Oeckler	
41	Transmission electron microscopy and electron crystallography		Oeckler	
42	Soft Colloidal Particles as Tool for Bioanalytical Sensing and Biomimetic Cellular Probe	investigated.	Pompe	
43	Presentation mode of signalling molecules	The presentation mode of signalling molecules (mobile vs. bound) modulates downstream events like proliferation and differentiation in living cells. We will develop biochemical plattforms to control the presentation mode of different signalling molecules and study their impact in in vitro cell systems.	Pompe	Beck-Sickinger

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44	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 understanding of their behavior.		Grundmann
45	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
46	Atomic-scale structure and vibrations in rare-earth pnictide chalcogenides	Rare-earth pnictide chalcogenides represent an intriguing, yet mostly unstudied, class of materials with exceptional physical properties, including charge density waves. To develop a fundamental understanding of these materials and their properties, the element-specific atomic-scale structure and atomic vibrations of RESbS and REBiTe with RE = La, Ce, Pr and Nd will be investigated by temperature-dependent X-ray absorption spectroscopy.	Schnohr	
47	Probing structural transitions of single- polymer chains with mechanical stress	In this project structural transitions in single polymer chains under external tension and torsion shall be investigated using magnetic and optical tweezers. Research objects are two different type of polymers: synthetic polymers and DNA chains. For the synthetic polymers the folding of such chains into well-ordered polymer crystals is investigated. In case of DNA a detailed understanding of structuarl reorginization processes upon extreme DNA twisting shall be obtained.	Seidel	Cichos
48	Self-assembly of nanoelectronic components with the help of DNA origami nanostructures	In this project DNA origami nanostructures shall be used to self assemble nanoelectronic devices. It involves the development of programmable assembly strategies of DNA nanostructures with complex shape that support the deposition of metallic and semiconducting materials. Furthermore, the nanoelectronic properties of the obtained structures will be characterized.	Seidel	Grundmann
49	Real-time observation of single enzymes that bind and process DNA	Aim of the project is to develop and apply state-of-the art biophysical techniques, such as optical/magnetic tweezers and advanced fluorescence techniques, to follow the activity of single enzymes (DNA repair proteins, CRISPR-CAs enzymes) in real time on a single DNA molecules that are targeted by these enzymes.	Seidel	Cichos
51	Non-equilibrium and non-linear dynamical phenomena in quantum systems	We will investigate novel emergent phenomena that can arise in quantum systems that are open and in a non-equilibrium or driven regime. For example investigate novel phenomena occurring in Floquet systems coupled to heat baths, and novel effects driven by electron's Berry phase in solids in regimes beyond linear response. (https://home.uni-leipzig.de/qcmt/home.html)		

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52		We will investigate phases of matter that feature emergent particles with fractionalized quantum numbers and anyonic statistics, such as quantum Hall and quantum spin liquids, which could be used as "hardware" for topological quantum computation. One of goals is to understand characteristic propeties of these states that could be useful in guiding their experimental discovery in systems such as quantum magnets. Another goal is to study ideal models of states that display exotic interplays of symmetry and fractionalization. (https://home.uni-leipzig.de/qcmt/home.html)	Sodemann	
53	Non-perturbative methods for strongly interacting states of quantum matte	We will investigate methods that allow to capture the properties of strongly interacting phases of matter. In particular, we will focus on gapless fermionic phases and employ methods such as higher dimensional generalizations of bosonization maps, non-perturbative field theoretic dualities. We will use this to compute concrete quantities relevant to experiments in correlated materials, such as thermal, optical, and electrical properties. (https://home.uni-leipzig.de/qcmt/home.html)	Sodemann	
50	Interaction of cells and tissue with smart materials for biomedical applications	The interaction of cells and tissue in contact with biomaterials play a crucial role for many biomedical applications such as implants and other tissue replacements. Within the project we aim to investigate the physical behavior of cells such as migration, adhesion and their mechanical properties in contact with nano- and microstructured surfaces, as well as nanoparticles.		Mayr

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