

Faculty of CHEMISTRY & PHARMACY

People and their research



Universität Regensburg
FACULTY OF CHEMISTRY AND PHARMACY

Our JUNIOR SCIENTISTS



Dr. Robert Kretschmer
Inorganic Chemistry

Research in the Kretschmer Group focusses on the design and synthesis of low-valent polynuclear Group 13 and 14 compounds. Besides the investigation of structure and bonding in these unique organometallic compounds, we are interested in their application towards small molecule activation.

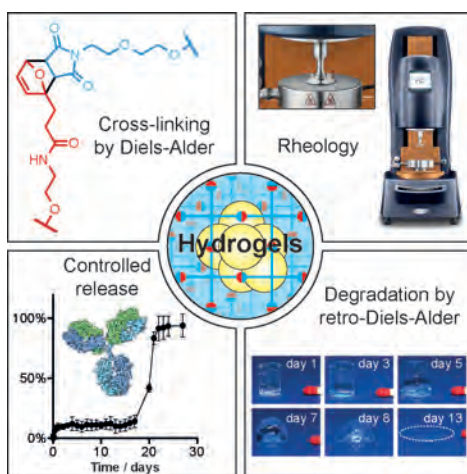
Tailored chelating ligands are used to systematically modify the oxidation states of the metals, the metal-metal distances and the electronic interactions between them. The well-directed variation of the cooperativity between the metal(loid) centers may lead to novel and exciting chemistry, beyond the scope of conventional monometallic Group 13 and 14 reagents.



The main research areas are the synthesis of polymers and the development of hydrogels for biomedical applications. The Diels-Alder/retro-Diels-Alder reaction is employed as a reversible cross-linking reaction for biodegradable hydrogels. The prepared hydrogels are characterized by rheological experiments and degradation studies. Such hydrogels can accommodate high loads of proteins, such as therapeutic antibodies, and release their payload in a controlled manner. Potential applications are seen in the treatment of age-related macular generation, a major cause of visual impairment worldwide.

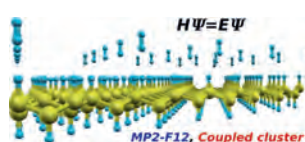


Dr. Ferdinand Brandl
Pharmaceutical Technology



The main focus of my research is development of first-principle quantum-chemical methods for calculating the electronic structure of periodic systems and related properties. The developed computational

schemes and efficient algorithms allow for application of the methods to complex extended systems. The quantum chemical hierarchical approach, which combines periodic and finite-cluster treatments, makes it possible to reach a very high precision for the interaction energies, which is comparable to or even surpassing the experimental precision. The applications of the developed methods are targeting molecular crystals, crystals with a complex binding pattern (stacked polymers or sheets, etc.), molecules adsorbed on surfaces, i.e.

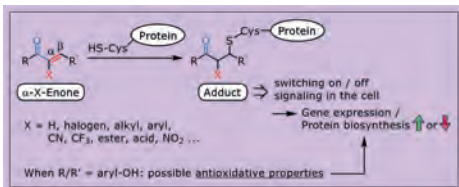


PD Dr. Denis Usyat
Theoretical Chemistry



systems, where the intermolecular interaction, which is rather difficult to describe accurately, substantially contributes to binding.

PD Dr. Sabine Amslinger
Organic Chemistry



In the Amslinger group we try to influence biological pathways relevant for inflammation and cancer, but also neuroprotection. Therefore, we synthesize small molecules often based on natural products, such as chalcones, flavones, terpenes, diarylheptanoids and so-called phosphoantigens. One general approach to modulate biological activities by these molecules is based on thiol-mediated processes which can be addressed by oxidation or alkylation of cysteine residues of proteins. Molecules with an α,β -unsaturated carbonyl system, often polyphenolic compounds, proved to be particularly useful in this context. We do not only synthesize new enones/phenolic compounds based on natural products, we also combine the enone moiety with heterocycles like oxadiazoles. And, moreover, we assess their chemical reactivity towards thiols as well as their biological activities in multiple cell-based assays.

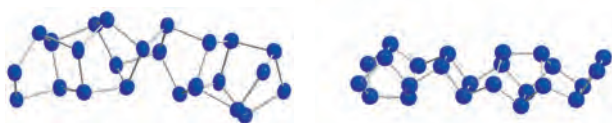




Prof. Dr. Arno Pfitzner

His research is centered in the large field of inorganic solid state and material chemistry. The main focus is on synthesis of new compounds and characterization of their physical properties.

The synthesis of new adducts of molecules composed of elements from the 5th and 6th main group of the periodic system of elements (P, As, Sb, O, S, Se, Te) with metal halides has been investigated for some time. The use of Copper(I)-halides (CuX, X = Cl, Br, I) as solid solvents yields new allotropic phosphor modifications.



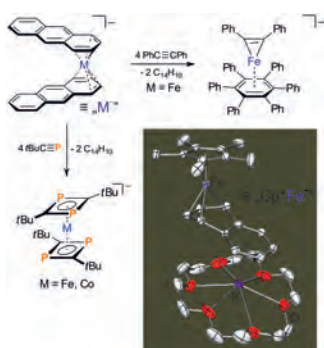
This basic research extends to application-oriented topics, like the synthesis and optimization of new ionic and semiconductors, new thermoelectric or luminescent materials as well as heterogeneous photocatalysts.



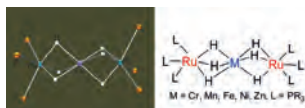
Ionic conductors are materials, in which charge is not transported by electrons but by cations or anions instead. In doing so, ion mobility is not only dependent on temperature, but also e.g. on their chemical environment.

The research interest is focussed on the field of preparative organometallic chemistry and homogeneous catalysis.

New anionic transition metal compounds with metals in low oxidation states become easily accessible employing a new synthesis strategy. Using these as starting materials metal clusters, "functionalized" transition metal anions and novel multimetallic complexes can be prepared. Particularly, research is focussed on the element iron, that is of special interest for sustainable catalytic processes as it is accessible easily, non-toxic and without hazards for the environment.



In addition, the synthesis and reactivity of transition metal hydrides with one or more metal atoms is investigated. These compounds are able to activate both C-H- and C-C-bonds, allowing their use in organic catalysis.



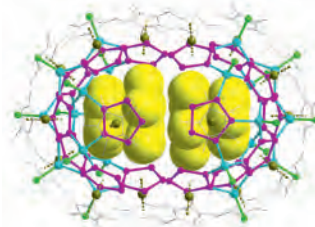
Prof. Dr. Robert Wolf

Prof. Dr. Manfred Scheer

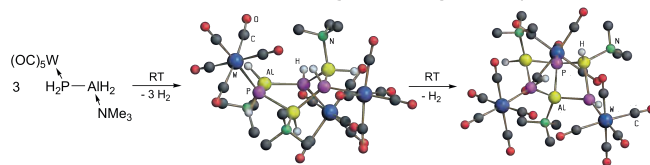


The group is active in the field of molecular chemistry with the focus on the application of the synthesized compounds for material sciences.

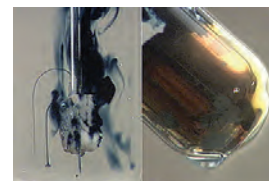
By the reaction of unsubstituted E_n ligand complexes with Lewis acidic metal units, spherical fullerene-like balls and nano-capsules are synthesized. These reactions based partially on template controlled formations, however, latest results show the self-assembly of certain systems. In the presence of organic multitopic linkers such reactions lead to the formation of novel extended organometallic-organic hybridmaterials.



Another major field of interest is the synthesis of new main group element-rich heterocycles. One focus lays on the synthesis of group 13/15 element (B, Al, Ga; P, As, Sb) containing aggregates and polymers. These compounds represent the inorganic analogues of hydrocarbons.



The research of the group is focussed on the preparation and chemical transformation in water-free liquid ammonia. While ammonia, NH_3 , is a gas at room temperature, it can be liquified by cooling below -33°C , yielding a versatile solvent.

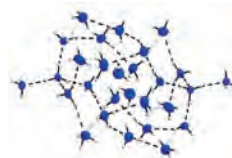


Solution of sodium in liquide ammonia

Especially important is its stability in presence of strong reducing agents like highly charges anions or even free electrons. Many of the species under investigation can be solvated in ammonia only, like e.g. Sb_5^{5-} , As_6^{4-} , Sb_9^{4-} or PbSe_3^{4-} . These element clusters can be used for opening up new elementary classes of compounds.

Further attention is on the structural chemical investigation of N-H-N hydrogen bond systems in ammoniates. In contrast to the O-H-N hydrogen bonds in aqueous solvent crystals, the hydrates, the former ones hardly have been studied.

Aim of the studies is to prepare crystals as rich in ammonia as possible, to classify the structures systematically and to work out similarities and differences compared to hydrates.



Protonated ammonia complex
 $[\text{N}_{28}\text{H}_{68}]^{2+}$



Prof. Dr. Nikolaus Korber



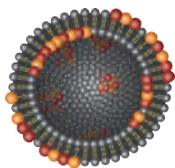
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Thank you!



Prof. Dr. Burkhard König

Visible light photocatalysis finds an increasing number of applications in organic synthesis. We use visible light photocatalysis with one or more photons in arylation, alkylation, oxidation and reduction reactions. The reaction mechanisms are determined by spectroscopic methods. LEDs are used as efficient light sources.

The co-embedding of amphiphilic receptors, catalysts or dyes into vesicle membranes yields functionalized dynamic lipid-water interfaces. The close proximity of the embedded molecules favors synergistic and cooperative action, which is useful for sensing and catalysis.



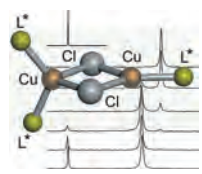
Receptor ligands and drugs, which are photochromic are investigated in close collaboration with researchers in pharmacy and biochemistry. The goal is the remote control of biological function by light.



Prof. Dr. Ruth Gschwind

In the focus are structures and molecular ways of action of catalysts and supramolecular reagents. Especially weak intermolecular interactions of reactants in reactive intermediates are of interest.

The underlying reaction mechanisms of organo catalysis are only poorly understood. The group investigates central links for the course of action of typical organo-catalyzed reactions, like e.g. enamine intermediates of prolin-catalyzed aldol reactions.



Another topic are copper catalysts and organo copper compounds. Cu(I) and Cu(III) are stabilized as reaction intermediates of organo cuprates to gain a structural understanding of these reactions. In addition structure and functionality of phosphoamidite copper catalysts and their intermediates are studied.

The research of the group is dedicated to the development of modern metal-catalyzed reactions for the refinement of basic chemicals as well as organo- and photocatalytic synthesis of functionalized intermediates.



In cooperation with industry sustainable protocols using iron catalysis for cross coupling are developed as an alternative for established palladium- and nickel catalysis which is disadvantageous from both economic and ecological point of view.

Another research focus revolves around the utilization of visible light for organic transformations. Major emphasis is laid on the photocatalytic reactions at the gas/liquid interphase. Current projects include photooxygenations, photocarbonylations and the design of new reactor technologies.



Prof. Dr. Axel Jacobi von Wangelin

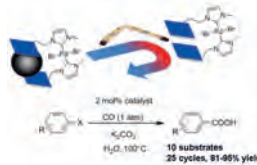


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Institute of ORGANIC CHEMISTRY

Prof. Dr. Oliver Reiser

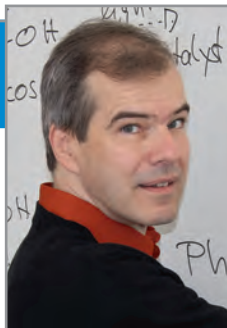
In the field of catalysis both metal- and organo catalysts are employed. Major emphasis is put on the development of asymmetric processes for the production of fine chemicals based on renewable resources.



In the synthesis of manyfold biologically active γ -butyrolacton natural compounds tricyclic guanoldis are of special interest

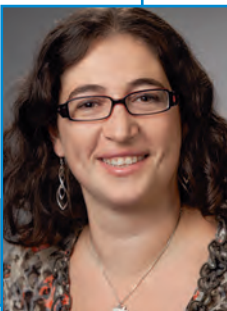
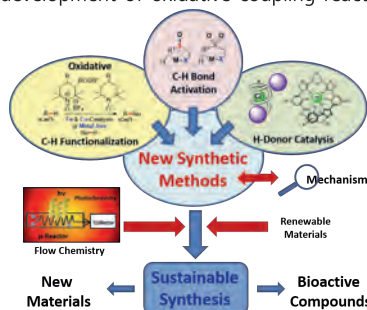
to develop more selective and active drugs against certain types of cancer.

The central topic of peptide foldamers is the use of unnatural in combination with natural aminoacids for the design of stabile secondary structures. These can be employed as ligands for biologically important molecules and may serve as organo catalysts.



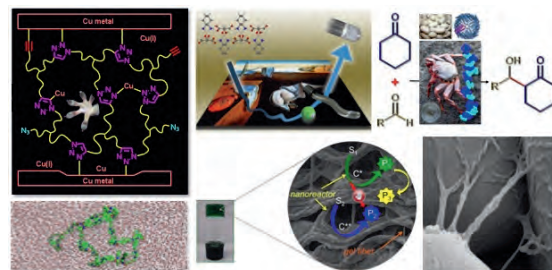
Our research program is dedicated to the development, understanding and application of new synthetic methods to achieve more efficient and sustainable organic transformations.

We are committed to tackle modern synthetic challenges, including the development of oxidative coupling reactions using non-toxic and easy to handle oxidants, transition metal-catalyzed selective C-H activation and the design of unique novel non-covalent organocatalysis.



Prof. Dr. Olga Garcia Mancheño

Our main research interest is focused on the development of advanced multi-functional materials, through hierarchical self-assembly processes, with applications in areas such as biomedicine, catalysis, molecular sensing, coatings, environmental remediation and energy. Within this context, the study of chemical and physical softgels with increasing technological importance constitutes a core activity in our group.



Prof. Dr. David Díaz Díaz

Institute of PHYSICAL & THEORETICAL CHEMISTRY

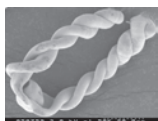


Prof. Dr. Werner Kunz

Liquids and solutions are in the focus of our research. We develop and characterize green und sustainable solvents, Ionic Liquids and emulsifiers for various formulations and applications, e.g. in cosmetics, for cleaning products, and for industrial processes such as plant extraction or new material design.



When silicates and carbonates are precipitated from aqueous solutions, the precipitates show quite astonishing morphologies, like they have been only known in living nature up to now. Fungi-like structures and even double helices can form by a spontaneous self-assembly of these simple mineral salts.



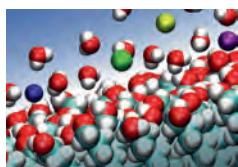
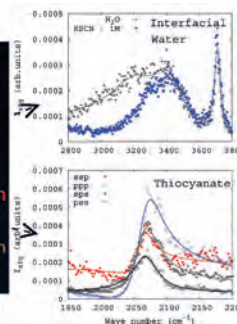
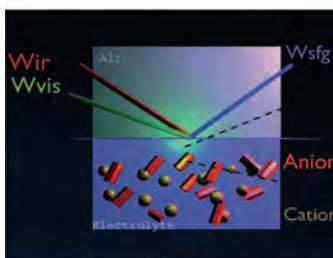
Main part of the research is dedicated to an understanding of molecular surfaces and their significance for colloidal systems. The small particle size of colloidal systems of between 1 and 1000 nanometers leads to an uncommonly large ratio of surface to volume. Therefore, the surface mainly determines the behaviour of the system.

Further information:
"Solution Chemistry"



Prof. Dr. Hubert Mutschmann

The research aims on an understanding of the self-assembly of molecules at surfaces and to establish a connection between microscopic and macroscopic parameters. Central problems are ion-specific effects and surface rheology. A classical description is based upon the Poisson-Boltzmann theory which takes into account the interplay of the ions' electrostatic and thermal energy.



The modeling of liquids, surfaces and biopolymers is in the center of the research.

All kinds of salt solutions exhibit so-called ion-specific Hofmeister effects. It is calculated how salts behave within the solutions, whether they will be attracted or repulsed by different surfaces and what are the consequences for the properties of the solvent.

The stability of proteins in aqueous solution is influenced by the presence of several additives. However, the mechanisms coming into play have not been resolved without doubt yet. Thus, the binding of cosolutes like ammonia to peptide chains is investigated.



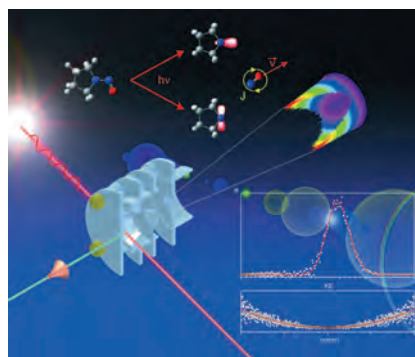
Prof. Dr. Dominik Horinek



Prof. Dr. Bernhard Dick



We investigate the dynamics of photo dissociation reactions in the gas phase: Isolated molecules are cooled down to a temperature of a few Kelvin and excited by a photon of defined energy. Selected quantum states of the products are measured with Velocity Map imaging or 3D-REMPI spectroscopy. The distribution of the velocities and the directions of the dissociation fragments as well as the population of rotational and vibrational states yield detailed insight into the dynamics of photo dissociations.



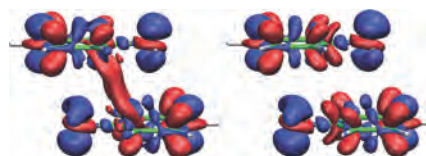
Many organisms possess sensors for light which consist of a protein that binds a light sensitive molecule, e.g. retinal or flavin. Measurements of temporally and spectrally resolved light-absorption after fast laser excitation allow to identify intermediates of the photochemical reaction chain and thus to elucidate the operating mode of these photo receptors.



Further information:
"Spectroscopy"

Research is focussed on development and application of precise theoretical methods to predict the structure and properties of expanded molecular systems, especially so-called local correlation methods. These allow the efficient use of the

spacial short-range of dynamic correlation effects. The computing time of such methods is drastically reduced in comparison to conventional procedures (linearly scaling methods). The pure development of methodologies is always accompanied by work on several applied projects.



Prof. Dr. Martin Schütz



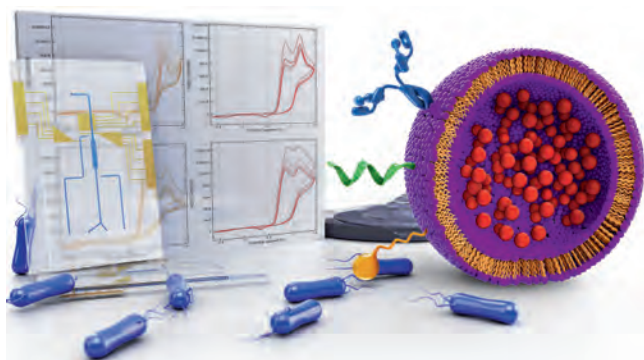
Further information "Theoretical Chemistry".
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Prof. Dr. Antje Bäumner

Microbiosensors and lab-on-a-chip systems are developed to specifically detect pathogenic organisms and toxins. We also develop nanomaterials such as liposomes, nanoparticles and nanofibers to serve as functional components within the sensors and assays.

The surface chemistries of microfluidic channels and the nanomaterials are optimized for the immobilization of biological molecules such as DNA probes, antibodies and receptors. Sample preparation components such as concentration, filtration, and molecular amplification are developed to work directly on-chip. Our detection strategies include electrochemical, optical and luminescence approaches with the goal to establish simple-to-use sensors that can be used on-site, in the field and for point-of-care applications.



Institute of ANALYTICAL CHEMISTRY

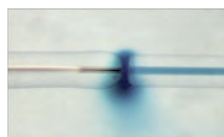
Prof. Dr. Frank-Michael Matysik



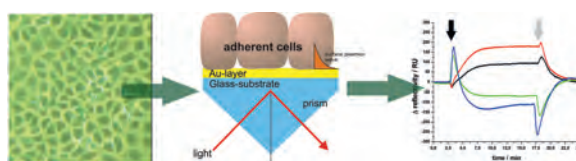
The Matysik group is focused on instrumental analysis, in particular electrochemical techniques, mass spectrometry and separation techniques. A major research objective is state-of-the-art methodological development of analytical procedures for ultrasmall sample volumes.

The investigation of these ultrasmall volumes (10^{-9} – 10^{-12} L) creates special challenges in sample collection and detection. Microfluidic systems in capillary and chip format are used to handle very small amounts of liquids in analytical settings.

In addition, new techniques for the determination of arsenosugars and lipids present in only trace amounts especially in marine organisms are developed. A further improvement of analytical tools for these species is essential for a realistic assessment of their hazardous potentials.



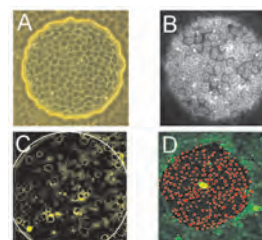
The development of biosensors with animal cells as sensing elements are the major research focus in the Wegener lab. This approach is based on the fact that living cells respond very sensitively to biological, chemical and physical stimuli. The sensor cells are interfaced with label-free, non-invasive physical transducers (optical, electrochemical, piezoelectric) so that the measurement itself does not interfere with cell physiology.



In addition to using cells as sensors the lab tries to integrate physical means to manipulate the cells in a well-defined and reproducible way. This combination of sensors and actuators will allow to address new problems in cell-based analytics. Cell manipulation includes a short and reversible opening of the cell membrane for the intracellular delivery of non-membrane permeable compounds, the fusion of cells as well as local cell killing for cell migration and wound healing studies.

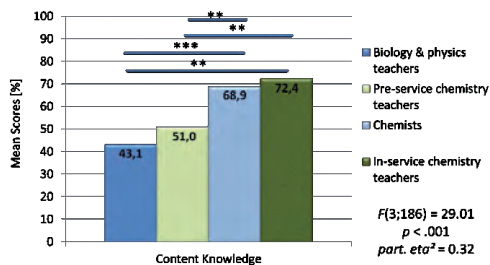


Prof. Dr. Joachim Wegener



Further information:
"Analytical Chemistry,
Chemo- and Biosensors"

Further information:
"Chemistry Education"



The research of our working group focuses on the connection between the various degrees of professional competence of chemistry teachers and the way in which the teachers act in the classroom as well as making differentiated predictions about the effect of professional competence on students' growth of knowledge and motivation. In order to analyze teaching and learning processes empirical methods like video-based test instruments and paper-pencil-tests are used. Recent results reveal that the professional competence of chemistry teachers is domain specific and differs by school type and the level of education. Currently, we are investigating how experiments/models, technical language and student errors are handled in classroom situations. In addition, the development of an innovative teaching concept for university students in a teacher training program is being developed and evaluated.



Chemistry EDUCATION

Prof. Dr. Oliver Töpner





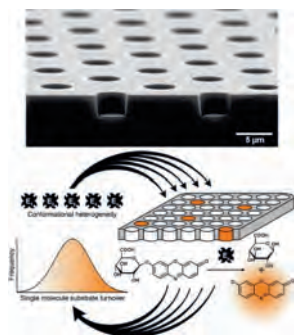
Dr. Hans-Heiner Gorris

Bioanalytical Chemistry

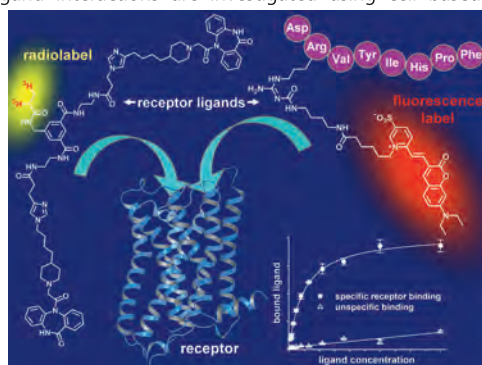
Fluorescence spectroscopy is one of the most versatile and sensitive detection methods in analytical chemistry with the potential to reach the single-molecule level. Autofluorescence and light scattering of the surrounding medium, however, typically lead to background interference. The fluorescence background can be

strongly reduced by performing a fluorogenic enzyme reaction in a femtoliter (μm^3) volume.

We have devised femtoliter arrays consisting of 62.500 femtoliter-sized chambers in the surface of fused silica slides to analyze the substrate turnover of hundreds of individual enzyme molecules in parallel. In a different approach, we avoid autofluorescence and light scattering in the first place. So-called photon-upconverting nanoparticles emit visible light under near-infrared excitation (anti-Stokes luminescence), where autofluorescence and light scattering are minimized.



Research projects are aiming at the design, synthesis and pharmacological characterization of non-peptidic and peptidic ligands for G-protein coupled receptors (GPCRs). Targets of interest are, for example, muscarinic acetylcholine, neuropeptide Y, neurotensin, angiotensin II and neuropeptide FF receptors. Special focus is put on the development of molecular and pharmacological tools such as radio- and fluorescence labeled ligands, highly selective ligands and bivalent ligands. Receptor-ligand interactions are investigated using cell based functional assays (e.g. Ca^{2+} assay) and binding assays.



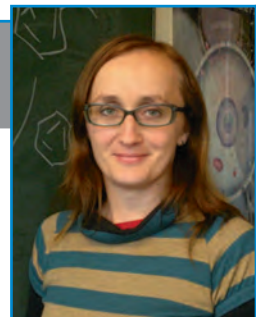
Dr. Max Keller

Pharmaceutical and Medicinal Chemistry

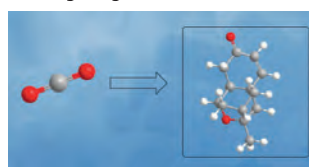
Our JUNIOR SCIENTISTS

Dr. Ivana Fleischer

Organic Chemistry



Our research focuses on the development of new catalytic transformations for the organic synthesis. The main subjects of our investigations are non-classical C1 building blocks for metal- and organocatalyzed reactions. The most attractive and especially challenging C1 source is carbon dioxide, which constitutes the dream target of our studies. In addition, we are investigating new tandem reactions of carbonyl compounds based on



metal- and organocatalyzed transformations. We are interested in the whole picture: from the mechanistic understanding of the reactions to useful synthetic applications.

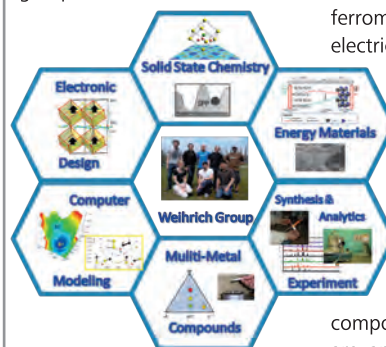


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<http://www.uni-regensburg.de/chemie-pharmazie/fakultaet/>



Our research is situated in solid state chemistry and functional materials. Experimental and theoretical methods are combined to synthesize novel compounds and to study structure-property relations within the ternary phase diagram M-A-X (transition-metals M, main group metals A and non-metals X). Examples therein are half metal



ferromagnetic $\text{Sn}_2\text{Co}_3\text{S}_2$, thermoelectric $\text{InSnCo}_3\text{S}_2$, superconducting $\text{Bi}_2\text{Rh}_3\text{X}_2$, semiconducting PtSnSe and electrodes for high voltage lithium ion batteries like $\text{Li}(\text{Co},\text{Ni})\text{PO}_4$. Various methods are applied (high temperature, high pressure, sol-gel, solvothermal) to synthesize nanosize and crystalline

compounds. Samples are analyzed by XRD ($8\text{ K} < T < 900^\circ\text{C}$), thermal analysis and microscopic methods. DFT modeling is applied to identify target compounds with interesting magnetic or electronic properties or novel metastable compounds and structures (SPP1415).



PD Dr. Richard Wehrich

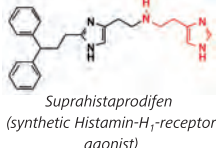
Inorganic Chemistry



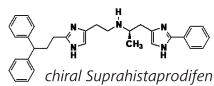
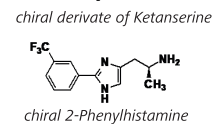
Prof. Dr. Sigurd Elz

The group is looking for new drugs with agonistic, partially agonistic or antagonistic activity at G protein coupled receptors of the histamine- and serotonin family. For example, the compound suprahistaprodifen, a novel and potent histamine H₁-receptor antagonist, has been developed which exhibits an activity much higher than the natural messenger histamine.

In addition work is dedicated to the synthesis and pharmacological characterization of stereoisomeric drugs, like enantiomers. In this field contributions regarding stereoselectivity of agonists and antagonists could be made for both the area of serotonin and histamine.



chiral derivate of Ketanserine



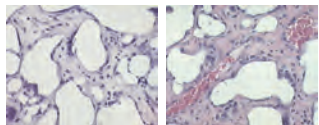
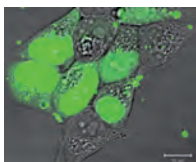
In the focus of our medicinal chemistry projects are G-Protein-coupled receptors (GPCRs), such as histamine and neuropeptide Y (NPY) receptors as typical representatives of aminergic and peptidergic GPCRs (cf. www.GRK1910.de), and modulators of ABC transporters. It is the aim to gain deeper insight into the molecular mechanisms of function of these biological targets. This interdisciplinary approach includes computer-assisted methods, the design and chemical synthesis of subtype-selective ligands (agonists, antagonists, inverse agonists) and molecular tools (radiolabeled and fluorescent ligands), supported by models of wild-type and mutant receptors, novel concepts of bioisosteric replacement, the study of ligand-receptor interactions (binding and function), the elaboration of functional selectivity by analysis of ligand-specific signaling as well as the development of appropriate assays.

Projects in the field of experimental tumor pharmacology deal with strategies to overcome both chemoresistance of malignant tumors and the blood-brain barrier. Efforts are spent to exploring the potential of modulators of ABC transporters in the treatment of glioblastoma.



Prof. Dr. Armin Buschauer

General subject of the group's research are interactions between materials and cells or tissues down to the nanoscale. The aim is to investigate such interactions and to make them available for the development of therapeutically relevant biomimetic materials. Material design projects aim at providing carriers for proteins and nucleic acids for biomedical applications. Examples are polymer hydrogels that serve as drugs carriers or nanoparticles that are able to interact with cell surface receptors via multivalent binding mechanisms. Such materials allow for better cell recognition and concomitantly hold a tremendous



therapeutic potential for the treatment of retinal diseases such as macular degeneration or diabetic retinopathy. Tissue engineering, i.e. the generation of living tissues in vitro and in vivo, is yet another research direction of the group. The development of suitable materials for the cultivation and implantation of cells is thereby in focus.

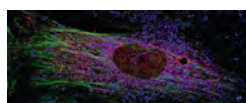
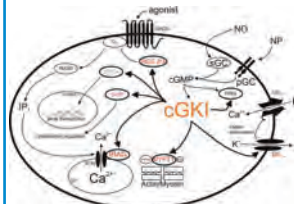
Prof. Dr. Achim Goepferich



Prof. Dr. Jens Schlossmann

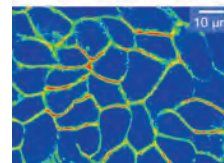
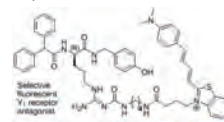


The group deals with an analysis of the nitrogen oxide (NO)/cyclic guanosine monophosphate (cGMP)-mediated signal transduction in order to identify the molecular, physiological and pathophysiological mechanisms of this signal pathway. Studies are done using both cellular systems and transgenic mouse models.

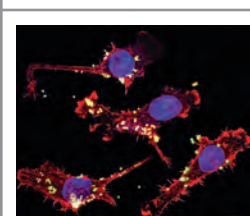
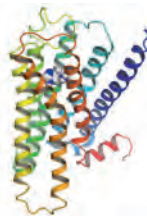


With the help of heterologous expression systems and primary cell cultures ligands, kinases and kinase substrates (amongst others) are analyzed as well as changes in intracellular calcium levels, of the cytoskeleton and the proliferation are tested.

In addition the cGMP-dependent protein kinases I and II are expressed (in SF9 insect cells) and kinase activators and inhibitors are studied. Using the mouse models cardiovascular, renal and hematological functions are analyzed currently.



Detection of NPY Y₁ receptors in the membrane of human MCF-7 breast cancer cells by confocal microscopy



The research of the group is focussed on cytotoxic, antiproliferatory, antioxidative, antiinflammatory and immunomodulatory properties of natural compounds. In vitro assays established for the characterization of extracts and single compounds also serve for the isolation of natural compounds guided by their bioactivity. Secondary compounds are of special importance for plants with respect to their interactions with pollinators (color of blossoms, i.e. dyes, olfactory compounds). Ecological changes influencing the production of secondary compounds may lead to respective changes in habitat-specific interactions. These ecological factors are characterized in relation to the qualitative and quantitative composition of the profile of secondary compounds in order to establish the influence on the production of secondary compounds.

Prof. Dr. Jörg Heilmann



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Thank you!