

# DEPARTMENT OF CHEMISTRY AND PHARMACY

## PROFILE 2018









## DEPARTMENT OF CHEMISTRY AND PHARMACY— SYNTHESIS OF THE FUTURE

Chemical sciences play an integral role in today's life and are fundamental for the progress in technology and medicine. Hence, chemistry and pharmacy are situated at the intellectual heart of many scientific disciplines as science has become increasingly interdisciplinary. With a strong commitment to excellence in education and research, we are dedicated to the fundamental chemical sciences as well as to exploring fundamental scientific problems at the interface to other disciplines.

The Department of Chemistry and Pharmacy at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) has a long-standing tradition of excellence—because of our vast resources, cutting-edge facilities, and outstanding faculty—and is ranked among the best in the country. This is documented by the quality of its programs, the caliber of its faculty, and the excellence of its students.

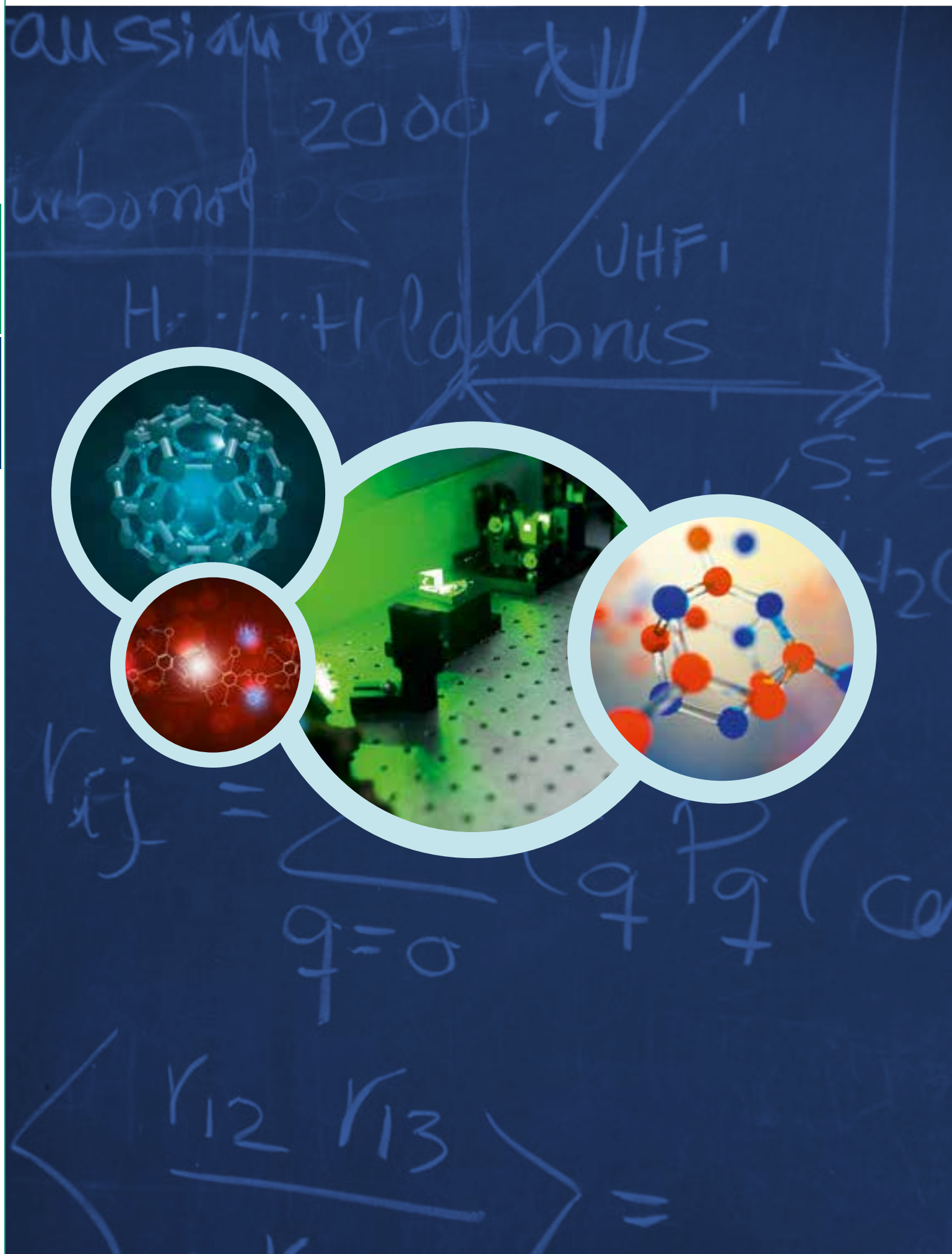
The faculty and staff of the Department of Chemistry and Pharmacy provide an environment, where students at all levels explore, discover, and learn chemical sciences through coursework and research. Undergraduate, graduate, and post-doctoral research associates join the Department of Chemistry and Pharmacy from across the country and from a great number of countries all over the world to study in specific research programs directed by FAU's chemistry and pharmacy professors.

The Department employs 31 professors pursuing research in all areas of chemistry and pharmacy. The foci of our renowned and well-funded research programs are molecular materials and catalysis as well as bioactive molecules. Modern research cuts across traditional disciplinary boundaries, and our faculty plays key roles at the forefront of multiple interdepartmental research units at Friedrich-Alexander-Universität Erlangen-Nürnberg including the Cluster of Excellence, several Collaborative Research Centers, Research Units and Research Training Groups.

*Peter Gmeiner*

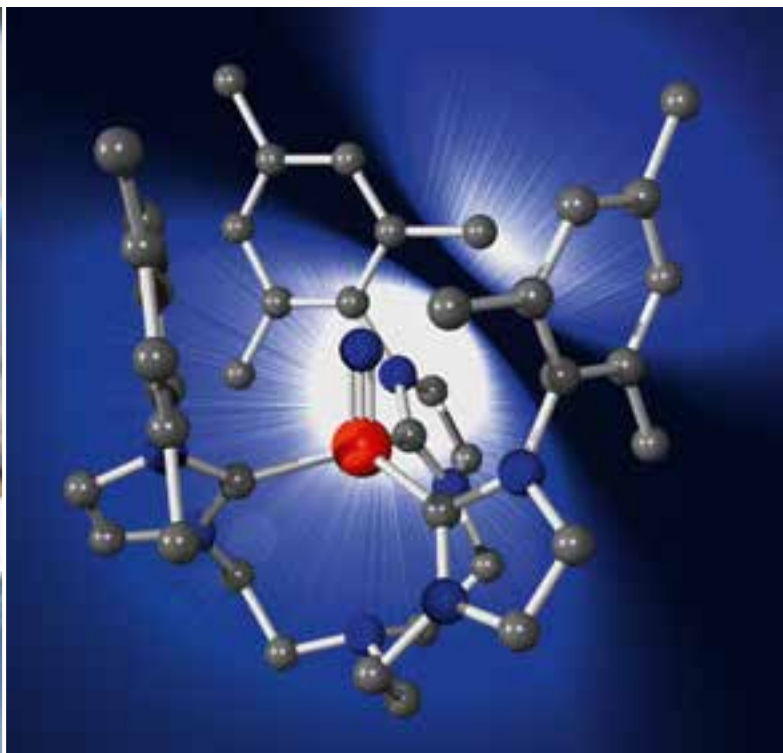
Head of the Department of Chemistry and Pharmacy







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## DEPARTMENT OF CHEMISTRY AND PHARMACY

### PROFILE

Founded in 1743, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) has a rich history. It is a strong research university with an international perspective and one of the largest universities in Germany, with 39,780 students, 265 degree programs, 4,000 academic staff (including 579 professors), 199.6 million Euros third-party funding in 2017, and 500 partnerships with universities all over the world.

FAU is committed to the unity of research and education. Teaching at the University is closely linked to research and focuses on training students in both theory and practice to enable them to think critically and work independently. The research itself also strikes the perfect balance between a theoretical approach and practical application. The goals are to specialize in areas of research that will shape the future and to create a network of interdisciplinary cooperation between technical, scientific, and traditional subjects.

Among the five FAU faculties the Faculty of Sciences features five departments, Biology, Geography and Geosciences, Mathematics, Physics, as well as Chemistry and Pharmacy.

The **Department of Chemistry and Pharmacy (DCP)** is made up of two separate units, namely Chemistry, on one hand, and Pharmacy and Food Chemistry, on the other hand. Both are cooperating closely with other Faculties within FAU, especially with the Faculties of Engineering and Medicine as well as with other departments within the Faculty of Sciences. The cooperations range from joint research projects and interdisciplinary research centers to extensive exchange of students at the undergraduate and graduate levels.

**DCP** comprises 9 chairs in Chemistry for Inorganic, Organic, Physical, and Theoretical Chemistry and 4 chairs in Medicinal Chem-

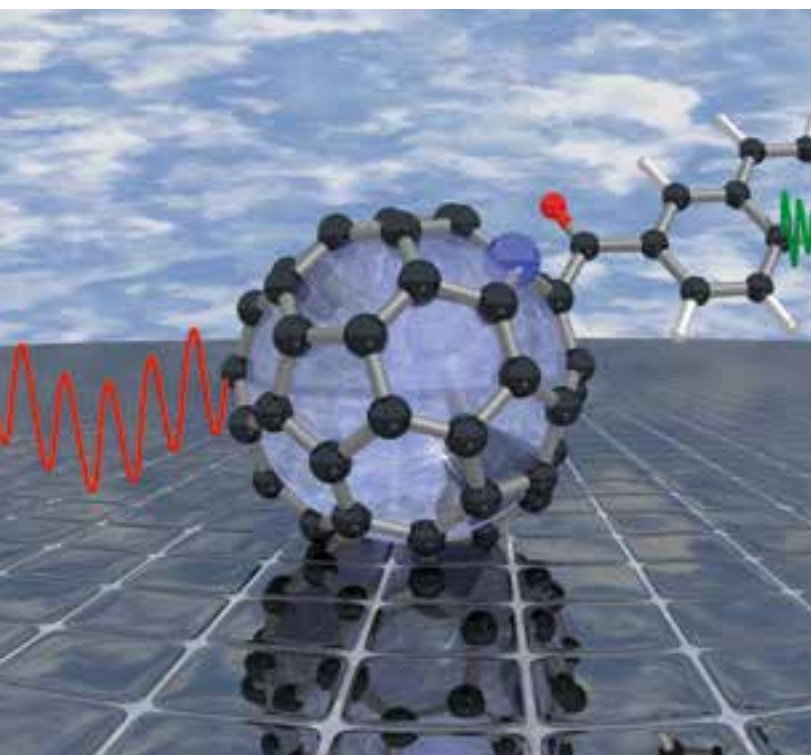
istry, Pharmaceuticals, Food Chemistry, and Flavour Research. A total of 31 professors hold appointments in the various areas. Additional support is provided by about 30 permanent and 130 non-permanent scientific staff members. External research funds that total up to an average of more than 10 million Euros per year enable the means to finance more than 180 additional scientists.

Overall, the compelling research at **DCP** has received top rankings not only at the national but also at the international level. The latest research funding ranking of the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) confirms Erlangen's third place in third-party funding of German chemistry departments. This is rounded off by the Shanghai Academic Ranking of World Universities in 2015, which lists FAU's Chemistry in the TOP 75 worldwide and 7 in Germany. QS World University Ranking placed **DCP** among the TOP 150 in 2018.

Current developments, as outlined in the following sections, are reflections of the national and international standing of the Department:

Since 2015, **DCP** is a central part of the Cluster of Excellence—„Engineering of Advanced Materials (EAM)”, which is funded by the Federal Government via DFG. Among the 25 lead Principal Investigators (PI), 6 come from Chemistry. The PIs from **DCP** contribute to the cluster research areas “Multiscale Modelling and Simulations”, “Engineering of Nanoelectronic Materials”, and “Engineering of Catalytic Materials”. In 2012, funding for the Cluster of Excellence EAM was renewed until end of 2018. Furthermore, 8 additional project leaders from **DCP** are associated with the Cluster of Excellence, which includes substantial funding for personal and instrumentation.





In 2012, DFG approved funding for the Collaborative Research Center SFB 953 “Synthetic Carbon Allotropes” and the Research Training Group GRK 1910 “Medicinal Chemistry of Selective GPCR Ligands”. SFB 953 with about 24 Mio Euro for 8 years supports a total of 21 groups with 9 PIs directly linked to **DCP**. The GRK 1910, which is a collaborative effort together with the University of Regensburg, finances 7 groups belonging to **DCP** with 5 Mio Euro for 4.5 years.

In 2012, the State of Bavaria initiated an interdisciplinary consortium “Solar Technologies Go Hybrid—SolTech” by chemists and physicists at five different Bavarian universities. In Erlangen, 14 out of the 15 funded groups come from **DCP** and are supported with 5 Mio Euro for a period of 5 years.

Finally, in 2013, the Research Unit FOR 1878 “Functional Molecular Structures on Complex Oxide Surfaces” (funCOS) was established by DFG. It supports 14 research groups, 8 of which are located at **DCP**. The total funding until 2020 amounts to 6.5 million Euros.

## RESEARCH FOCI

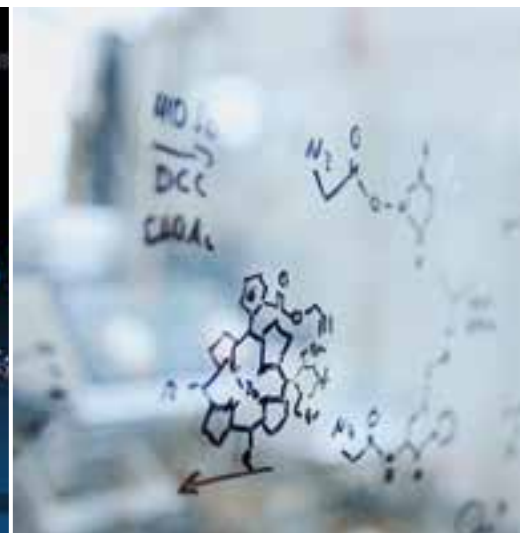
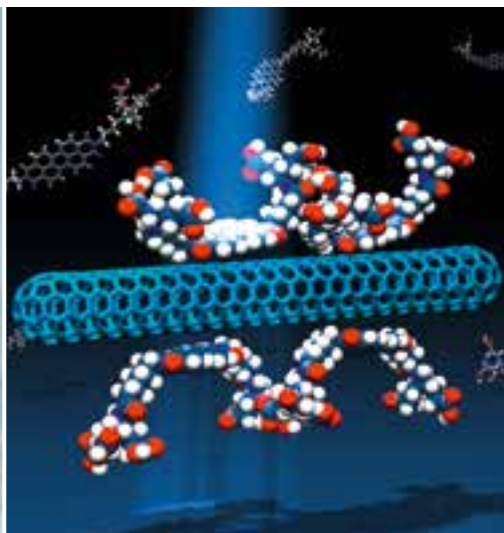
The research activities of **DCP** cover a wide spectrum in the areas of Chemistry, Materials Science, Biology, and Pharmaceutical Science. The two major research foci of **DCP**, namely Molecular Materials and Bioactive Molecules, constitute the basis for the FAU research foci “New Materials and Processes” and “Medicine, Life Sciences and Health”.

The synthesis and characterization of molecular materials with special emphasis on electronic, photophysical, and catalytic properties constitutes one of the two major research foci of **DCP**, that is, Molecular Materials. To this end, different forms of carbon allotropes and redox-active metal complexes represent some of the most in-

tensively studied classes of molecules. Bioactive molecules, in general, and the design, synthesis, and examination of novel neurotropic agents for their activity towards signaling proteins—G-protein-coupled receptors—in particular, represent the second major research focus, that is, Bioactive Molecules, of the Department. The research activities integrate chemical synthesis, biological and pharmacological testing, structure-activity relationships, the technology of drug delivery, and investigations of molecular mechanisms of action.

The research foci create the molecular bridge between the Faculty of Engineering, on one side, and the Faculty of Medicine, on the other. The strongly interwoven and multiple interaction nature of these research activities are the inception to a large number of interdisciplinary collaborative research projects within the University (Collaborative Research Centers (SFB), Research Training Units (GRK)) and with other nationally and internationally leading institutions (DFG Priority Programs, EU, BMBF, NIH (US), Volkswagenstiftung, DAAD, Humboldt-Foundation, Bayerische Forschungsförderung, etc.), in which **DCP** participates in addition to the above presented collaborative research projects lead by **DCP**.

Moreover, the research foci of **DCP** are vital for the FAU research focus “Future Energy Systems”. Microscopic understanding of processes relevant for energy, environment, and climate again means understanding at the molecular level. The research activities of **DCP** furthermore contribute and are related to the FAU research foci “New Materials and Processes”, “Electronics, Analytics and Digital Transformation”, “Medicine, Life Sciences and Health”, and “Optics and Optical Technologies”. In other words, **DCP** is active in 5 of the 8 FAU research foci.



### RESEARCH ENVIRONMENT AND INFRASTRUCTURE

The research activities of **DCP** are embedded in a number of centers at FAU. For example, the Interdisciplinary Center for Molecular Materials promotes fundamental and interdisciplinary research at the frontier areas between Chemistry, Physics, and Materials Science. The Interdisciplinary Center for Interface Controlled Processes aims at strengthening interdisciplinary research considering interfaces of materials, the Computer Chemistry Center amalgamates competences of the Department with respect to simulation and computational science. The Emil Fischer Center comprises research groups from the Pharmaceutical Sciences, Food Chemistry and Molecular Medicine and, as such, crosslinks scientific work on bioactive molecules, target proteins and bioanalytics. These centers are coordinated or, in case of the Computer Chemistry Center, formed by members of **DCP**.

In addition, **DCP** is a vital member in the Erlangen Catalysis Resource Center, the Central Institute for Scientific Computing, and the Interdisciplinary Center for Neuroscience. All of the aforementioned foster interdisciplinary research activities across disciplines and are instrumental in joint funding efforts. Moreover, **DCP** runs the elite Graduate School Molecular Science, which is based on the interdisciplinary curriculum Molecular Science as a collaborative effort of Chemistry and Pharmacy. A second graduate program run by **DCP** through the Emil Fischer Center is the Emil Fischer Graduate Programme of Pharmaceutical Sciences & Molecular Medicine. Last but not least, the Helmholtz-Institut Erlangen-Nürnberg as well as the Energie Campus Nürnberg, which both are research platforms for the development and presentation of a closed renewable energy chain, contribute to the stimulating and productive research environment.

### TEACHING PROFILE

The Bachelor and Master programs Chemistry and Molecular Science are highly modularized, research-oriented (B.Sc.) and research-focused (M.Sc.) curricula. Both the Pharmacy and Food Chemistry degree programs have been expanded in the last 5 years and continue to attract large numbers of undergraduates with top school grades.

In the Master programs, which are completely taught in English, a tight interplay between contemporary research and teaching leads to a high-class, modern education based on the scientific activities of the Department. Therefore, the aforementioned scientific foci are well reflected in the modules of the M.Sc. curricula. Additionally, the wide spread nature of the offered subjects put the students in a position to select courses according to their personal interest. The teaching philosophy aims at the development of students into well-rounded scientists who can take on leadership roles in industry, and academia.

In addition to the scientific education, the personnel progress of the students is supported by offered language course and the opportunity to study parts of all study programs abroad. The quality of all study programs is ensured by a tight evaluation and supervision process.

### INTERNATIONALIZATION OF RESEARCH AND TEACHING

Internationality is a key character of **DCP**. A steadily increasing number of foreign scholars and exchange programs—funded through DAAD/RISE, SCS-IREU/DAAD, and ERASMUS—are a clear documentation for the internationalization of undergraduate and graduate studies. The latter is complemented by international doctoral and post-doctoral students—funded through DAAD, Alexander von Humboldt Foundation, and EU programs. Cooperation with, for example, Shenzhen University in China and the University of Wollongong in Australia are initiated by excellence in research and teaching and are often build up by committed members of **DCP**. They include frequent exchanges of students and researchers. 5 out of 13 chairs have an international background.



# DEPARTMENT OF CHEMISTRY AND PHARMACY

## INORGANIC CHEMISTRY

### Inorganic and Organometallic Chemistry

**Prof. Dr. S. Harder**

Prof. Dr. N. Burzlaff

### Inorganic and General Chemistry

**Prof. Dr. K. Meyer**

Prof. Dr. R. Dorta

### Bioinorganic Chemistry

**Prof. Dr. I. Ivanović-Burmazović**

### Chemistry of Thin Film Materials

**Prof. J. Bachmann PhD**

## PHYSICAL / THEORETICAL CHEMISTRY

### Physical Chemistry I

**Prof. Dr. D. M. Guldi**

Prof. Dr. C. Kryschi

Prof. Dr. T. Drewello

### Physical Chemistry II

**Prof. Dr. H.-P. Steinrück**

Prof. Dr. R. Fink

Prof. Dr. J. Libuda

### Theoretical Chemistry

**Prof. Dr. A. Görling**

Prof. Dr. D. Zahn

## ORGANIC CHEMISTRY

### Organic Chemistry I

**N.N.**

Prof. Dr. J. Schatz

Prof. Dr. S. Tsogoeva

### Organic Chemistry II

**Prof. Dr. A. Hirsch**

Prof. Dr. A. Mokhir

Apl. Prof. Dr. N. Jux

## PHARMACY AND FOOD CHEMISTRY

### Medicinal Chemistry

**Prof. Dr. P. Gmeiner**

Prof. Dr. J. Eichler

Prof. Dr. M. Heinrich

### Pharmaceutics

**Prof. G. Lee PhD**

### Food Chemistry

**Prof. Dr. M. Pischetsrieder**

### Aroma and Smell Research

**Prof. Dr. A. Büttner**

### Molecular and Clinical

Pharmacy

**N.N.**

## COMPUTER CHEMISTRY CENTER (CCC)

Techn. Director: Apl. Prof. T. Clark PhD

## INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS (ICMM)

Prof. Dr. F. Gröhn

Prof. Dr. B. Meyer

## DIDACTICS OF CHEMISTRY

Prof. Dr. A. Kometz

## CLINICAL PHARMACY

Prof. Dr. F. Dörje MBA

## INTERDISCIPLINARY CENTERS

- Emil Fischer Center (EFC)
- Erlangen Catalysis Resource Center (ECRC)
- Institute of Advanced Materials and Processes (ZMP)
- Interdisciplinary Center for Interface-Controlled Processes (ICICP)
- Cluster of Excellence: Engineering of Advanced Materials (EAM)
  - Centre for Scientific Computing (ZISC)

## GRADUATE SCHOOLS

- Emil Fischer Graduate Programme
  - Graduate School Advanced Materials and Processes
  - Graduate School Molecular Science

# DEGREE PROGRAMS

## CHEMISTRY

(B.Sc. / M.Sc.)

## MOLECULAR SCIENCE NANO SCIENCE / LIFE SCIENCE

(B.Sc. / M.Sc.)

## CHEMISTRY TEACHING DEGREE

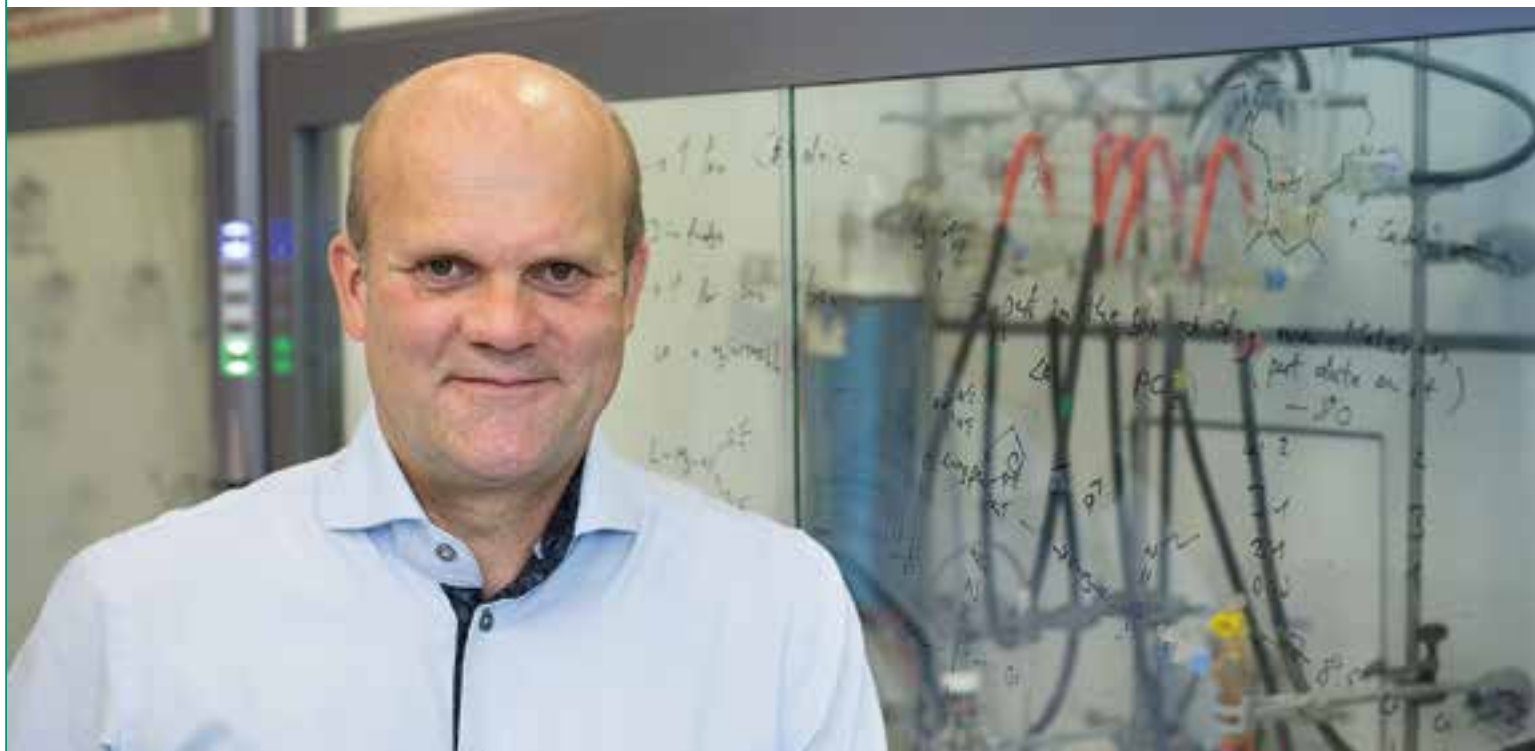
(State Examination)

## PHARMACY

(State Examination)

## FOOD CHEMISTRY

(State Examination)



## CHAIR OF INORGANIC AND ORGANOMETALLIC CHEMISTRY

### PROF. DR. SJOERD HARDER

[sjoerd.harder@fau.de](mailto:sjoerd.harder@fau.de) • [www.chemie.fau.de/harder](http://www.chemie.fau.de/harder)

#### CURRICULUM VITAE

- Since 2012** University Full Professor, Chair of Inorganic and Organometallic Chemistry at the University of Erlangen-Nürnberg, Germany
- 2009 – 2012** Chair of Molecular Inorganic Chemistry at the University of Groningen, Netherlands
- 2004 – 2009** Professor of Inorganic Chemistry at the University of Duisburg-Essen, Germany
- 1998 – 2003** Lecturer at the University of Konstanz, Germany, and the University of Cape Town, South Africa
- 1994 – 1998** Habilitation in Inorganic and Organometallic Chemistry at the University of Konstanz, Germany
- 1993 – 1994** Post-doc (Hans-Herbert Brintzinger) at the University of Konstanz, Germany
- 1992** Post-doc (Andrew Streitwieser) at the University of California, Berkeley, USA
- 1991** Post-doc (Paul R. von Schleyer) at the University of Erlangen-Nürnberg, Germany
- 1990** PhD in Organic Chemistry at the University of Utrecht, Netherlands

#### OBJECTIVES

- Further development of a fundamental understanding of organometallic compounds and reactions
- Application of organometallic chemistry in various fields like catalysis, polymerization chemistry, enantioselective conversions, luminescence, surface science and subjects related to a sustainable energy economy
- Mastering and teaching the skills of working with highly air-sensitive compounds under an inert atmosphere using Schlenk techniques

#### SCIENTIFIC BACKGROUND

Our group works at the frontiers of the organometallic chemistry of the early main group metals with a special focus on the heavier group 2 metals (Ca, Sr, Ba). This corner in the periodic table has been forgotten for a long time but its chemistry is now starting to develop rapidly. The work with these highly reactive, and consequently also very air-sensitive, organometallic compounds is not only challenging but also requires techniques that allow handling of these complexes under an inert atmosphere. Although we partially work in gloveboxes, we master and develop the original Schlenk techniques at a high level and believe that this is the key to doing chemistry with highly



reactive compounds. The high reactivity of our complexes is exploited in catalysis. Our general motto “Cheap Metals for Noble Tasks” has led to pioneering breakthroughs in the field of calcium-based catalysis. These offer a cheap alternative to transition metal catalysts and are also attractive for reasons of biocompatibility. Our interests, however, are much broader and also venture into areas like lanthanide chemistry and early (Ti, Zr) as well as late (Au, Cu, Zn) d-block metals or in the field of highly Lewis-acidic late main group metal chemistry (Al).

### RESEARCH HIGHLIGHTS

We are among the pioneers using early main group metals in catalysis and developed for example methods for the strictly controlled catalytic hydrosilylation of alkenes, a highly atom-efficient key transformation for the production of silicon compounds. The catalyst in this unique reaction is a calcium hydride species that we could also isolate and structurally characterize. Surprisingly, we could use this catalyst also in the hydrogenation of alkenes with  $H_2$  and this method represents a first demonstration of transition metal-free alkene hydrogenation catalysis. Other highlights of our research are the isolation of first calcium carbene complexes of the form  $Ca=CR_2$  and our work with “superbulky” ligands among which  $Cp^{BIG}$ , a large penta-aryl cyclopentadiene. The latter ligand is the key to a set of interesting lanthanide sandwich complexes with an unusual strong luminescence. Our expertise in group 2 metal hydride chemistry evolved to the synthesis of larger magnesium hydride clusters that represent model systems for hydrogen storage materials like bulk  $MgH_2$ . Especially rewarding are the investigations on metal amidoborane complexes for hydrogen storage.

### PERSPECTIVES

We will continue to explore the organometallic chemistry of heavier group 2 metals but also strongly focus on Mg and the closely related Zn chemistry. We currently start to explore their redox chem-

istry and use in Frustrated Lewis Pair chemistry but also actively pursue the use and development of nonheterocyclic carbene ligands (NHC's). Investigations of their reactivity towards small molecules will contribute to new catalytic protocols. The high abundance and low prices of these simple metals is the part of the key to a sustainable society based on renewable materials. Apart from that, our future focus will further concentrate on energy-related research themes and polymerization catalysis.

### SELECTED PUBLICATIONS

- H. Bauer, M. Alonso, C. Färber, H. Elsen, J. Pahl, A. Causero, G. Ballmann, F. De Proft, S. Harder, *Nature Catalysis*, **2018**, 1, 40–47
- M. Wiesinger, B. Maitland, C. Färber, G. Ballmann, C. Fischer, H. Elsen, S. Harder, *Angew. Chem. Int. Ed.*, **2017**, 56, 16654–16659
- B. Maitland, M. Wiesinger, J. Langer, G. Ballmann, J. Pahl, H. Elsen, C. Färber, S. Harder, *Angew. Chem. Int. Ed.*, **2017**, 56, 11880–11884
- A. Causero, H. Elsen, J. Pahl, S. Harder, *Angew. Chem. Int. Ed.*, **2017**, 56, 6906–6910
- J. Langer, B. Maitland, S. Grams, A. Ciucka, J. Pahl, H. Elsen, S. Harder, *Angew. Chem. Int. Ed.*, **2017**, 56, 5021–5025
- J. Penafiel, L. Maron, S. Harder, *Angew. Chem. Int. Ed.* **2015**, 54, 201–206
- S. Harder, J. Spielmann, J. Intemann, H. Bandmann, *Angew. Chem. Int. Ed. Engl.*, **2011**, 50, 4156–4160

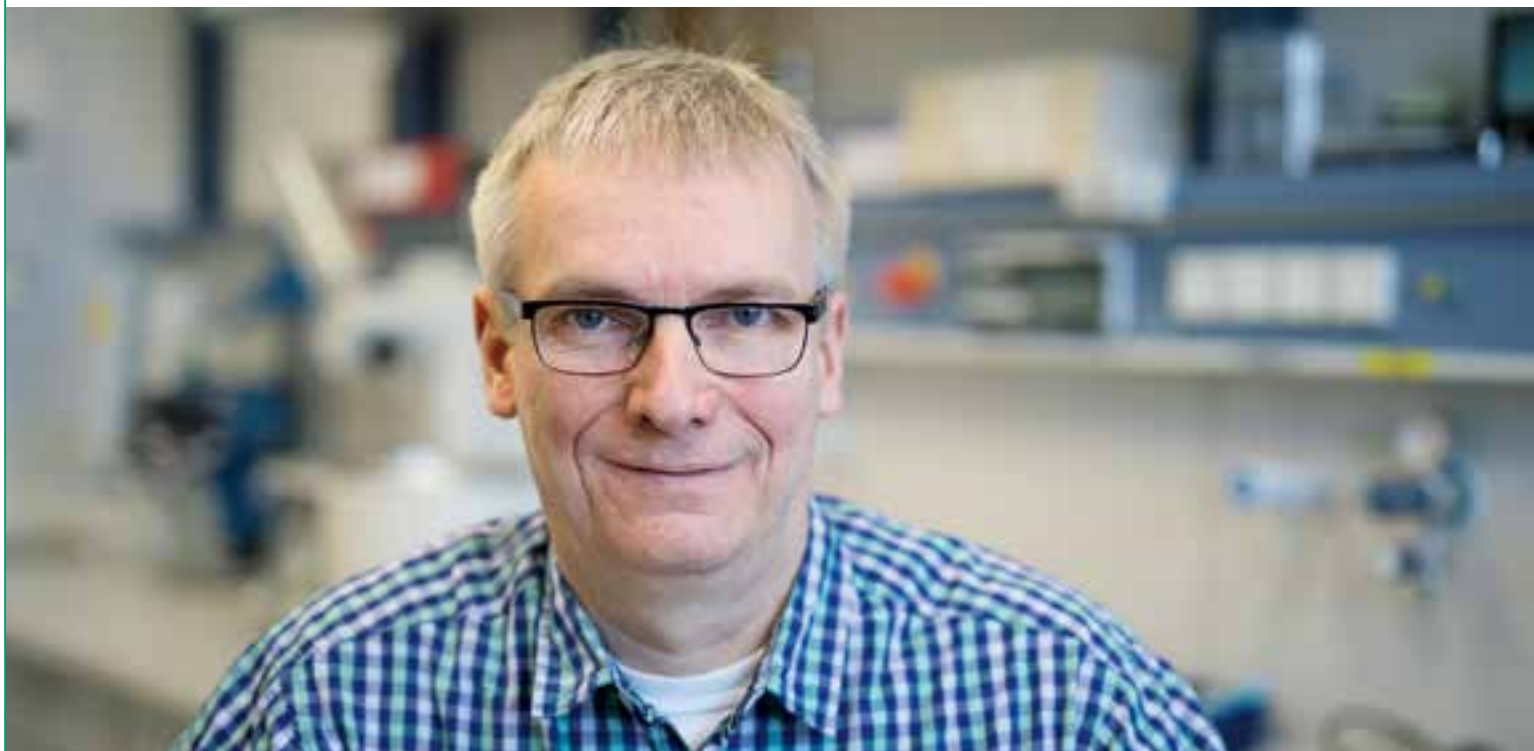
### SELECTED REVIEWS

- S. Harder, Molecular early main group metal hydrides: synthetic challenge, structures and applications, *Chem. Comm.*, **2012**, 48, 11165–11177
- S. Harder, From limestone to catalysis: Application of calcium compounds as homogeneous catalysts, *Chem. Rev.*, **2010**, 110, 3852–3876

### SELECTED AWARDS

- 2017 Schlenk Lecture Award (University of Tübingen/BASF)
- 1994 European Community—Marie Curie Fellowship
- 1993 European Community—Human Capital & Mobility Fellowship
- 1992 NATO Fellowship
- 1991 Alexander von Humboldt Fellowship
- 1990 H. J. Backer Prize of the Royal Dutch Society of Chemistry (Organic Chemistry)





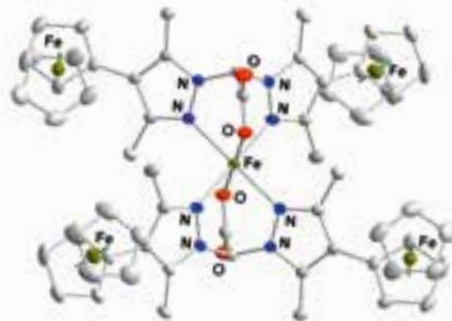
# PROFESSOR OF INORGANIC CHEMISTRY

## PROF. DR. NICOLAI BURZLAFF

nicolai.burzlaff@fau.de • [www.chemie.fau.de/burzlaff](http://www.chemie.fau.de/burzlaff)

### CURRICULUM VITAE

- Since 2004** University Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
- 1999 – 2004** Habilitation at the University of Konstanz, Germany
- 1997 – 1999** Postdoctoral Fellow at the Dyson Perrins Laboratory, Oxford, Great Britain
- 1997** PhD at the University of Würzburg, Germany



### OBJECTIVES

To design innovative heteroscorpionate ligands as a toolbox for metalloenzyme models, organometallics, supramolecular chemistry, and hybrid materials.

### SCIENTIFIC BACKGROUND

In the past decades, protein structures of several 2-oxoglutarate dependent iron oxygenases have been reported by various groups. Two iron binding histidines and one aspartate or glutamate—the so called 2-His-1-carboxylate facial triad—are conserved throughout the whole family of enzymes. This *N,N,O* binding motif, which is also found in some zinc peptidases, is the key research target of the Burzlaff group. Thus, to mimic this motif is the task of most of our model complexes for these iron and zinc dependent enzymes. Small heteroscorpionate ligands such as  $\kappa^3$ -*N,N,O* coordinating ligands are applied for this purpose. These ligands can be tailored with bulky

substituents to modify their sterical hindrance and with linker groups for solid phase fixation or copolymerization. One ongoing goal of such hybrid materials is to develop artificial enzymes, e.g. by applying imprinted polymer techniques or by embedding the model complexes in a protein.

### RESEARCH HIGHLIGHTS

Bioinorganic model complexes of various bis(pyrazol-1-yl)acetato or bis(imidazol-2-yl)propionato ligands mimic the 2-His-1-carboxylate facial triad of mononuclear non-heme iron oxygenases. With iron and ruthenium models bearing such ligands our group tries to mimic certain steps in the catalytic cycle of the enzymes. Coordination of substrates or substrate analogs and inhibitors to the models are also investigated. Related zinc complexes are structural models for the active sites of gluzincins. These are useful tools to develop



and test new zinc binding groups (ZBGs) to identify new lead structures for peptidase inhibitors. Several ligands have been grafted on Merrifield resins or on silica. Moreover, copolymers of several scorionate ligands with MMA/EGDMA have been synthesized. Ongoing work focuses on the generation of imprinted polymers by template complexes to generate artificial enzymes. Furthermore, various 1D and 2D coordination polymers as well as metal organic frameworks (MOFs) are accessible with the heteroscorpionates or new bidentate ligands. The heteroscorpionate ligands are also useful in organo-metallic and coordination chemistry and allow a chemistry comparable to that of cyclopentadienyl (Cp) or hydrido(trispyrazol-1-yl) borato ligands (Tp). Several transition metal oxo, carbonyl, carbene, vinylidene, allenylidene, dinitrogen, hydrido and hydrogen complexes have been synthesized so far. Recently, we focus especially on carbon-rich allenylidene complexes as a new concept to modify semi-conducting organic materials. New chiral enantiopure tripod ligands are designed from cheap compounds of the chiral pool such as (+)-camphor or (–)-menthone, which are suitable for transition metal mediated enantioselective catalysis. Moreover, in cooperation with university hospitals (FAU and LMU), we study small molecules that control the erythropoietin (EPO) formation by stabilization of the hypoxia inducible transcription factor HIF. Finally, kidney stones of mice models are studied by PXRD.

## PERSPECTIVES

In the future, we would also like to extend our efforts on five new topics: First, dioxygen activation by copper(I) complexes bearing bis(pyrazol-1-yl)acetic acids as chelating ligands. Depending on the substituents either hydroxylation of the ligand or H<sub>2</sub>O<sub>2</sub> generation is observed. Second, the synthesis of one-dimensional coordination polymers that might show conducting or semi-conducting properties. Third, the cation induced self assembly of tri- and tetranuclear complexes that might establish a route to models for the oxygen evolving center (OEC) of the photosystem II (PSII). Forth, carbon-rich molecules such as pentacenes will be transformed to organometallic

cumulenyldiene complex fragments to vary the electronic properties of the semi-conducting materials. Finally, in cooperation with the university hospital, we search for new leads that control the erythropoietin (EPO) formation by stabilization of the hypoxia inducible transcription factor HIF. New inhibitors are identified by coordination studies with ferrous model complexes, by *in silico* docking and by *in vitro* and *in vivo* bioassays. Fluorescing inhibitors are developed as tools to monitor the uptake and kinetics of this promising new class of drugs.

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# CHAIR OF GENERAL AND INORGANIC CHEMISTRY

## PROF. DR. KARSTEN MEYER

karsten.meyer@fau.de • [www.chemie.fau.de/kmeyer](http://www.chemie.fau.de/kmeyer)

### CURRICULUM VITAE

- Since 2006** University Full Professor, Chair of Inorganic and General Chemistry at the University of Erlangen-Nürnberg, Germany
- 2001 – 2005** Assistant Professor at the University of California, San Diego (UCSD), USA
- 1998 – 2000** Postdoctoral Studies at the Massachusetts Institute of Technology (MIT), Cambridge, USA
- 1995 – 1998** PhD at the Max-Planck-Institute (MPI) for Radiation Chemistry (now MPI for Chemical Energy Conversion), Mülheim/Ruhr, Germany
- 1989 – 1995** Study of Chemistry at the Ruhr-University of Bochum (RUB), Germany, Diploma in Chemistry

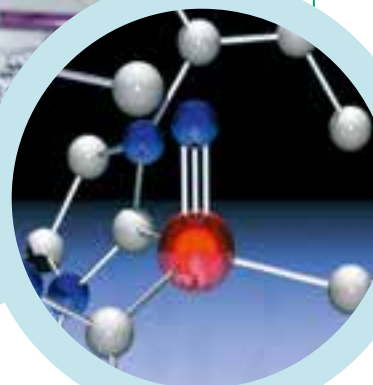
### OBJECTIVES

Synthetic Chemistry is at the heart of the Meyer lab research. General objectives are the syntheses of new chelating ligands and their reactive transition and actinide metal coordination complexes. These complexes often exhibit unprecedented coordination modes and unusual electronic structures, which result in enhanced reactivities towards small molecules of industrial and biological relevance, such as  $H_2$ ,  $H_2O$ ,  $CH_4$ ,  $CO$ ,  $CO_2$ ,  $N_2$ ,  $NO_x$ ,  $O_2$ ,  $O_3$ ,  $P_4$ ,  $As_4$ ,  $SO_x$ , etc. The synthetic results are complemented by detailed and often challenging spectroscopic investigations; requiring high sample purity and reproducibility. High-level spectroscopic investigations, supplemented by computational analyses, aid the understanding of the molecular and electronic structures that are origin of the specific compound reactivity.

### SCIENTIFIC BACKGROUND

Small molecules – such as alkanes, carbon dioxide, and water – are attractive natural resources for the synthesis of fine chemicals and fuels. This is particularly true for the greenhouse gases  $CO_2$  and  $CH_4$  but also for  $H_2O$  that holds promise to be the “coal of the future”. Activation and functionalization of these molecules, however, is difficult due to their thermodynamic stabilities. One approach to circumvent this limitation is to coordinate the inert molecules to a redox-active, low-valent metal ion, which can serve as an electron source to reduce strong bonds. Based on the versatile reactivity of uranium and transition metal complexes it is expected that novel complexes are capable of unprecedented transformation of small molecules; thus, opening opportunities for activation and functionalization of chemical feedstock.



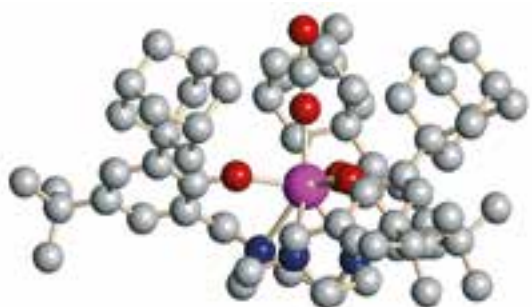


## RESEARCH HIGHLIGHTS

The Meyer research program is focused on the activation of small molecules of biological and industrial interest using redox-active uranium and transition metal complexes in molecularly engineered ligand environments. Benchmarks of the Meyer research work include the activation, cleavage, and multiple-bond metathesis of carbon dioxide at uranium complexes and the synthesis of reactive peroxy-, imido-, and nitrido-complexes for the functionalization of organic molecules via atom and group transfer chemistry. We were successful in synthesizing entire series of actinide and transition metal complexes that are unique as they are isostructural with varying oxidation states, e.g. Fe(I) to Fe(V) and U(II) to U(VI), enabling a complete and systematic analysis of the structure—reactivity relationships. Highlights are the identification of a new, previously unknown U(II) oxidation state and the electrocatalytic reduction of H<sub>2</sub>O for the production of H<sub>2</sub>; thus, opening new avenues to uranium reactivity. The analysis of complex series with structural continuity through the oxidation states presents a distinct benefit for the understanding of fundamental uranium and transition metal coordination chemistry. Topics such as the nature of *f*-orbital covalency in uranium complexes and the role of electronic structure in coordination complex reactivity are under continuous investigation and have become trademark areas of the Meyer lab research.

## PERSPECTIVES

Ultimate long-term objectives of the fundamental synthetic research in the Meyer lab are the development of efficient (electro-) catalysts for the metal complex-assisted conversion of abundant natural substrate resources and the discovery of renewable energy sources. Future research will therefore continue to focus on the advancement of novel actinide and transition metal-based catalytic transformations involving simple chemical feedstock, such as carbon dioxide and water, that are the key to sustainable energy resources.



## SELECTED PUBLICATIONS

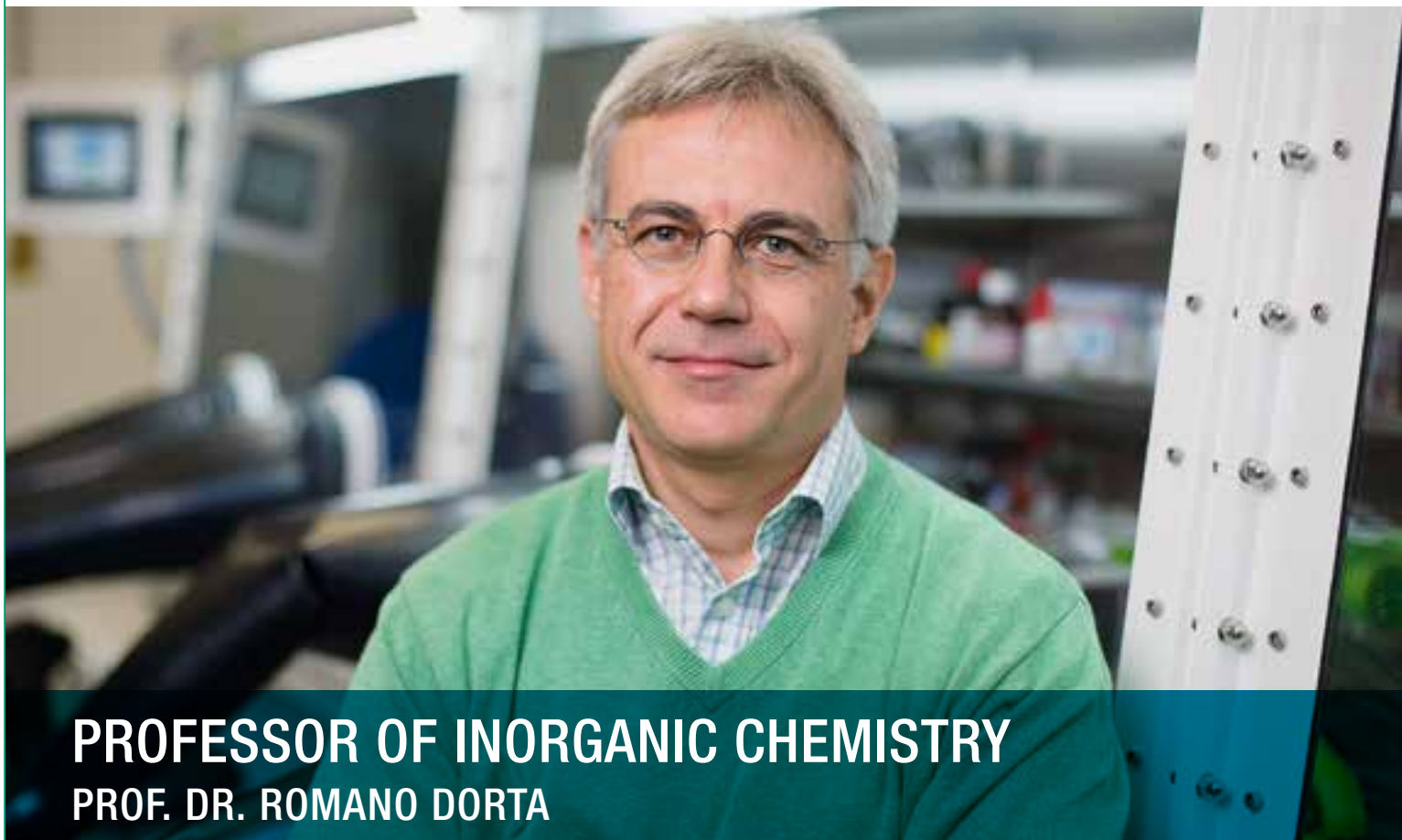
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## SELECTED REVIEWS

- H. S. La Pierre, K. Meyer, Activation of Small Molecules by Molecular Uranium Complexes, *Progress Inorganic Chemistry*, **2014**, 58, 303–415
- J. Hohenberger, K. Ray, K. Meyer, The Biology and Chemistry of High-Valent Iron Oxo and Nitrido Complexes, *Nature Commun.*, **2012**, 51, 781–783
- S. C. Bart, K. Meyer, Highlights in Uranium Coordination Chemistry, *Structure & Bonding*, **2008**, 127, 119–176
- A. R. Fox, S. C. Bart, K. Meyer, C. C. Cummins, Towards Uranium Catalysts, *Nature*, **2008**, 455, 341–349

## SELECTED AWARDS

- 2018 Visiting Professorship, ETH Zürich, Switzerland
- 2017 Ludwig Mond Award, Royal Society of Chemistry, Great Britain
- 2017 L. A. Chugaev Commemorative Medal, Russian Academy of Sciences
- 2017 Elhuyar-Goldschmidt Award, Spanish Royal Society of Chemistry
- 2015 Visiting Professor at the Nagoya Institute of Technology, Japan
- 2015 JSPS Professorship Award “Brain Circulation Project”, Nagoya, Japan
- 2012 Visiting Professorship, Université Paul Sabatier, Toulouse, France
- 2012 Visiting Professorship, University of Manchester, Great Britain
- 2011 Fellow of the Royal Society of Chemistry, Great Britain
- 2010 Dalton Transactions European Lectureship Award, Great Britain
- 2009 Israel Chemical Society Lifetime Honorary Membership
- 2004 Alfred P. Sloan Award, USA



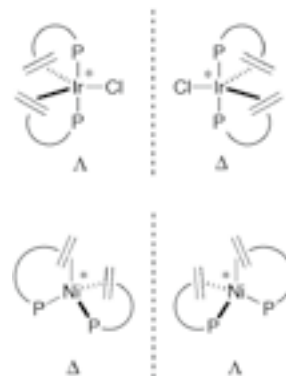
# PROFESSOR OF INORGANIC CHEMISTRY

## PROF. DR. ROMANO DORTA

romano.dorta@fau.de • [www.chemie.fau.de/dorta](http://www.chemie.fau.de/dorta)

### CURRICULUM VITAE

- Since 2013** Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany  
**2002 – 2013** Full Professor of Inorganic Chemistry, Universidad Simón Bolívar, Caracas, Venezuela  
**2000 – 2002** Research fellow at the Instituto Venezolano de Investigaciones Científicas, Venezuela  
**1998 – 2000** Postdoctoral fellow at the Weizmann Institute of Science, Rehovot, Israel  
**1993 – 1998** PhD, ETH, Zürich, Switzerland  
**1988 – 1993** Study of Chemistry, Université de Lausanne, Switzerland, and Università degli Studi di Parma, Italy



### OBJECTIVES

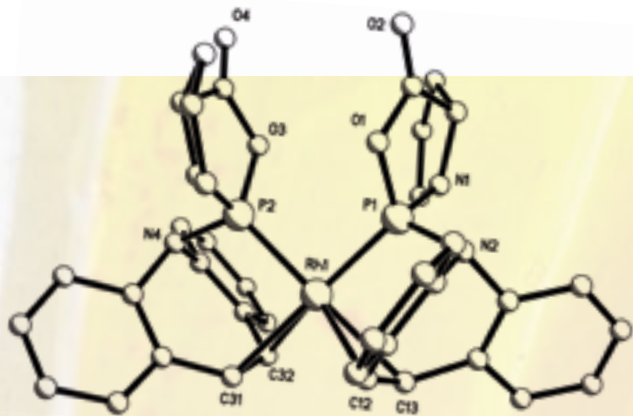
Our research efforts are directed towards the design of novel chiral organometallic complexes, which serve as catalysts for the asymmetric synthesis of optically active organic molecules. The development of alternative synthetic tools, such as functional ionic liquids is also part of our objectives.

### SCIENTIFIC BACKGROUND

Chiral molecules are ubiquitous in nature and biochemical processes. The enantiomers of a biologically active chiral molecule may elicit very distinct responses in living organisms. Many active pharmaceutical ingredients are chiral molecules, which nowadays are mostly commercialized in their non-racemic forms, due also to regulatory constraints. However, the synthesis of enantiomerically pure mole-

cules is costly, and indeed the added value of such products is very high. Annual single-enantiomer drug sales worldwide are estimated to be worth well over 200 billion Euros. Therefore, the development of new enantioselective synthetic methodologies has high priority. Amongst them, asymmetric catalysis represents a most elegant approach, a fact that was highlighted by the 2001 Chemistry Nobel Prize. The idea behind asymmetric catalysis is that the spatial information residing on a catalytically active chiral metal complex be transmitted as efficiently as possible onto the substrate molecules. Ideally, every chiral catalyst molecule would be able to generate thousands or even millions of product molecules of a defined chirality, thereby acting as a chirality multiplier. This technology can be superior to the classic separation of racemates or other stoichiometric enantioselective methods.





## RESEARCH HIGHLIGHTS

The design of new chiral ligand systems is the first and most challenging step toward the synthesis of reactive, optically pure metal complexes that are to be used as catalysts for asymmetric organic transformations. Some time ago, we came up with a chiral P-alkene hybrid ligand architecture that proved to be synthetically flexible enough to create small ligand libraries. Lately, we have expanded this design to sophisticated stereogenic P-donors and elements of planar chirality. Our P-alkene ligands exhibit hemilabile behavior thanks to the weakly coordinating alkene function. Such ligands protect reactive metal centers from premature decomposition without affecting their inherent reactivity, which is an important aspect in homogeneous catalysis. This is evidenced by our Ni(0)-P-alkene complexes that are perfectly air-stable in the solid state, but once in solution readily activate small molecules, thus maintaining the high reactivity typical of electron rich Ni(0) species but doing away with their characteristic air-sensitivity. Hemilability is operational in important catalytic reactions but structural proof thereof is scarce, and we have succeeded to authenticated it by X-ray crystallography in various P-alkene metal complexes. More recently, the design of novel  $C_2$ -symmetric sulfoxide-based pincer ligand systems as a rigid platform for chiral metal complexes is being investigated. For catalytic applications we only employ well-defined molecular organometallic species and try to avoid *in situ* formed catalyst mixtures. Examples are our chiral cationic mononuclear Rh-P-alkene complexes that catalyze the asymmetric formation of C–C bonds with almost perfect enantioselection ( $> 99\%$  ee). Finally, functional ionic liquids represent promising new synthetic tools for stoichiometric and catalytic transformations. Transition metal salts that are liquid at room temperature may be used as biphasic, self-supported catalysts for oxygen atom transfer reactions.

## PERSPECTIVES

We are currently developing novel P-stereogenic, planar-chiral P-alkene hybrid ligand systems and  $C_2$ -symmetric sulfoxide-based pincer ligands for the synthesis of highly reactive chiral complexes of early and late transition metals. We are exploring their rich organometallic chemistry, which ranges from activations of small molecules and specific bonds, to new catalytic reactivities. Catalysis development in our group is centered on the atom-economical, enantioselective formation of C–C, C–N, and C–O bonds. On the other hand, highly reactive functional ionic liquids are also being investigated as new synthetic tools.

## SELECTED PUBLICATIONS AND REVIEWS

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## CHAIR OF BIOINORGANIC CHEMISTRY

### PROF. DR. IVANA IVANOVIĆ-BURMAZOVIĆ

ivana.ivanovic-burmazovic@fau.de • [www.chemie.fau.de/ivanovic-burmazovic](http://www.chemie.fau.de/ivanovic-burmazovic)

#### CURRICULUM VITAE

<b>Since 2008</b>	University Full Professor, Chair of Bioinorganic Chemistry at the University of Erlangen-Nürnberg, Germany
<b>2008</b>	Offer for a professorship of Bioinorganic Chemistry at the University of Texas, Arlington, USA
<b>2008</b>	Habilitation in Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
<b>2001 – 2003</b>	Alexander von Humboldt Postdoctoral Fellow at the University of Erlangen-Nürnberg, Germany
<b>2000 – 2003</b>	Assistant Professor of General and Inorganic Chemistry at the University of Belgrade, Serbia
<b>1996 – 2000</b>	Research and Teaching Assistant of Inorganic Chemistry at the University of Belgrade, Serbia
<b>1999</b>	PhD, Faculty of Chemistry, University of Belgrade, Serbia

#### OBJECTIVES

The general goal of our Chair of Bioinorganic Chemistry is elucidation of the metal-tuned redox processes of biological and catalytic relevance at the molecular level. In a focus is the activation of small molecules (superoxide radical anion ( $O_2^-$ ), nitric oxide (NO), peroxynitrite ( $ONOO^-$ ), hydrogen sulphide ( $H_2S$ )) by redox-active metal complexes, which can have physiological or pathophysiological consequences in biological systems, but at the same time can find application in bioinspired catalysis and biotechnology. We study reaction mechanisms to understand elementary reaction steps of complex bioinorganic processes involved in redox signaling and design efficient enzyme mimetics, metal based human pharmaceuticals and chemical catalysts. The approach is to rationally design bio/catalytically-active metal complexes with desirable physiological/catalytic

effects based on understanding of their kinetic, thermodynamic, redox and mechanistic behavior, paving the way for improvements in human health and the energy conversion.

#### SCIENTIFIC BACKGROUND

Syntheses of redox-active transition metal complexes of different coordination geometry and their versatile solution/reaction behavior are the general interests of our research group. We explore a wide range of intermolecular interactions in solutions (multiple proton-coupled electron transfer processes, weak secondary interactions and host-guest chemistry in solution, interactions with solvent molecules, solvent exchange processes, stabilization of reactive superoxide via electrostatic interaction in ionic liquids) and reaction mech-

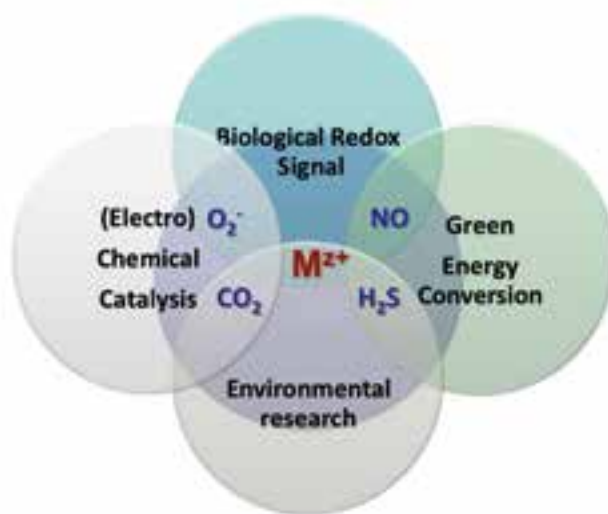
anisms in order to predict a potential application of metal based structures and tune their desirable activity. We apply a wide range of instrumentation methods in our research: time-resolved UV/vis low-temperature (down to -90 °C) and high-pressure stopped-flow measurements, high-pressure fluorescence stopped-flow measurements, high-pressure NMR measurements, temperature and pressure dependent electrochemical measurements, cryo time-resolved preparative spectroelectrochemistry, time-resolved solution IR, low-temperature mass spectrometry and cell culture and biochemical studies.

### RESEARCH HIGHLIGHTS

- SOD mimetics: experimental methodology, mechanisms and biological effects
- Water exchange on metal centers for understanding bio- and catalytic processes
- HNO generation by SOD mimetics and metal centers in biological systems
- 100 years old question, why nitrite acts as an antidote for hydrogen sulfide, is now solved: heme-catalyzed reaction between  $\text{NO}_2^-$  and  $\text{H}_2\text{S}$  generates HNO in mitochondria
- Interaction between  $\text{H}_2\text{S}$  and  $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}]$  as a new pharmacological source of HNO
- HSNO as a new signalling (shuttle) molecule
- Cross-talk between  $\text{H}_2\text{S}$  and NO
- Homogeneous and heterogeneous catalytic removal of  $\text{H}_2\text{S}$
- Mechanism of fast  $\text{CO}_2$  fixation by Ni-OH species
- Confined space reverses the high-pressure behavior of an iron-center, relevant for operation of heme-proteins in deep-sea organisms and a reverse spin-crossover effect

### PERSPECTIVES

Our long-term goals is to develop an emerging field of Medicinal Redox Inorganic Chemistry at a global level and to increase the impact of (bio)inorganic chemistry research on health care. Our efforts are directed to conceive the basic chemical processes behind the pharmacological treatment of oxidative and nitrosative stress, which are generators of aging and pathophysiological processes. In a time ahead of us, we see utilization of redox-active metal complexes in regulation of the cells redox status, activation of immune system mechanism, and as pharmaceuticals for treating the disease states related to immunodeficiency, inflammation/infection, and neuropathology. With the same goal we work on the effects of  $\text{H}_2\text{S}$  in triggering beneficial physiological mechanisms in the cells with an extreme redox status. Thus, development of new compounds that will at the same time act as SOD mimics,  $\text{H}_2\text{S}$  and/or  $\text{NO}^-$  donors as potential pharmaceuticals is challenging for us. We will also apply our knowledge on tuning the redox reactions by pressure for clarifying and increasing the efficiency of proton coupled electron transfer involved in the energy conversion processes.



### SELECTED PUBLICATIONS

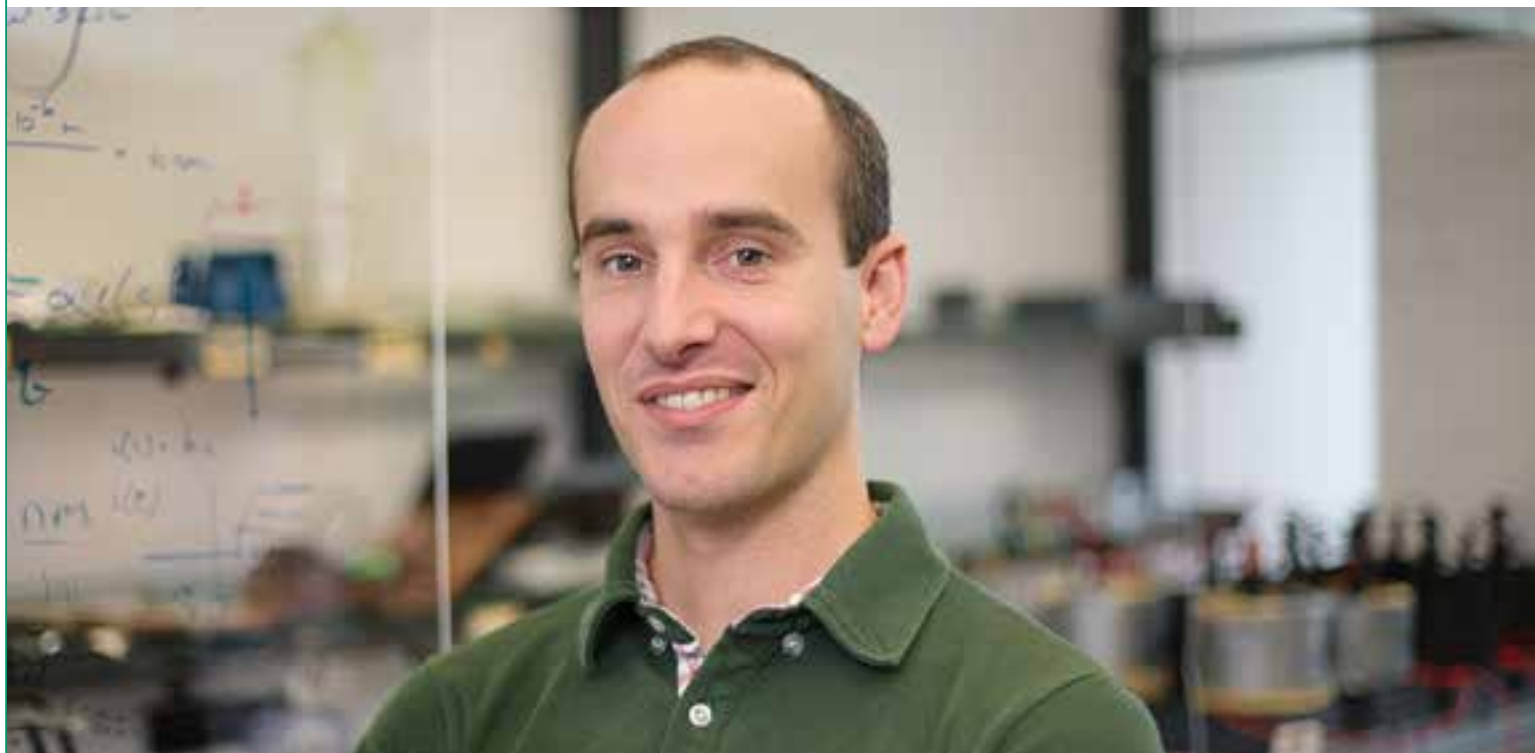
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- I. Ivanović-Burmazović, M.R. Filipović, *Removal of Hydrogen Sulphide (H2S): Catalytic oxidation of sulphide species*, **2012**, WO 2012175630 A1 20121227

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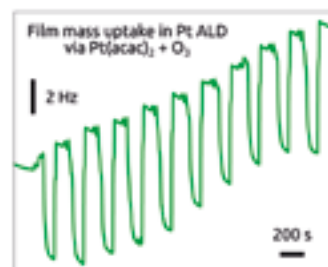
## CHAIR FOR CHEMISTRY OF THIN FILM MATERIALS

### PROF. JULIEN BACHMANN PHD

julien.bachmann@fau.de • [www.chemie.fau.de/bachmann](http://www.chemie.fau.de/bachmann)

#### CURRICULUM VITAE

- Since 2017** Full Professor, Chemistry of Thin Film Materials, University of Erlangen-Nürnberg, Germany
- 2012–2017** Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
- 2009–2012** Junior Professor of Chemical Physics (Physics and Chemistry Departments) at the University of Hamburg, Germany
- 2007–2009** Scientist at the Institute of Applied Physics, University of Hamburg, Germany
- 2006–2007** Postdoctoral Fellow at the Max Planck Institute of Microstructure Physics, Halle, Germany
- 2006** PhD in Inorganic Chemistry at the Massachusetts Institute of Technology, USA
- 2001** Chemistry Diploma at the University of Lausanne, Switzerland



#### OBJECTIVES

The overarching theme of our research is the systematic investigation of structure-property relationships in nanostructured inorganic materials. To achieve this goal, we develop innovative preparative methods designed for engineering ordered arrays of elongated structures, the geometry of which is accurately tunable, and the surface chemistry of which can be defined at will. We then quantify how the performance indicators of the material depend on the geometric parameters of the structures. We pay particular attention to the interplay of transport and interface phenomena in various types of energy conversion devices, such as the electrodes of fuel cells, electrolyzers, and batteries, as well as solar cells. We also aim at controlling data storage in adequately shaped magnetic elements.

#### SCIENTIFIC BACKGROUND

Research in nanostructured materials has long been justified by the size- and shape-dependent variation of properties expected, and observed, in confined systems. Their applications in modern solar cells, various types of electrodes, and magnetic data storage media mostly rely on their large specific surface area. Colloidal synthesis has been most instrumental towards fundamental advances and in applied devices, but is limited to disordered, suspended particles. In contrast to this, in our group we start from bulk solid pieces of macroscopic size, then we treat them in order to generate large amounts of parallel structures ordered on a surface or in a matrix. We pay particular attention to the generality of our preparative methods, and the accurate tunability of the geometry.



Julien Bachmann's dual background in molecular coordination and redox chemistry, on the one hand, and in the chemical and physical preparative and characterization methods of solids and interfaces, on the other hand, is perfectly suited to addressing the challenges of this highly interdisciplinary field of research.

## RESEARCH HIGHLIGHTS

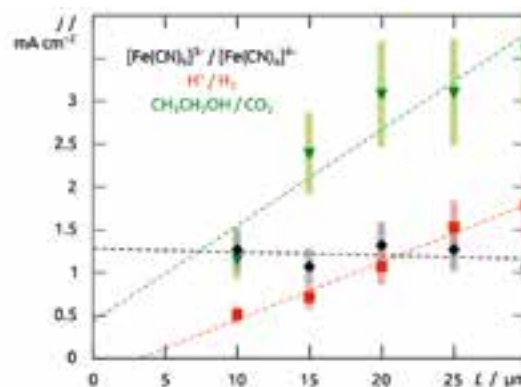
We use electrochemical methods (‘anodization’) to generate hexagonally arranged arrays of parallel, cylindrical pores, the length of which can be set to any value between 0.5  $\mu\text{m}$  and 100  $\mu\text{m}$  and the diameter between 10 nm and 300 nm. We introduce diameter modulations, if needed, at arbitrarily defined points along the pores’ length. Subsequently, we use galvanic techniques to either fill the pores completely with solid metallic wires, or to grow hollow metal tubes along the pore walls. These metallic structures may consist of one pure metal, of alloys, or even of alternating segments with different composition. An alternative is provided by atomic layer deposition (ALD), a thin film deposition technique that exploits well-defined surface chemistry to enable the conformal coating of our deep pores with thin layers of oxides and sulfides. One or several consecutive ALD layers can be applied, the thicknesses of which we set between 1 nm and 20 nm typically. With the ‘solution ALD’ method that we developed recently, we extend the range of materials that can be deposited as thin films based on self-limiting surface reactions. Our samples and reactions are characterized by electron microscopy, spectroscopic ellipsometry, piezoelectric microbalance, various steady-state and dynamic electrical, electrochemical, and photoelectrochemical methods, impedance spectroscopy, and magnetometry.

In the magnetic realm, segmented structures enable us to define a large number of ‘bits’ along the length of each object. The shape and length of each segment, as well as the distances between the segments, define the magnetization orientation, the switching field, and the interactions between bits. In ‘extremely thin absorber’ (ETA) solar cells, we find an optimal thickness for the intrinsic light-absorbing layer which balances the requirements of sufficient light absorption and efficient charge carrier collection. For many electrochemical fuel cell reactions at noble metal surfaces, we increase the current density by elongating the electrode’s pores while minimizing the catalyst loading via very thin coatings. We also experiment with broadly available alternative materials in electrochemical, photoelectrochemical and photovoltaic devices, whereby we compensate for the materials’ intrinsically poor physical or chemical properties by increasing their interface area geometrically.

## PERSPECTIVES

The generality of our methods enables us to combine materials in a modular manner to create electrochemically and photoelectrochemically optimized systems, in which several functional materials (such as electron conductor, light absorber, and water oxidation catalyst) are combined in a coaxial geometry on the sub-micrometer scale. In parallel, we will also pay renewed attention to the molecular aspect of multielectron reactivity at solid surfaces, in order to better

understand the interfacial catalysis aspects of our work. The physical-chemical insight gained from our geometrically controlled model systems will finally be exploited towards the construction of energy conversion devices based on abundant elements and cost-efficient materials.

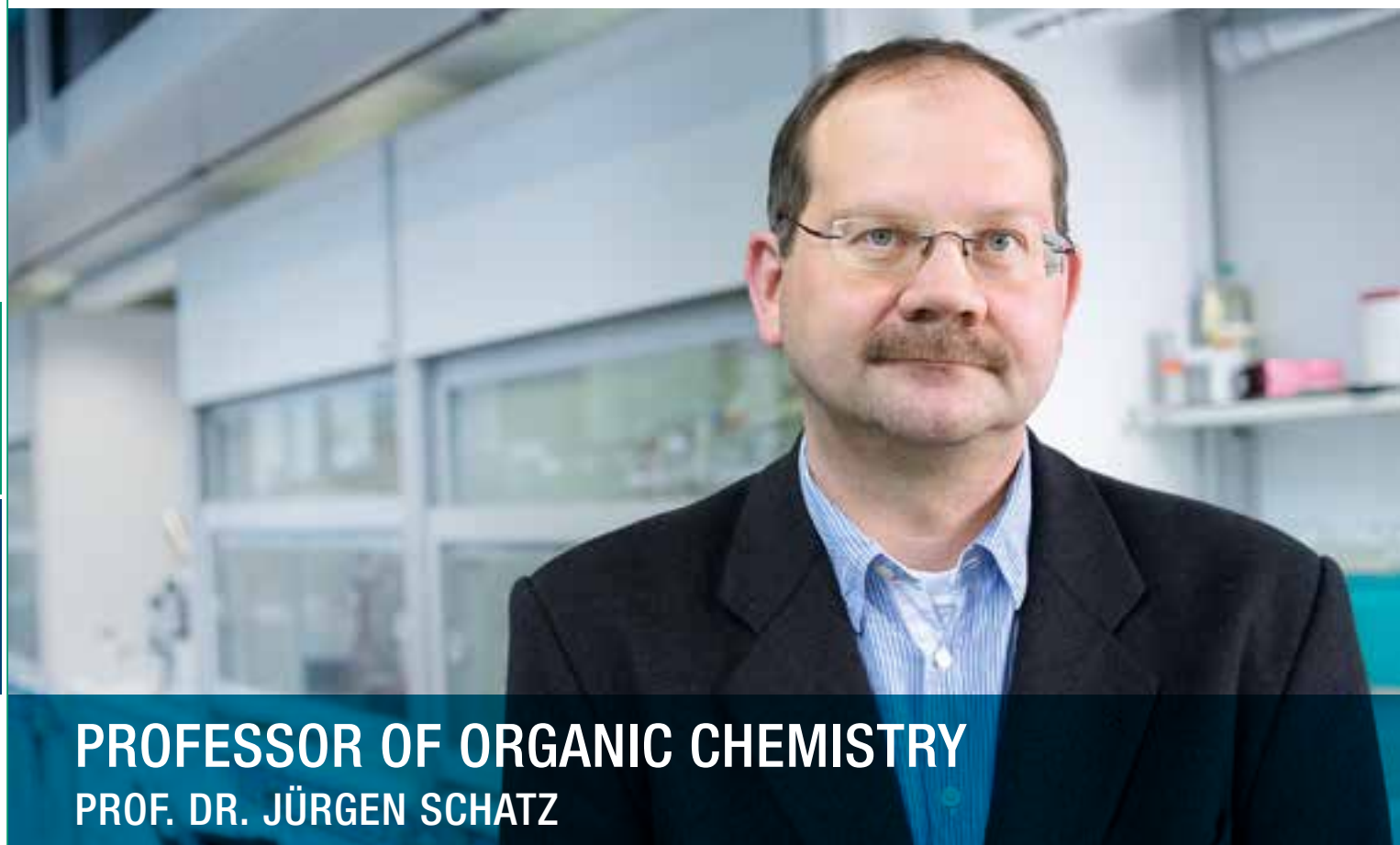


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- S. Bochmann, A. Fernandez-Pacheco, A. Neff, M. Mačković, E. Spiecker, K. R. Siefertmann, R. Cowburn, J. Bachmann, *RSC Advances*, **2017**, 7, 37627–37635
- O. Brummel, D. Besold, Y. Wu, S. Bochmann, F. Lazzari, F. Waidhas, T. Döpfer, U. Bauer, P. Bachmann, C. Papp, H.-P. Steinrück, A. Göring, J. Libuda, J. Bachmann, *ChemSusChem*, **2016**, 9, 1424–1432
- Y. Wu, D. Döhler, E. Oks, M. Wolf, M. Barr, L. Santinacci, J. Bachmann, *Nano Lett.*, **2015**, 15, 6379–6385
- L. Assaud, J. Schumacher, A. Tafel, S. Bochmann, S. Christiansen, J. Bachmann, *J. Mater. Chem. A*, **2015**, 3, 8450–8458
- Y. Wu, L. Assaud, C. Krysch, B. Capon, C. Detavernier, L. Santinacci, J. Bachmann, *J. Mater. Chem. A*, **2015**, 3, 5971–5981

## SELECTED AWARDS

- 2015 ERC Consolidator Grant, European Research Council
- 2013 Starting Grant, Cluster of Excellence ‘Engineering of Advanced Materials’, Erlangen, Germany
- 2009–2012 Six teaching prizes (four times first prize, twice second prize), University of Hamburg, Department of Physics, Germany
- 2006 Humboldt Research Fellowship, Alexander von Humboldt Foundation
- 2002 Award for Excellence in Teaching by a Graduate Student, MIT, Department of Chemistry, USA
- 2001 Presidential Fellowship, MIT, USA



## PROFESSOR OF ORGANIC CHEMISTRY

### PROF. DR. JÜRGEN SCHATZ

[juergen.schatz@fau.de](mailto:juergen.schatz@fau.de) • [www.chemie.fau.de/schatz](http://www.chemie.fau.de/schatz)

#### CURRICULUM VITAE

<b>Since 2007</b>	University Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
<b>2007</b>	Lecturer, Department of Chemistry and Pharmacy, Ludwig-Maximilians-Universität (LMU), München, Germany
<b>2002 – 2007</b>	Privatdozent, University of Ulm, Germany
<b>1995 – 2002</b>	Habilitation, University of Ulm, Germany
<b>1994 – 1995</b>	Postdoctoral Fellow, Department of Chemistry, Imperial College, London, Great Britain
<b>1994</b>	PhD in Organic Chemistry at the University of Regensburg, Germany

#### OBJECTIVES

To use (pure) water as an alternative medium for organic and supramolecular chemistry. Here, we want to design molecular systems based on weak (supramolecular) interactions and to exploit such arrays for catalysis, biological applications or as sensors.

#### SCIENTIFIC BACKGROUND

Organic Chemistry is usually performed in its corresponding environment—organic solvents. However, the interest in environmentally friendly (“green”) and sustainable processes has recently increased dramatically.

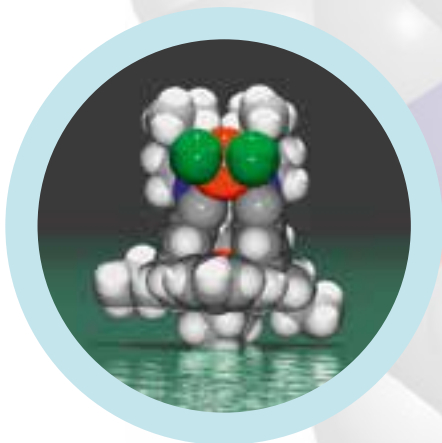
Here, our general interest in organic chemistry, which uses pure water as a solvent, can help to develop methodologies which allow organic transformations in aqueous media. We focus on the use of water-soluble macrocycles, e.g., calixarenes, cyclodextrins, cyclo-

phanes, or cucurbiturils, to adjust the solubility of both reagents and catalysts by supramolecular, non-covalent interactions. However, on the way to catalysis using self-assembled, non-covalently linked catalysts in water, many fundamental scientific problems have to be tackled: The supramolecular interactions between all components have to be elucidated both structurally and quantitatively. Therefore, we study the host-guest chemistry of artificial receptor molecules with cations, anions, or neutral molecules as guests.

Supramolecular interactions are also the underlying theme of a second research topic: The use of calixarene-based gadolinium complexes for applications in magnetic resonance imaging (MRI).

#### RESEARCH HIGHLIGHTS

Over the last years, we developed methods to perform standard organometallic reactions in pure water. For example, Suzuki cross



coupling as well as Grubbs-type metathesis reactions can now be realized in pure aqueous solution. The design, syntheses, and optimization of water-soluble macrocycles, which can be used as additives in these reactions, proved to be decisive. Especially, imidazolium salt based systems were very successful. This class of compounds can also act as precursors for N-heterocyclic carbenes (NHCs) which are ligands for both Palladium and Ruthenium used in Suzuki couplings and Grubbs metathesis reactions, respectively. In this way, both solubility and catalysis could be addressed using the same type of compounds.

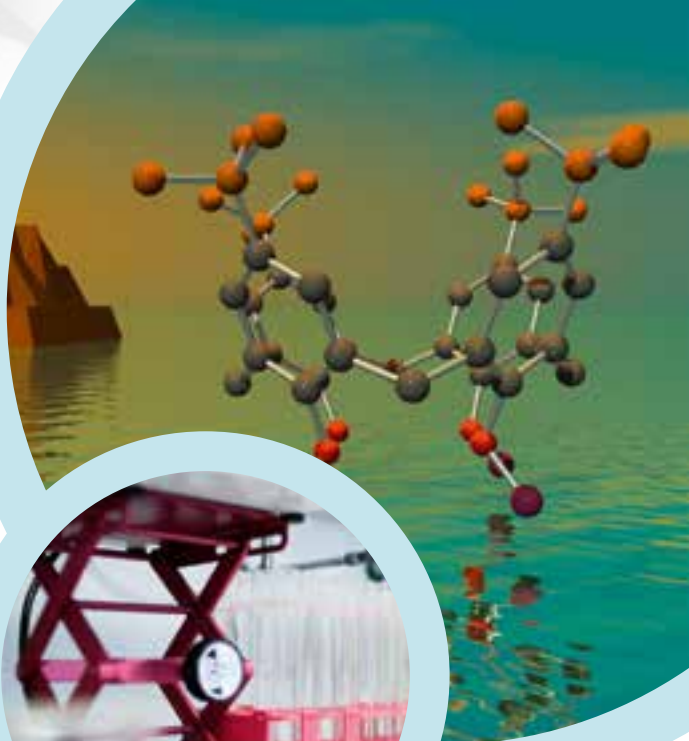
Imidazolium salts were also extremely useful in the recognition of small inorganic and organic anions. Recently, we succeeded in developing a naked-eye detection of small amounts of fluoride, acetate or benzoate using a calixarene-based anion receptor molecule.

In the supramolecular chemistry of cations Gadolinium-azacrown-ether-calixarene hybrids were synthesized which exhibit an outstanding performance in MRI applications.

## PERSPECTIVES

In future, we want to pursue three main areas of research: organometallic catalysis in water, anion recognition especially in polar environment, and novel MRI contrast agents.

In the first area, we want to develop efficient, tailor-made catalysts for applications in aqueous solution as medium. Additionally, we are working on the combination of various methods available in the “catalysts tool box”. Multi-step, one-pot procedures exploiting transition metal-, organo- and biocatalysis—disciplines well represented here in Erlangen—are here an appealing target. The quest for “naked-eye” receptors which detect anions with high efficiency and selectivity in pure water as an environment can be regarded as a holy grail in supramolecular chemistry. We want to address the challenge using organic cations as molecular platforms for anion receptors because these building blocks provide both colour, necessary for the optical read-out, and increased binding strength. Chiral discrimination in non-covalent recognition processes will also be an attractive issue for further research. Third, we will incorporate MRI contrast agents in biological structures such as liposomes, vesicles, or membranes.



## SELECTED PUBLICATIONS

- J. Schatz, R. Tammer, *Erste Hilfe – Chemie und Physik für Mediziner*, **2018**, Springer-Lehrbuch
- J. Schatz, *Übungsbuch Chemie für Mediziner*, **2017**, Springer-Lehrbuch
- I. Hoffmann, J. Schatz, *RSC Advances*, **2016**, 6, 80692–80699
- I. Hoffmann, B. Blumenröder, S. Onodi, S. Dommer, J. Schatz, *Green Chem.*, **2015**, 17, 3844–3857
- J. Tomasek, M. Seßler, H. Gröger, J. Schatz, *Molecules*, **2015**, 20, 19130–19141
- J. Tomasek, J. Schatz, *Green Chem.*, **2013**, 15, 2317–2338
- J. Schatz, M. Seßler, *Chem. Unsere Zeit*, **2012**, 46, 48–59
- K. Tenbrink, M. Seßler, J. Schatz, H. Gröger, *Adv. Synth. Catal.*, **2011**, 353, 2363–2367

## PATENTS

- J. Schatz, S. Onodi, A. Hätzelt, T. Gerke, Active ingredients which improve primary detergent power, **2016**, WO 2016008788 A1, DE 102014010505 A1

## SELECTED REVIEWS

- I. Hoffmann, J. Schatz, Thiophene Metallation and Cross-Coupling Chemistry, *Top. Heterocycl. Chem.*, **2015**, 39, 3844–3857
- J. Schatz, D. Schühle, Supramolecular Metal Complexes for Imaging and Radiotherapy, *Supramolecular Systems in Biomedical Fields*, **2013**, 10, 300–330
- I. Hoffmann, J. Schatz, Organometallic reactions in aqueous phase, *Nachrichten aus der Chemie*, **2013**, 61, 748–753
- D. T. Schühle, J. A. Peters, J. Schatz, Metal Binding Calixarenes with Potential Biomimetic and Biomedical Applications, *Coord. Chem. Rev.*, **2011**, 255, 2727–2745

## SELECTED AWARDS

- 2008–2013 Teaching Awards, University of Erlangen-Nürnberg, Faculty of Medicine
- 2002 Lehrbonus University of Ulm (Teaching Award)
- 1994 E.ON Bayern – Kulturpreis Ostbayern (PhD Award)





## PROFESSOR OF ORGANIC CHEMISTRY

### PROF. DR. SVETLANA B. TSOGOEVA

svetlana.tsogoeva@fau.de • [www.chemie.fau.de/tsogoeva](http://www.chemie.fau.de/tsogoeva)

#### CURRICULUM VITAE

- Since 2007** University Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany  
**2002 – 2007** Juniorprofessor at the Institute of Organic and Biomolecular Chemistry, University of Göttingen, Germany  
**2000 – 2002** Postdoctoral Research Fellow at the Fine Chemicals Division of Degussa AG, Hanau, Germany  
**1998 – 2000** Postdoctoral Research Fellow at the Johann Wolfgang Goethe University, Frankfurt am Main, Germany  
**1995 – 1998** PhD at the St.-Petersburg State University, St. Petersburg, Russia

#### OBJECTIVES

The development, application, and teaching of modern synthetic methods in asymmetric catalytic synthesis and chiral resolution is a central goal in our group. Computations and experiment are often both employed to address specific problems and in the same project. State-of-the-art analytical techniques and skills are used to carry out experiments, notably for design and evaluation of chiral organocatalysts and iron catalysts. Interdisciplinary and international collaborations round off our profile, where both sides mutually profit from the synergy of the expertises existing in different research groups.

#### SCIENTIFIC BACKGROUND

Many bioactive compounds are chiral and there is an ever-growing demand in contemporary pharmaceuticals or material science for compounds with high enantiopurity, e.g., for single enantiomer chiral drugs and their precursors. Stereochemistry therefore aims at intro-

ducing chiral centers of defined absolute configuration at desired positions into molecules and with high conversion rates from prochiral reactants. Hence, there is a continued need to design more active, more versatile and more enantioselective catalysts. In addition, we endeavour to find successful new synthetic methods and/or catalytic systems in enantioselective organocatalysis, aiming at high throughput, high enantioselectivity and diastereoselectivity, a wide substrate or reaction scope and use of environmentally benign solvents (e.g., water). To achieve this goal, computational methodologies and tools are employed to predict enantioselectivities or for finding clues for improved catalyst lead structures. Novel organic process techniques are being developed in our lab, accessing autocatalysis and crystal engineering. A further area of research interest is the design of synthetic hybrids of natural bioactive compounds with potential applicability in medicinal chemistry. Further, novel organocatalytic multi-

step domino reactions, which provide straightforward, sustainable and atom economical route to difficult-to-access complex bioactive heterocyclic compounds, are being developed in our group.

## RESEARCH HIGHLIGHTS

Research in our group is centered around *Asymmetric Organocatalysis, Iron Catalysis, Multi-Step Domino Reactions, One-Pot Processes and Natural Product Hybrids for Medicinal Chemistry*.

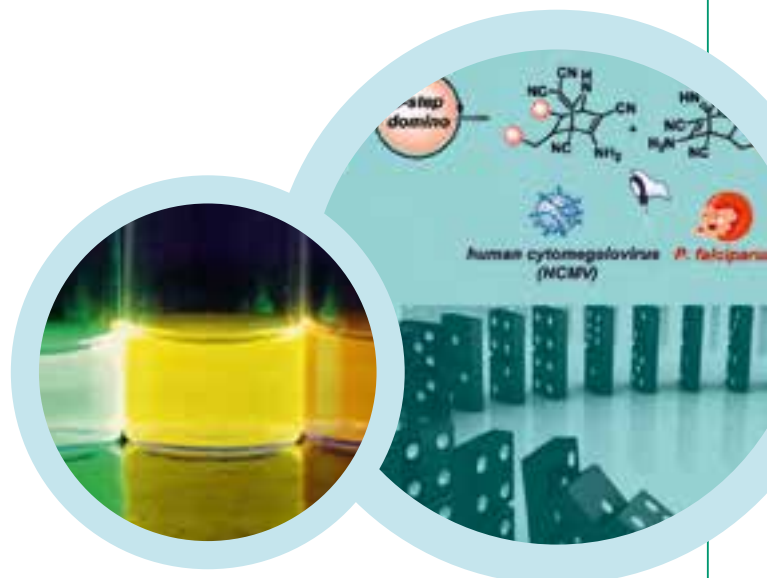
In the flourishing research area of *Asymmetric Organocatalysis* we focused early on the design, synthesis and application of novel *chiral bifunctional organocatalysts* for different organic transformations. We found and applied the first primary amine containing *unmodified dipeptides and thiourea-amine organocatalysts* for highly enantioselective C-C bond formation reactions (e.g., nitro-Michael, Mannich, aldol reactions). We discovered lately the first *organo-autocatalytic reactions*. Combining the novel concept of product catalysis with that of asymmetric amplification, we first demonstrated spontaneous enantioenrichment in fully organic reactions.

Recently we extended the spectrum of our research to domino reactions and one-pot processes, which are of prominent importance for preparation of complex molecules starting from simple and readily available compounds and are among the most recent, elegant, sustainable and environmentally attractive synthetic methods. Such synthetic strategy is desirable, concerning environmental aspects and sustainability, and with respect to reduction of costs and potentially hazardous waste.

*Medicinal chemistry* involves the identification, synthesis and development of promising new compounds suitable for therapeutic use. It also includes the study of existing drugs, their biological properties, and their structure activity relationships. *Hybridization of bioactive natural and unnatural compounds* rates among the most promising recent approaches in this field. Our interest focuses on the development of new lead structures and the design of promising candidates for potent drugs in the field of medicinal chemistry.

## PERSPECTIVES

The future of asymmetric catalysis and of the technologies used in generation of enantiomerically pure compounds in the industry might look rather different from what we know today. The discovery of organoautocatalysis is evidence that seemingly already well-understood organic reactions might possess much more complicated mechanisms than hitherto believed. To uncover the exact nature of stereoselective reactions could offer new opportunities for catalyst design and process development in catalytic asymmetric synthesis, e.g., in more efficient reactions that are more atom-economical or which produce less waste. In this context, one-pot multicomponent reactions in which different catalytic steps proceed successively and without the need of intermittent product extraction, catalyst retrieval and purification steps plays a promising role for the future development of asymmetric synthesis. The exploitation of novel chiral resolution techniques like crystal engineering in combination with conventional asymmetric synthesis has a high potential for future



optimizations to attain high-throughput and efficient production of single enantiomer compounds, which have a tremendous economic potential.

## SELECTED PUBLICATIONS

- F. E. Held, A. A. Guryev, T. Fröhlich, F. Hampel, A. Kahnt, C. Hutterer, M. Steingruber, H. Bahsi, C. von Bojničić-Kninski, D. S. Mattes, T. C. Foertsch, A. Nesterov-Mueller, M. Marschall, S. B. Tsogoeva, *Nature Commun.*, **2017**, 8, 15071
- C. M. Bock, G. Parameshwarappa, S. Bönisch, C. Neiss, W. Bauer, F. Hampel, A. Görling, S. B. Tsogoeva, *Chem. Eur. J.*, **2016**, 22, 5189–5197
- A. Fingerhut, Y. Wu, A. Kahnt, J. Bachmann, S. B. Tsogoeva, *Chem. Asian J.*, **2016**, 11, 1232–1239
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- D. A. Yalalov, S. B. Tsogoeva, T. E. Shubina, I. M. Martynova, T. Clark, *Angew. Chem. Int. Ed.*, **2008**, 47, 6624–6628
- C. Baudequin, A. Zamfir, S. B. Tsogoeva, *Chem. Commun.*, **2008**, 4637–4639
- S. B. Tsogoeva, S.-W. Wei, *Chem. Commun.*, **2006**, 1451–1453

## SELECTED REVIEWS

- T. Fröhlich, A. Çapci Karagöz, C. Reiter, S. B. Tsogoeva, Artemisinin-Derived Dimers: Potent Antimalarial and Anticancer Agents, *J. Med. Chem.*, **2016**, 59, 7360–7388
- F. E. Held, S. B. Tsogoeva, Asymmetric cycloaddition reactions catalyzed by bifunctional thiourea and squaramide organocatalysts: *Recent advances*, *Catal. Sci. Technol.*, **2016**, 6, 645–667
- S. B. Tsogoeva, When chiral product and catalyst are the same: Discovery of asymmetric organoautocatalysis, *Chem. Commun.*, **2010**, 46, 7662–7669
- S. B. Tsogoeva, Recent Progress in the Development of Synthetic Hybrids of Natural or Unnatural Bioactive Compounds for Medicinal Chemistry, *Mini Rev. Med. Chem.*, **2010**, 10, 9, 773–793

## SELECTED AWARDS

- 2012 Otto-Röhm Research Award
- 2008 Tetrahedron: Asymmetry “Most Cited Paper 2005–2008 Award”
- 2007 Thieme Journal-Preis



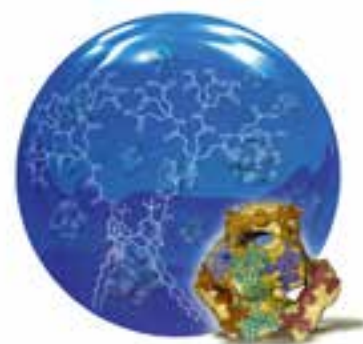
## CHAIR OF ORGANIC CHEMISTRY II

### PROF. DR. ANDREAS HIRSCH

andreas.hirsch@fau.de • [www.chemie.fau.de/hirsch](http://www.chemie.fau.de/hirsch)

#### CURRICULUM VITAE

- Since 1995** University Full Professor, Chair of Organic Chemistry II at the University of Erlangen-Nürnberg, Germany
- 1995** Professor for Organic Chemistry at the University of Karlsruhe, Germany
- 1991 – 1995** Habilitation at the Institute of Organic Chemistry, University of Tübingen, Germany
- 1990 – 1991** Postdoctoral research with Prof. Fred Wudl at the Institute for Polymers and Organic Solids, Santa Barbara, USA
- 1987 – 1990** PhD in Organic Chemistry at the University of Tübingen, Germany



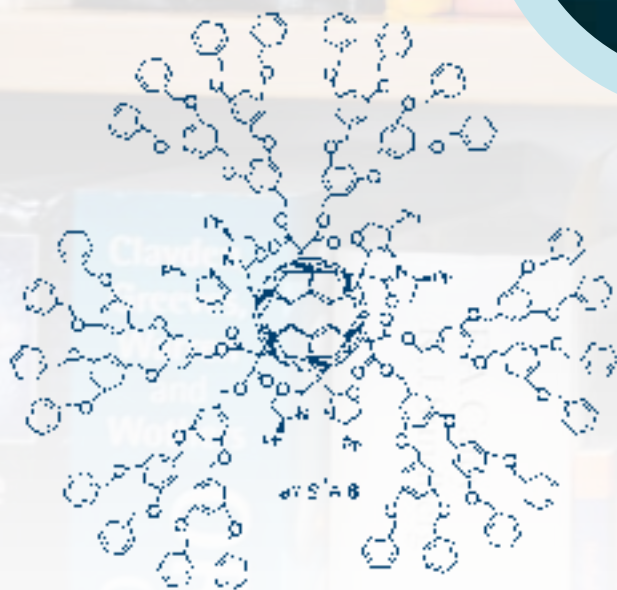
#### OBJECTIVES AND SCIENTIFIC BACKGROUND

Hirsch's laboratory has been pioneering and is at the forefront of carbon allotrope chemistry and is well-known for the investigations of basic principles for the functionalization of the 0-dimensional fullerenes, the 1-dimensional carbon nanotubes and the 2-dimensional graphene, which lead to synthesis of numerous examples of derivatives with tailor-made structural, electronic, photophysical and biomedical properties. Andreas Hirsch's work in synthetic organic chemistry includes synthesis of oligoynes, development of new covalent, ionic and H-bonded dendrimers, porphyrines, calixarenes, perylenes and redox-active ionic liquids. Currently the Hirsch laboratories are extending their interests into 2D materials such as black phosphores and MoS<sub>2</sub>.

#### RESEARCH HIGHLIGHTS

The research of the Hirsch group is characterized by its uncompromising commitment to interdisciplinarity. Among the most important achievements are: control over the regiochemistry of multiple addition reactions, the shape dependent difference of endohedral and exohedral functionalization, the  $2(n+1)^2$ -rule for the description of spherical aromaticity of fullerenes, which is named as Hirsch rule, the introduction of water solubility into these carbon rich systems and the first p-type doping of carbon nanotubes, the synthesis of self-assembled dendrimers, the generation of shape persistent micelles and switchable Buckysomes, the synthesis and investigation of well defined monodisperse polyelectrolytes, the retrofunctionalization of carbon nanotubes and finally the first systematic investigation on the covalent and non-covalent functionalization of graphene. Numer-

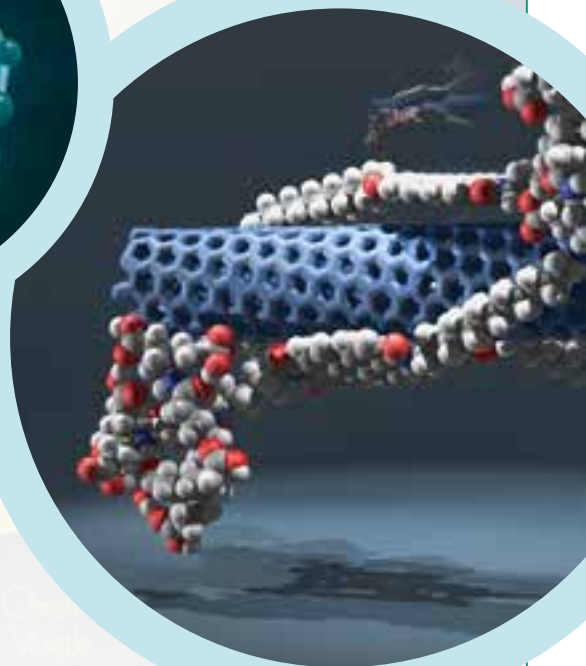
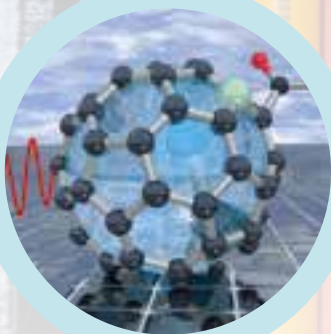




ous examples of fullerene, nanotube and graphene derivatives with tailor-made properties such as a) donor-acceptor hybrids suitable to undergo photoinduced energy and electron transfer, b) synthetic mimics for globular hemeproteins, c) dendrizymes, d) heterofullerenes, e) cluster opened fullerenes, f) the largest polyelectrolytes with completely defined and monodisperse structures, g) nanotube based carriers for gene delivery, h) giant bis-fullerene dipoles, i) the first example of fullerene amphiphiles that aggregate completely in shape persistent micelles, whose structure could be determined with molecular precision and j) water soluble fullerene derivatives that act as very potent superoxide dismutase models in the field of biomedical chemistry. The PI's work in synthetic chemistry includes synthesis of acetylenic compounds such as polyynes and stabilized oligoynes which are of interest in approaching a new hypothetical allotrope of carbon, the one-dimensional carbene  $sp-C_{\infty}$ .

## PERSPECTIVES

The systematic investigation of the carbon allotrope chemistry and the development of new concepts in supramolecular chemistry will pave the way to high performance applications as molecular materials. Examples are printable electronics, organic photovoltaic devices, redox-active as potent neuro-protective drugs.



## SELECTED PUBLICATIONS

- P. Vecera, J. C. Chacon-Torres, T. Pichler, S. Reich, H. R. Soni, A. Görling, K. F. Edlthammer, H. Peterlik, F. Hauke, A. Hirsch, *Nat. Commun.*, **2017**, 15192
- G. Abellán, P. Ares, S. Wild, E. Nuin, C. Neiss, D. R. San Miguel, P. Segovia, C. Gibaja, E. Michel, A. Görling, F. Hauke, J. Gomez-Herrero, A. Hirsch, F. Zamora, *Angew. Chem. Int. Ed.*, **2017**, 56, 14389–14394
- P. Vecera, J. Holzwarth, K. F. Edlthammer, U. Mundloch, H. Peterlik, F. Hauke, A. Hirsch, *Nat. Commun.*, **2016**, 7, 12411
- R. Neubauer, F. W. Heinemann, F. Hampel, Y. Rubin, A. Hirsch, *Angew. Chem. Int. Ed.*, **2012**, 51, 11722–11726
- J. M. Englert, C. Dotzer, G. Yang, M. Schmid, C. Papp, M. J. Gottfried, H.-P. Steinrück, E. Spiecker, F. Hauke, A. Hirsch, *Nat. Chem.*, **2011**, 3, 279–286
- C. Ehli, C. Oelsner, D. M. Guld, A. Mateo-Alonso, M. Prato, C. D. Schmidt, C. Backes, F. Hauke, A. Hirsch, *Nat. Chem.*, **2009**, 1, 243–249

## SELECTED REVIEWS

- S. Eigler, A. Hirsch, Chemistry with Graphene and Graphene Oxide—Challenges for Synthetic Chemists, *Angew. Chem. Int. Ed.*, **2014**, 52, 7720–7738
- A. Hirsch, The era of carbon allotropes, *Nat. Mater.*, **2010**, 9, 868–871
- A. Hirsch, Functionalization of Single-wall Carbon Nanotubes, *Angew. Chem. Int. Ed.*, **2002**, 41, 1853–1859
- M. Bühl, A. Hirsch, Spherical Aromaticity of Fullerenes, *Chem. Rev.*, **2001**, 101, 1153–1183

## SELECTED AWARDS

- 2017 ERC Advanced Grant
- 2009 ERC Advanced Grant



## PROFESSOR OF ORGANIC CHEMISTRY

### PROF. DR. ANDRIY MOKHIR

andriy.mokhir@fau.de • [www.chemie.fau.de/mokhir](http://www.chemie.fau.de/mokhir)

#### CURRICULUM VITAE

- Since 2013** Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany  
**2011 – 2012** Associate Professor for Bioinorganic Chemistry, Ruprecht-Karls-Universität Heidelberg, Germany  
**2010** Habilitation at the Ruprecht-Karls-Universität Heidelberg, Germany  
**1997** PhD, Kiev Shevchenko University, Ukraine

#### OBJECTIVES

Development of switchable substrates for highly orthogonal chemical reactions in live cells: applications in medicine (disease-specific prodrugs targeting cancer and autoimmune diseases), bioanalytical and biochemical sciences (monitoring concentration and localization of nucleic acids in live cells).

#### SCIENTIFIC BACKGROUND

The group is involved in synthesis of organic and coordination compounds as well as bioconjugates of oligonucleotides with chemical fragments including redox active moieties, fluorescent dyes, reactive substrates and catalytic fragments. The activity of these substances is tested in cell free settings using NMR, UV-visible, fluorescence spectroscopy, chromatography (HPLC, TLC and others) and mass spectrometry (ESI, MALDI-TOF) as well as in cell cultures and (in cooperation) *in vivo*.

#### RESEARCH HIGHLIGHTS

We work on discovery of ferrocene-based prodrugs. In the cancer cell—specific microenvironment these compounds are converted in the quick autocatalytic reaction into highly toxic species, which kill cancer cells selectively. In the microenvironment of normal cells these metallodrugs are stable and not toxic (Figure 1).

We also develop nucleic acid controlled photocatalysts based on natural and semi-synthetic tetrapyrroles and their analogues. We use these catalysts to design catalytic and autocatalytic reactions, which are applied for the amplified detection of nucleic acids in living cells. The ultimate goal of this project is to develop a robust assay for detection of a single copy of a particular nucleic acid per cell (Figure 2). The same photocatalysts are used to design “caged” reagents (e.g. oligonucleotides, siRNAs), whose biological activity (antisense, RNAi or immunostimulatory activity) is controlled by non-toxic red light (Figure 3).

Figure 1

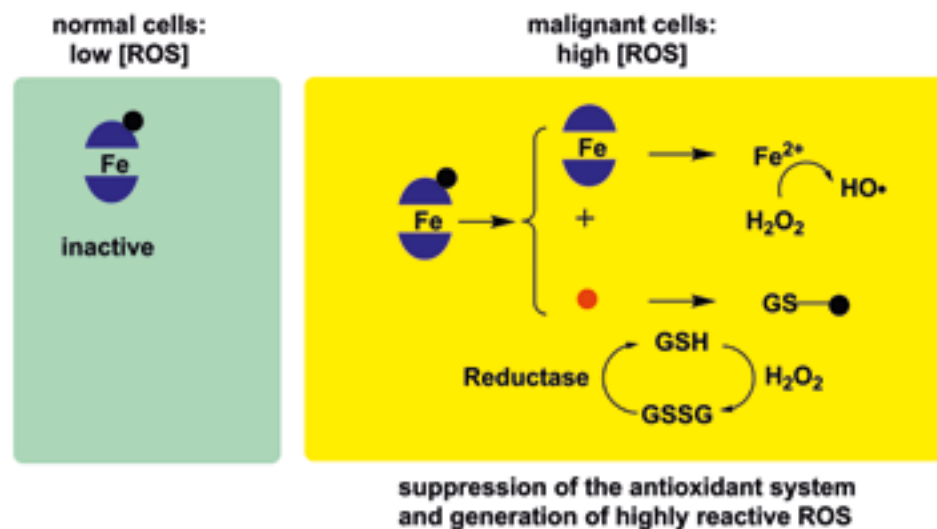


Figure 2

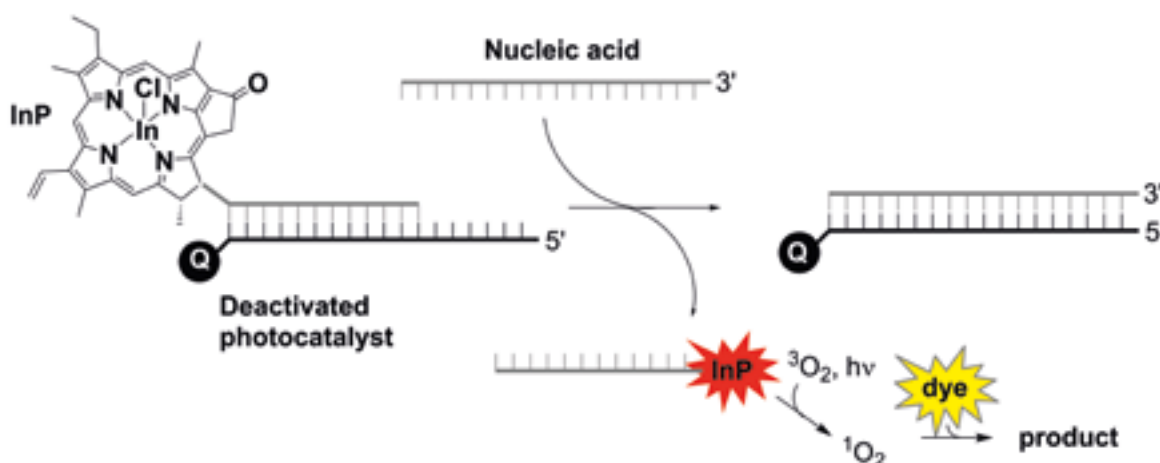
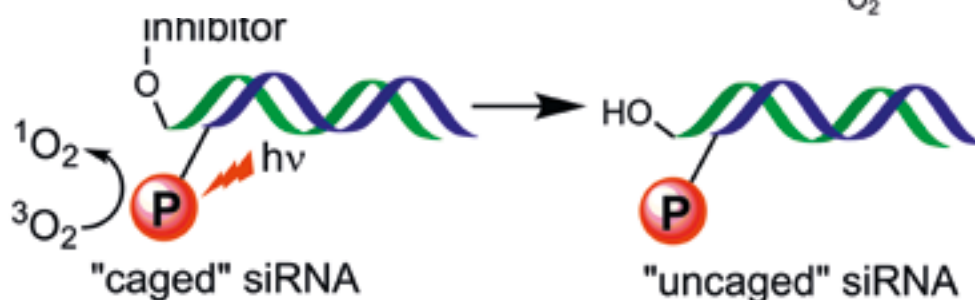


Figure 3



## PERSPECTIVES

Our long term goals include development of (a) side effect-free anticancer drugs and (b) membrane-permeable reagents for robust and highly sensitive detection of biomolecules in live cells and for regulation of their biological activity.

## SELECTED PUBLICATIONS

- S. Daum, V. Reshetnikov, M. Sisa, T. Dumych, M. D. Lootsik, R. Bilyy, E. Bila, C. Janko, C. Alexiou, M. Herrmann, L. Sellner, A. Mokhir, *Angew. Chem.*, **2017**, 56, 49, 15545–15549
- V. Reshetnikov, S. Daum, A. Mokhir, *Chem. Eur. J.*, **2017**, 23(24), 5678–5681
- H. Pieper, S. Chercheja, S. Eigler, C. Halbig, M. R. Filipovic, A. Mokhir, *Angew. Chem. Int. Ed.*, **2016**, 55, 1, 405–407
- A. Meyer, M. Schikora, A. Mokhir, *Chem. Comm.*, **2015**, 51, 13324–13326
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- D. Arian, L. Kovbasyuk, A. Mokhir, *J. Am. Chem. Soc.*, **2011**, 133, 11, 3972–3980

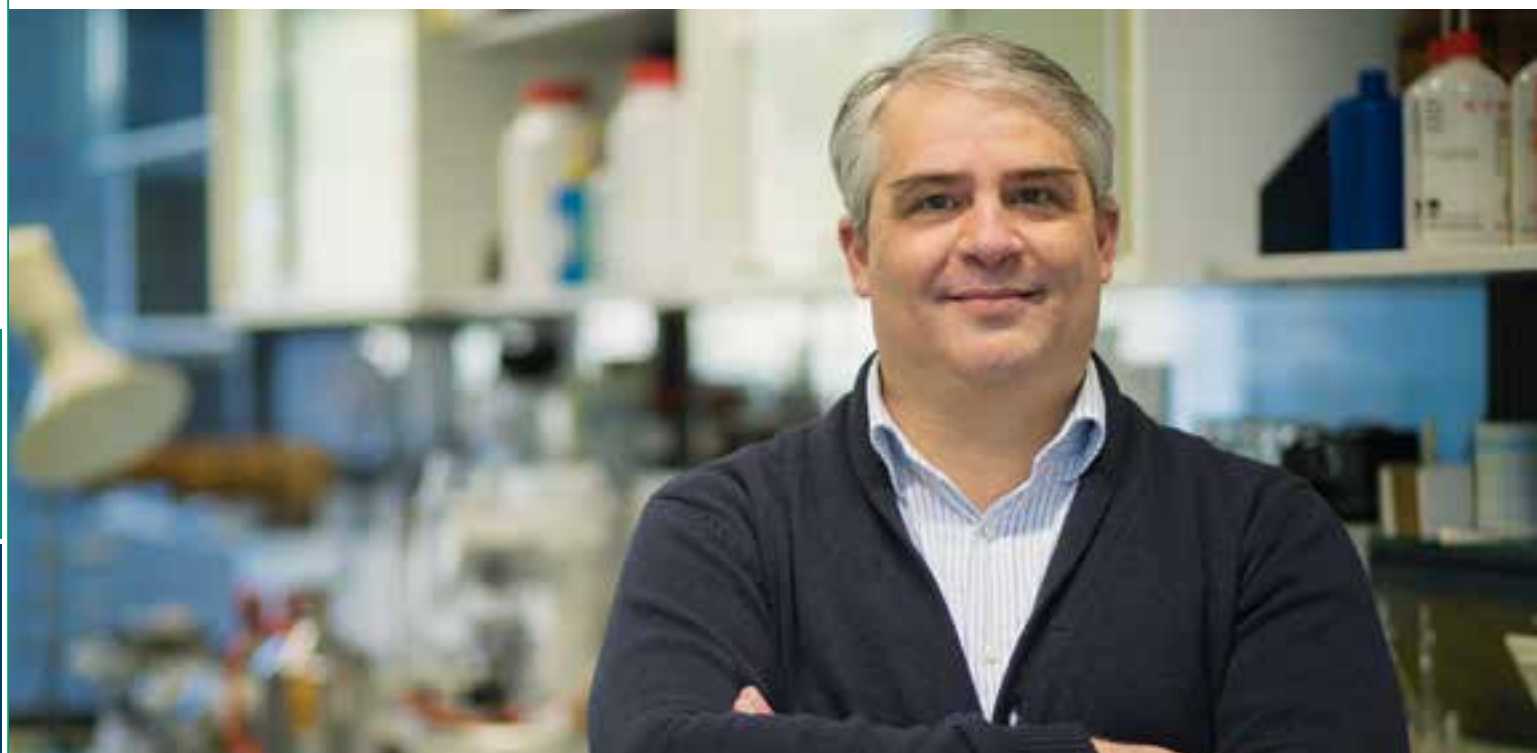
## SELECTED REVIEWS

- L. Kovbasyuk, A. Mokhir, Toxicity studies and biomedical applications of graphene oxide, in: A. Dimiev, S. Eigler, Wiley, **2017**
- A. Mokhir, Chemical reactions controlled by nucleic acids, in: E. Stulz, G. H. Clever, Wiley, **2014**

## SELECTED AWARDS

- 2005 selected in the Emmy Noether Programme of the Deutsche Forschungsgemeinschaft (DFG)
- 2011 selected in the Perspectives Program "PLUS 3" for independent young group leaders and endowed professorships of Boehringer Ingelheim Stiftung





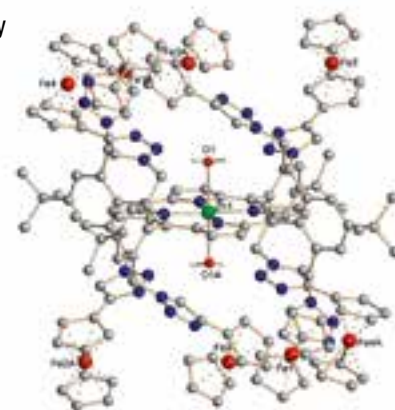
## PROFESSOR OF ORGANIC CHEMISTRY

### APL. PROF. DR. NORBERT JUX

[norbert.jux@fau.de](mailto:norbert.jux@fau.de) • [www.chemie.fau.de/jux](http://www.chemie.fau.de/jux)

#### CURRICULUM VITAE

<b>Since 2013</b>	Apl. Professor, Organic Chemistry at the University of Erlangen-Nürnberg, Germany
<b>2007</b>	Assistant Professor (PD), Organic Chemistry at the University of Erlangen-Nürnberg, Germany
<b>2006</b>	Habilitation in Organic Chemistry at the University of Erlangen-Nürnberg (Prof. A. Hirsch), Germany
<b>1997 – 2006</b>	Research Group leader in Organic Chemistry, University of Erlangen-Nürnberg, Germany
<b>1995 – 1996</b>	Postdoctoral Fellow, Department of Chemistry and Biochemistry, University of California, Los Angeles (Prof. Y. Rubin), USA
<b>1994</b>	PhD, University of Cologne (Prof. E. Vogel), Germany
<b>1990</b>	Diploma Degree in Chemistry, University of Cologne, Germany



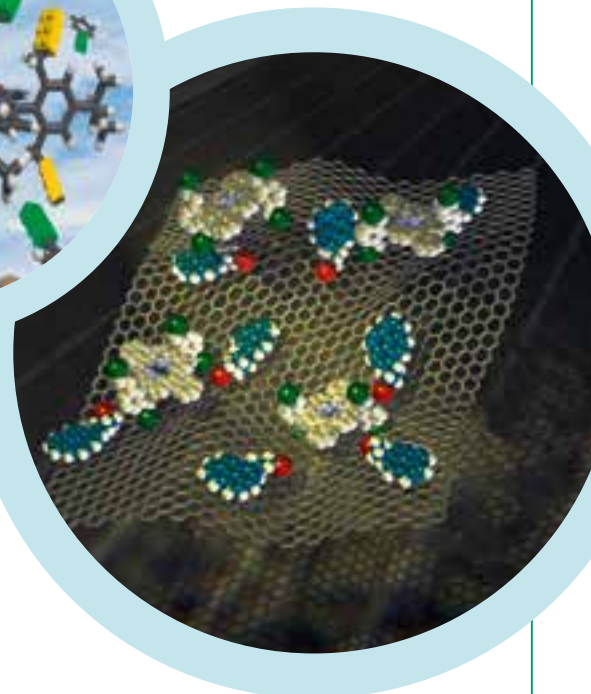
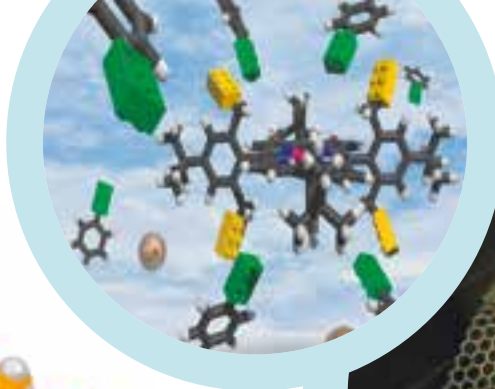
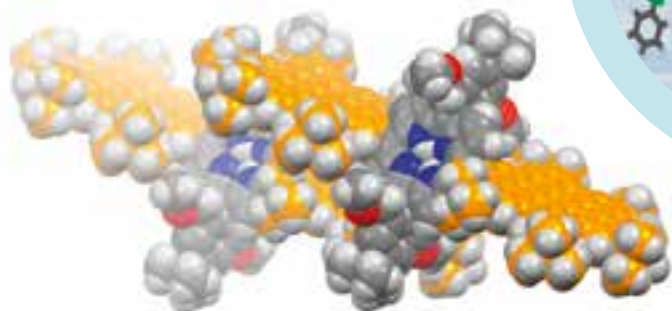
#### OBJECTIVES

To synthesize and characterize novel porphyrins and porphyrinoids, develop synthetic tools for their efficient functionalization; to explore their potential as a) components for solar energy conversion devices, b) as model systems for heme enzymes to gain insight into mechanisms of dioxygen activation and processing, c) as photosensitizers in elaborate modular carrier systems for photodynamic therapy of tumors and photodynamic inactivation of bacteria, fungi, molds, etc., d) as central parts of porphyrin-containing carbon-rich molecules and superstructures.

#### SCIENTIFIC BACKGROUND

Porphyrins are ubiquitous dyes in nature which govern the most important transformations in living organism—making them aptly named “pigments of life”.

Their inherent photophysical, photochemical, and redox properties are likely responsible for their extensive appearance in nature. In photosynthesis, porphyrins act as light harvesters in stunningly complex arrays, as electron donors in the reaction center and as electron transporting cofactors. In the respiratory chain, these cofactors play indispensable roles as dioxygen carriers, repositories



and activators, the latter essentially delivering the “energy of life” in cytochrome c oxidase. It is not surprising that huge efforts are made to better understand these vital processes, because this may lead to improved artificial solar energy conversion in terms of light—energy—gathering and water splitting. As heme enzymes catalyze very important oxidations in nature, they are also in the focus of intense pharmaceutical research. Even without looking at nature, porphyrins are fascinating molecules by themselves. They are able to form complexes with all metal ions, some half and even non-metals, often with several oxidation states available and strongly varying coordination geometries. Porphyrins act as sensitizer for singlet oxygen, thus are able to generate highly reactive species from dioxygen in the presence of light. This process, although detrimental in nature, is used in the photodynamic therapy of tumors (PDT) as well as the photodynamic inactivation of germs. The highly polarizable  $\pi$ -electron system of porphyrins, their ability to either take-up or give-up two electrons in often reversible manner offers a high potential in molecular electronics.

### RESEARCH HIGHLIGHTS

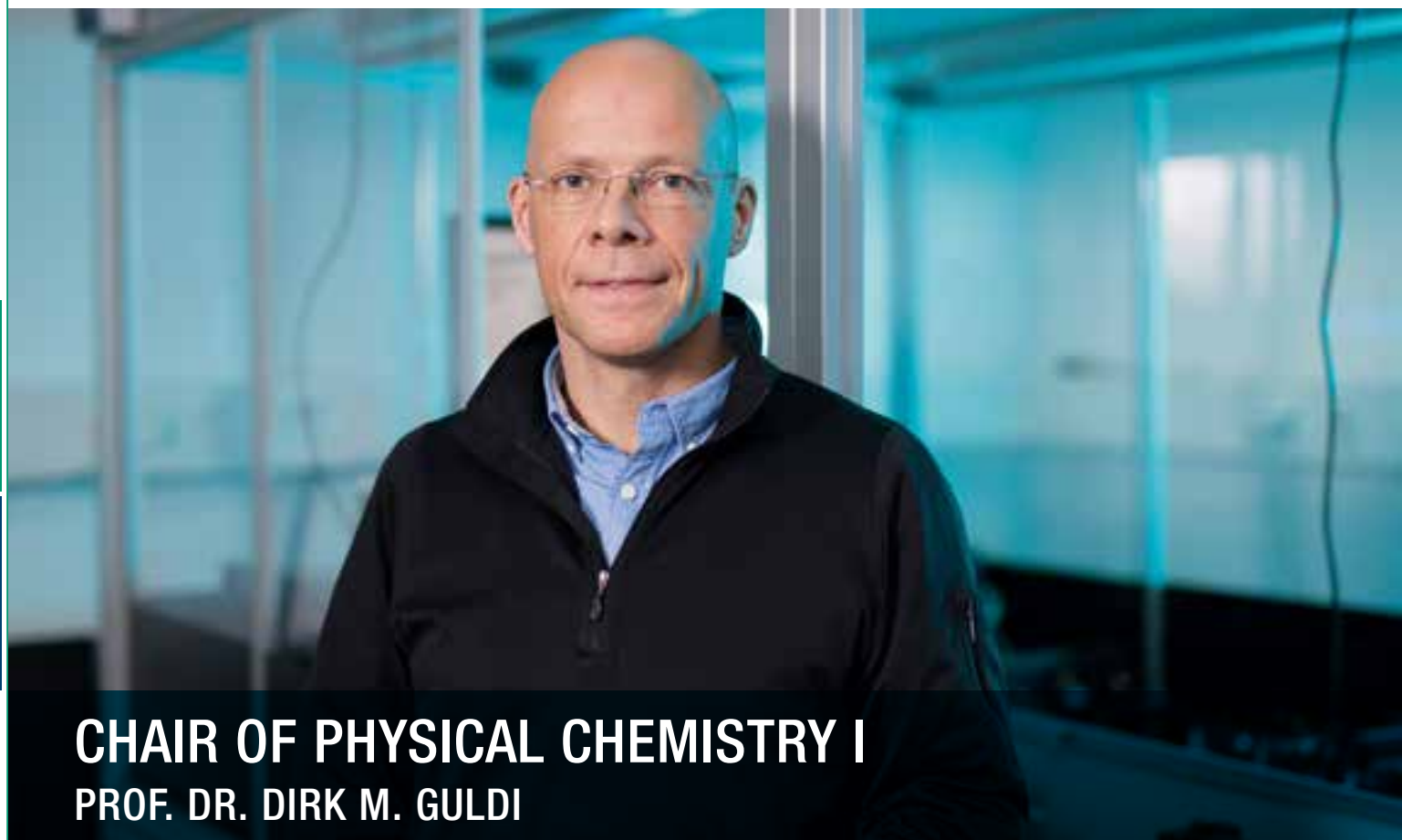
Our research is aimed at the synthesis and functionalization of porphyrins. Having the amazing properties of natural systems in mind, we prepare model compounds for, for example, enzymes, light harvesters, and reaction centers with organic chemical transformations—but we also look further into porphyrin chemistry. Recent highlights of our research are a) crown-ether appended metalloporphyrins which give deep insights into the mechanism of dioxygen activation, even under rather extreme high-pressure conditions as found for deep-sea organisms; b) antibody-conjugated modular carrier systems for the transport of photosensitizers for PDT; c) highly charged cationic and anionic metalloporphyrinoids in layer-by-layer-constructed photovoltaic devices; d) organization, metallation, and switching experiments of porphyrins on surfaces; and e) carbon-rich porphyrin conjugates containing hexa-peri-hexabenzocoronene (HBC) moieties. Our work is on the one side based on powerful organic synthetic methods and, on the other hand, highly interdisciplinary. We strongly collaborate with various groups in Erlangen within several initiatives, such as the Collaborative Research Center 953 “Synthetic carbon allotropes”, or the Bavarian project “Solar Technologies go Hybrid”.

### PERSPECTIVES

We are currently deeply involved in the preparation of porphyrins with high carbon content. Such compounds can be obtained by various approaches, such as introduction of acetylenic or polyaromatic hydrocarbon (i.e., HBC) substituents. Microwave-assisted transformations such as Diels-Alder reactions or Pd-catalyzed couplings are turning out to be more and more important. We have now established a flash-vacuum pyrolysis line where we investigate thermal reactions such as dehydrochlorinations or dehydrogenations of appropriately substituted porphyrins. We are convinced that carbon-rich porphyrins with their extended  $\pi$ -systems are ideal materials for molecular electronics and photovoltaics. We have shown that supramolecular interactions such as  $\pi$ - $\pi$ -stacking govern their structures in the crystal. Such effects may play a vital role in successful applications in the aforementioned fields.

### SELECTED PUBLICATIONS

- J. Holzwarth, K. Y. Amsharov, D. I. Sharapa, D. Reger, K. Roshchyna, D. Langerich, N. Jux, F. Hauke, T. Clark, A. Hirsch, *Angew. Chem. Int. Ed.*, **2017**, 129, 12352–12358
- D. Langerich, J. F. Hitzberger, W. Donaubaue, T. Drewello, N. Jux, *Chem. Eur. J.*, **2016**, 22, 16755–16759
- D. Langerich, D. Reger, H. Hoelzel, R. Riedel, M. M. J. C. Martin, F. Hampel, N. Jux, *Angew. Chem. Int. Ed.*, **2016**, 55, 5602–5605
- D. Langerich, J. F. Hitzberger, M. Marcia, F. Hampel, T. Drewello, N. Jux, *Angew. Chem. Int. Ed.*, **2014**, 53, 12231–12235
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- H. Maid, P. Böhm, S. Huber, W. Bauer, W. Hummel, N. Jux, H., *Angew. Chem. Int. Ed.*, **2011**, 50, 2397–2400
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- F. Rancan, M. Helmreich, A. Mölich, E. A. Ermilov, N. Jux, B. Röder, A. Hirsch, F. Böhm, *Bioconjugate Chem.*, **2007**, 18, 1078–1086
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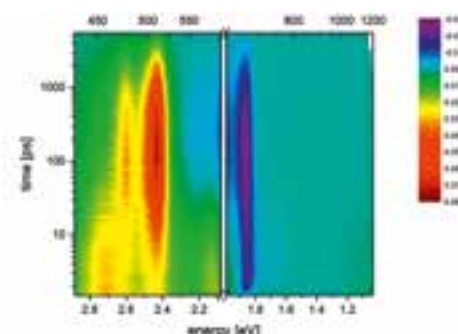
# CHAIR OF PHYSICAL CHEMISTRY I

## PROF. DR. DIRK M. GULDI

[dirk.guldi@fau.de](mailto:dirk.guldi@fau.de) • [www.chemie.fau.de/guldi](http://www.chemie.fau.de/guldi)

### CURRICULUM VITAE

- Since 2014** Member of Australian Research Council Centre of Excellence for Electromaterials Science, University of Wollongong, Australia
- Since 2013** Vice Dean for Research, Faculty of Sciences, University of Erlangen-Nürnberg, Germany
- Since 2004** University Full Professor, Chair of Physical Chemistry I at the University of Erlangen-Nürnberg, Germany
- 1995 – 2004** Faculty, University of Notre Dame, Radiation Laboratory, Notre Dame, USA
- 1992 – 1995** Researcher, Hahn-Meitner-Institute, Physical Chemistry, Berlin, Germany
- 1991 – 1992** Postdoctoral Fellow, National Institute of Standards & Technology, Gaithersburg, MD, USA
- 1988 – 1990** PhD, University of Köln, Germany



### OBJECTIVES

The research activities of the Guldi group cover the timely topic of designing, devising, synthesizing, and testing novel nanometer scale structures as integrative components for solar energy conversion including singlet fission. Nanocarbon materials are at the forefront of our studies by probing them in solution, in transparent films, and at electrode surfaces. Our experimental tools span from ultrafast spectroscopy and vibrational spectroscopy to electrochemistry and microscopy. Such conception is extremely valuable for the realization of solar energy conversion, photovoltaics, and catalytic reactivity, specifically to novel chemical and light driven systems.

### SCIENTIFIC BACKGROUND

Dirk M. Guldi is one of the world-leading scientists in the field of charge transfer/nanocarbons. In particular, he is well-known for his key contributions to the areas of charge-separation and singlet fission in molecular materials as well as the construction of nanostructured thin films for solar energy conversion. His scientific career has begun at the University of Köln, where he graduated in Chemistry (1988) and from where he received his PhD (1990). After a postdoctoral stay at the National Institute of Standards and Technology in Gaithersburg, USA (1991–1992), he took a position at the Hahn-Meitner-Institute Berlin (1992 – 1994). Following a brief stay as a Feodor-Lynen Fellow



at Syracuse University, USA, he joined the faculty of the Notre Dame Radiation Laboratory, USA (1995). Then, after nearly a decade in the USA, the University of Erlangen-Nürnberg succeeded in attracting Dirk M. Guldi back to Germany, despite major efforts by the University of Notre Dame (2004). He is among the Highly Cited Researchers based on a track record that includes around 550 publications and an H-index of 92.

## RESEARCH HIGHLIGHTS

A first highlight is that the Guldi group was among the first to demonstrate the outstanding electron acceptor properties of fullerenes in a set of donor-acceptor materials (*JACS* 1997/*Nature Chemistry* 2014) that give rise to photoinduced charge transfer events. Almost simultaneously with this pioneering work, they illustrated (*JACS* 1997) the beneficial features of fullerenes in artificial photosynthesis, that is, charge-recombination is located deep in the „inverted region“ of the Marcus parabola (*JACS* 2006/2008). This paved the way to their champion systems (*JACS* 2001/2004), in which all the primary events of photosynthesis are successfully mimicked. Impressive are the lifetimes of the spatially-separated radical ion pair states, the product of a sequence of energy and multi-step charge transfer reactions, which reach 1.6 s—a time domain that has never been accomplished so far in a molecular mimic of the photosynthetic reaction center.

The incentives for their ground-breaking work on carbon nanotubes were taken from using them as a versatile platform for charge management, namely charge transfer, charge transport, and charge storage (*Nature* 2007/*Nature Chemistry* 2014). A first breakthrough in the field of functional carbon nanotubes (*Angewandte Chemie* 2003/*Nature Chemistry* 2010) was the manifestation of an intramolecular charge transfer event triggered by light, which led to radical ion pair lifetimes in the range of several  $\mu$ s. To this end, a tremendous challenge is the characterization of radical ion pair states that involve different redox states of carbon nanotubes. Here, the Guldi group was first to succeed in establishing conclusively the spectroscopic signatures of reduced (*JACS* 2007) and oxidized forms (*Nature Chemistry* 2009) of carbon nanotubes, which evolve from donor-acceptor interactions. The outstanding tensile strength of carbon nanotubes is also notable. They realized values of  $220 \pm 40$  MPa in a revolutionary composite material (*Nature Materials* 2002).

In general, the charge separation in any of the highlighted materials has a lifespan long enough to dissipate and then utilize the charge carriers (*Chem* 2017). The Guldi group makes use of this and focuses on the systematic and molecularly controlled integration/organization of fullerenes (*Angewandte Chemie* 2000) and carbon nanotubes (*Angewandte Chemie* 2005) into photovoltaic devices, where again photo-induced charge transfer in the photoactive layers is the modus operandi as corroborated by in-situ measurements (*Nature Materials* 2009).

A more recent highlight from the Guldi group was to pioneer the field of singlet fission (PNAS 2015) by establishing a unified model for transforming spin-correlated triplets into uncorrelated pair of triplets (*Nature Communications* 2017).



## PERSPECTIVES

The major thrust of current and future work addresses the expanding global need for energy by developing a groundbreaking platform of different forms of nanocarbons to produce chemical fuels using solar energy with quantum yields of up to 200%. To advance to such a level of sophistication, future research in our group centers on constructing all nanocarbon based optoelectronic devices that make use of the unique and outstanding features of carbon allotropes ranging from fullerenes, carbon nanotubes, and carbon nanodots to carbon nanohorns and graphene, which will power the electrolytic formation of  $H_2$  and its conversion into a portable fuel-formic acid.

## SELECTED PUBLICATIONS

- B.S. Basel, J. Zirzmeier, C. Hetzer, B.T. Phelan, M.D. Krzyaniak, S.R. Reddy, P.B. Coto, N.E. Horwitz, R.M. Young, F.J. White, F. Hampel, T. Clark, M. Thoss, R.R. Tykwinski, M.R. Wasielewski, D.M. Guldi, *Nat. Commun.*, **2017**, 8, 15171
- J. Sukegawa, C. Schubert, X. Zhu, H. Tsuji, D.M. Guldi, E. Nakamura, *Nat. Chem.*, **2014**, 6, 899
- J. L. Lopez, C. Atienza, F. G. Brunetti, C. Romero-Nieto, D. M. Guldi, N. Martin, *Nat. Commun.*, **2014**, 5, 3763
- C. Ehli, C. Delsner, D. M. Guldi, A. Mateo-Alonso, M. Prato, C. Schmidt, C. Backes, F. Hauke, A. Hirsch, *Nat. Chem.*, **2009**, 1, 243

## SELECTED REVIEWS

- G. Bottari, M.A. Herranz, L. Wibmer, M. Volland, L. Rodriguez-Perez, D.M. Guldi, A. Hirsch, N. Martin, F. D'Souza, T. Torres Chemical Functionalization and Characterization of Graphene-Based Materials, *Chem. Soc. Rev.*, **2017**, 46, 4464
- G. Bottari, G. de la Torre, D. M. Guldi, T. Torres, Covalent and Noncovalent Phthalocyanine Carbon Nanostructure Systems: Synthesis, Photoinduced Electron Transfer, and Application to Molecular Photovoltaics, *Chem. Rev.*, **2010**, 110, 6768

## SELECTED AWARDS

- 2015 Richard E. Smalley Research Award (Electrochemical Society)
- 2013 ECS Fellow (Electrochemical Society)
- 2013 Honary Professorship (Xi'an Jiaotong University, China)
- 2013 RSC Fellow (Royal Society of Chemistry)
- 2010 Editorial Board Award (Royal Society of Chemistry)
- 2009 Elhuyar-Goldschmidt Award (Royal Spanish Chemical Society)



## PROFESSOR OF PHYSICAL CHEMISTRY

### PROF. DR. THOMAS DREWELLO

thomas.drewello@fau.de • [www.chemie.fau.de/drewello](http://www.chemie.fau.de/drewello)

#### CURRICULUM VITAE

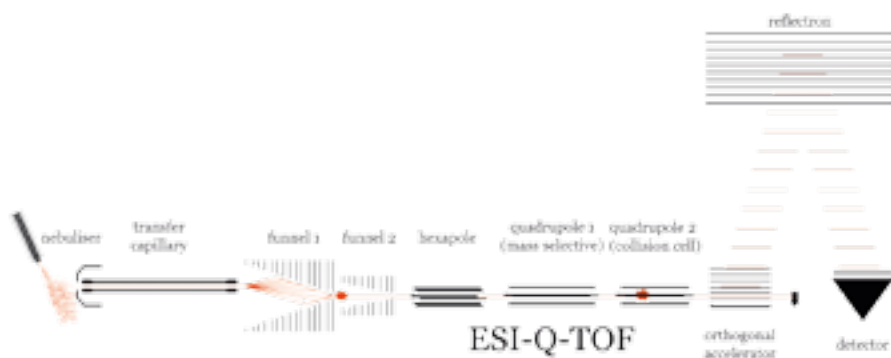
**Since 2008** University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany  
**1995 – 2007** Associate Professor at the University of Warwick, Great Britain  
**1990 – 1995** Researcher, Hahn-Meitner-Institute, Berlin, Germany  
**1989 – 1990** Postdoctoral Fellow, University of Amsterdam, Netherlands  
**1989** PhD, Technische Universität Berlin, Germany

#### OBJECTIVES

Research in this group is concerned with the development of mass spectrometry-based methods for the improved characterization of modern materials. Investigations into the mechanisms of gentle ionisation methods such as (Matrix-assisted) laser desorption / ionisation [(MA)LDI] and Electrospray ionisation [ESI] are essential in this context. Of major interest is the behaviour of cluster ions in the gas phase, which involves the production, reactivity (kinetic) and thermochemistry of different types of clusters, ranging from the loosely bound, van der Waals-type to strongly connected, covalent architectures. Modern mass spectrometry is developed and applied partly as an analytical tool and partly as a reaction vessel for the elucidation of geometries, energetics and reactivities of gas-phase species, aiming at the translation of these findings into the macroscopic world.

#### SCIENTIFIC BACKGROUND

Our research activities have always employed mass spectrometry as a tool in one form or another. Early investigations focussed on the use of large-scale multi-sector instrumentation for the study of the fragmentation behaviour of organic and organometallic species. The emphasis in these studies was on the thermochemical requirements connected with the formation of multiply charged ions in the gas phase and on the elucidation of metal-induced reactivity. We have been also involved with the application of synchrotron radiation to strictly single-photon-ionisation, studying inner shell excitation of different types of clusters and obtaining ionisation and appearance energies. The more recent activities focussed on reactivity studies of size-selected metal clusters with small molecules. For these investigations a metal cluster source was coupled with Fourier transform-ion cyclotron resonance (FT-ICR) mass spectrometry. We have also developed interest in the area of laser desorption / ionisation



both as an approach towards gentle ion formation and as a means to fuse and aggregate tailor-made precursors into larger architectures. Further recent interest is in on mechanistic aspects of electrospray-based ionisation. Current instrumentation is mainly based on quadrupole, time-of-flight and ion trap technologies.

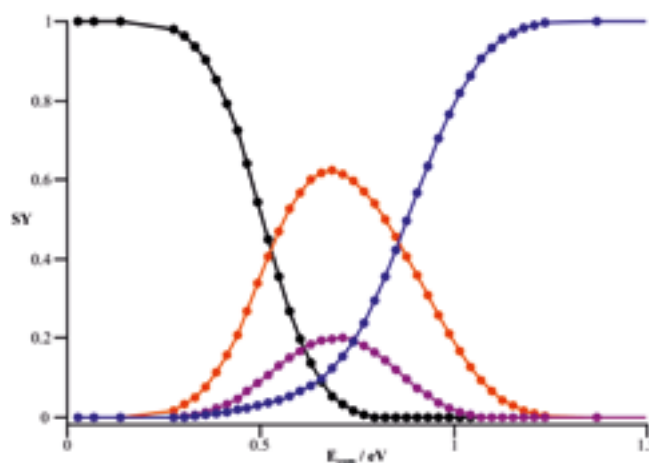
### RESEARCH HIGHLIGHTS

SFB 953 on New Synthetic Carbon Allotropes has greatly fostered the close collaborative research with the groups of K.Y. Amsharov, T. Clark, A. Görling, D.M. Guldi, A. Hirsch, N. Jux, M. Kivala, R.R. Tykwinski and others. Some of the resulting research highlights include:

- Introduction of Laser desorption / ionisation as a means to investigate the covalent bonding of porphyrins to graphene
- Comprehensive gas-phase investigation of the “carbyne”-like polyynes, cumulenes and their rotaxanes
- Formation and characterization of  $\pi$ -extended porphyrin-based systems
- Characterization of “electrospray-silent” metallo-porphyrins and-phthalocyanines through attachment of the formate anion
- Host / guest-chemistry: research into the noncovalent bonding between fullerenes and N-heterotriangulenes
- Formation and fragmentation dynamic of multiply charged true molecular anions of fluorofullerenes
- Laser-induced formation of fullerenes from strategically structured, non-fullerene precursor materials
- Application of electrospray as a means to produce large cluster ions from both molecular and salt-like building blocks

### PERSPECTIVES

Future activities will focus on the investigation of different carbon allotropes, elucidating their properties and reactivity by laser- and spray-based methods, with emphasis on affinities and interconversion. Of interest is the elucidation of bond and dissociation energies of ion / neutral and supramolecular complexes. The development of energy-dependent collision experiments will be of central importance in this context.



Future investigations will also focus on the formation and characterization of structure and reactivity of different types of clusters. We aim to promote electrospray as a method for cluster production.

Laser desorption / ionisation will be applied in device manufacturing for the elucidation of degradation processes.

### SELECTED PUBLICATIONS

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- I.D. Kellner, U. Hahn, T. Torres, T. Drewello, *J. Phys. Chem. A*, **2018**, 122, 6, 1623–1633
- D. Dasler, R.A. Schäfer, M.B. Minameyer, J.F. Hitznerberger, F. Hauke, T. Drewello, A. Hirsch, *J. Am. Chem. Soc.*, **2017**, 139, 34, 11760–11765
- J.F. Hitznerberger, P. Dral, U. Meinhardt, T. Clark, W. Thiel, M. Kivala, T. Drewello, *ChemPlusChem*, **2017**, 82, 2, 204–211
- D. Lungerich, J.F. Hitznerberger, W. Donaubaue, T. Drewello, N. Jux, *Chem. Eur. J.*, **2016**, 22, 47, 16754–16758
- I.D. Kellner, M.S. von Gernler, M.D. Tzirakis, M. Orfanopoulos, T. Drewello, *J. Phys. Chem. C*, **2016**, 120, 1, 786–792
- I.D. Kellner, U. Hahn, M. Duerr, T. Torres, I. Ivanovic-Burmazovic, T. Drewello, *J. Phys. Chem. A*, **2015**, 119, 46, 11454–11460
- R.W. Kirschbaum, D. Prenzel, S. Frankenberger, R.R. Tykwinski, T. Drewello, *J. Phys. Chem. C*, **2015**, 119, 5, 2861–2870
- R.W. Kirschbaum, M. Hausmann, O.V. Boltalina, S.H. Strauss, T. Drewello, *Phys. Chem. Chem. Phys.*, **2015**, 17, 35, 23052–23058
- D. Lungerich, J.F. Hitznerberger, M. Marcia, F. Hampel, T. Drewello, N. Jux, *Angew. Chem. Int. Ed.*, **2014**, 53, 45, 12231–12235





## PROFESSOR OF PHYSICAL CHEMISTRY

### PROF. DR. CAROLA KRYSCHI

carola.kryschi@fau.de • [www.chemie.nat.fau.de/person/carola-kryschi](http://www.chemie.nat.fau.de/person/carola-kryschi)

#### CURRICULUM VITAE

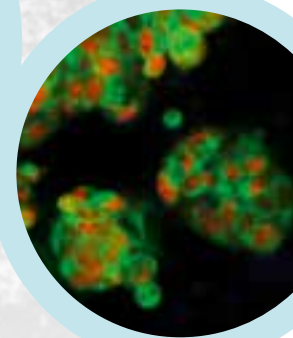
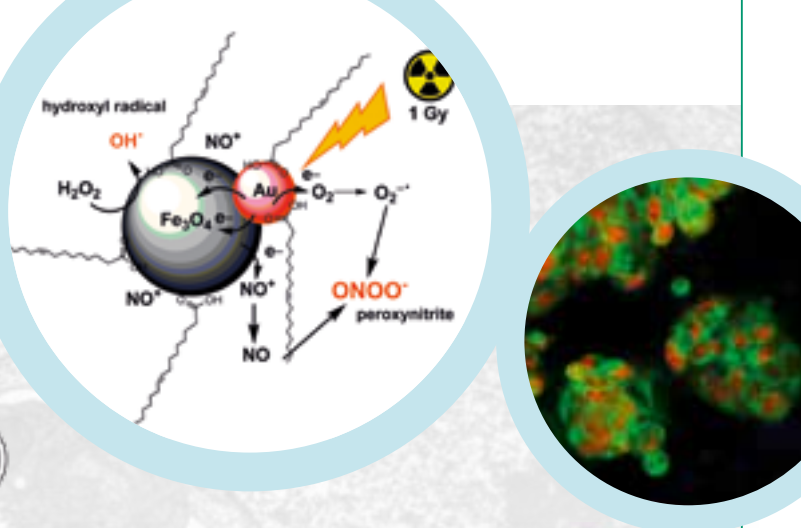
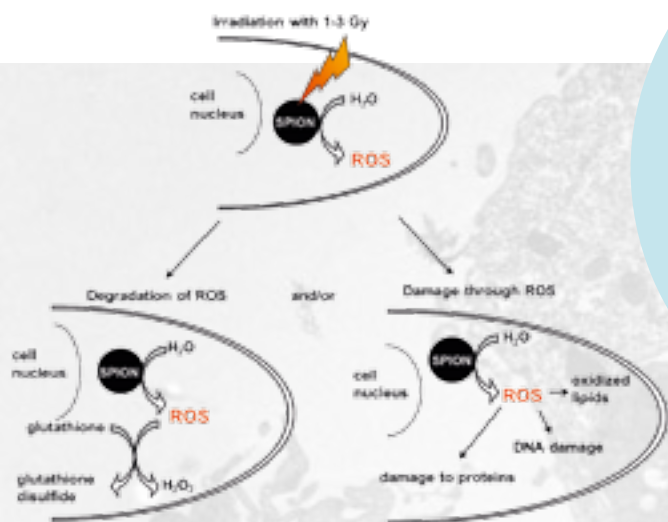
- Since 2000** University Professor, Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 1994 – 2000** Assistant Professor, Department of Experimental Physics (Solid-State Spectroscopy) at the University of Düsseldorf, Germany
- 1993** Habilitation in Experimental Physics: “Relaxation Dynamics in Molecular Crystals”
- 1988 – 1993** Assistant lecturer at the Department of Experimental Physics, University of Düsseldorf, Germany
- 1987** Postdoctoral Fellow, Department of Chemistry at Stanford University, USA
- 1983 – 1986** PhD, Institute of Physical Chemistry at the University of Düsseldorf, Germany

#### OBJECTIVES

Actual research activities of Carola Kryschi's work group are focused on tumor-targeted magnetoplasmonic Janus nanoparticles which serve as multifunctional nanotherapeutics for synergistic cancer therapies comprising X-ray radiation therapy and hyperthermia. An additional research objective is the development of luminescent gold nanocluster (AuNC) with adjustable sizes and defined surface structures, tailored for applications as transfection reagent in gene therapy. Other research efforts are devoted to the design of surface-stabilized complex metal oxide nanocomposites for photocatalysis as well as are directed to engineering of noble metal nanostructures for optoelectronic applications (e.g. nanolaser).

#### SCIENTIFIC BACKGROUND

Carola Kryschi began her scientific carrier in 1987 with a postdoctoral stay at Stanford University, USA (1987), where she achieved expertise on ultrafast laser spectroscopy techniques. Starting 1988 as assistant lecturer and continuing after postdoctoral lecture qualification (1993) as assistant professor at the Department of Experimental Physics of the University of Düsseldorf she focussed her research activities on studies of ultrafast excited-states relaxation dynamics, tautomerization reactions and phase transitions in molecular crystals and thin polymer films using ps resolving transient grating and photon echo spectroscopy. In cooperation with Prof. H.-D. Martin (University of Düsseldorf) and Prof. H.-P. Trommsdorff (UJF Grenoble) she successfully carried out a research project on optical switches in liquid and solid phase which are based on photochromic



dithienylethene compounds. An additional cooperation project with H.-D. Martin yielded the realization of nonlinear optical probes (hemicyanine dyes) suited for direct detection of cell membrane potential changes in living cells were successfully developed. Since 2000 she is Professor of Physical Chemistry at the University of Erlangen-Nürnberg.

## RESEARCH HIGHLIGHTS

One research highlight was the successful realization of molecular optical switches built on dithienylethene which reversibly operate on the picosecond scale by switching between a transparent and coloured state as well as allow switching on and off the emission of an attached fluorophore (J. Phys. Chem. 2001).

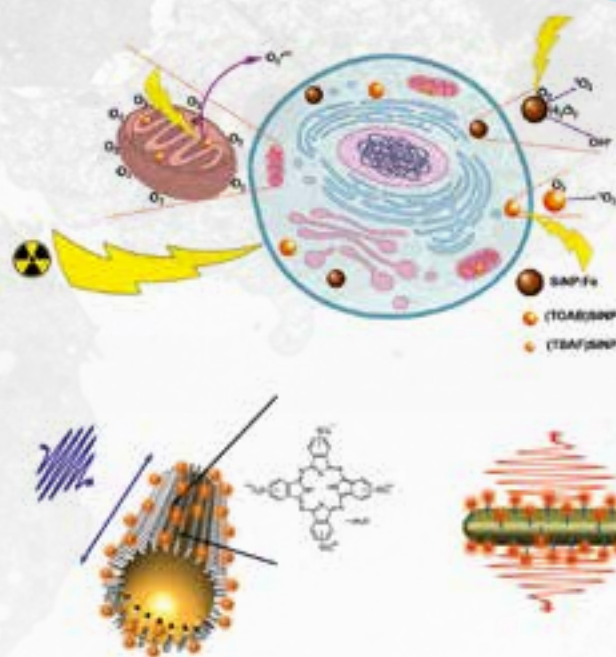
In cooperation with Evonik Industries AG we developed a two-step procedure enabling for the first time the fabrication of surface stabilized, oxide-free luminescent silicon quantum dots (EP 2 067743 A1) which were shown to function as transfection reagent for siRNA (BBRC 2009) that initiated RNAi mediated specific gene suppression.

Another actual research project is directed to the development of plasmonic nanolasers based on gold nanostructures (Condens. Matter 2017).

In an actual cooperative research project with departments of FAU's Faculty of Medicine, we are engineering surface-modified silicon clusters, tumor-targeted superparamagnetic iron oxide nanoparticles and magnetoplasmonic Janus nanoparticles that act as X-ray enhancer for low-dose radiation therapy (BBRC 2012, BBRC 2013, J. Phys. Chem. B 2014).

## PERSPECTIVES

Our future research activities are focused onto functionalized noble metal, metal oxide and semiconductor clusters, quantum dots and nanoparticles that are tailored for catalysis, optoelectronic or medical application. We will develop novel wet-chemistry recipes for the facile and sophisticated synthesis techniques for the inexpensive preparation of water-soluble luminescent silver and gold nanocluster being suited for applications in nanomedicine and photocatalysis. Actually we elaborate novel synthesis routes for multifunctional magnetoplasmonic Janus nanoparticles that may act as synergistic nano-platforms for radiation therapies of tumors.



## SELECTED PUBLICATIONS

- H.-P. Solowan, Carola Krysch, Facile Design of a Plasmonic Nanolaser, *Condens. Matter*, **2017**, 2, 8
- J. Hübner, M. Klumünzer, M. Comet, C. Martin, L. Vidal, M. Schäfer, C. Krysch, D. Spitzer, *Combustion and Flame*, **2017**, 184, 186–194
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- S. Klein, A. Sommer, L.V. R. Distel, J.-L. Hazemann, W. Kröner, W. Neuhuber, P. Müller, O. Proux, C. Krysch, *J. Phys. Chem. B*, **2014**, 118, 6159–6166
- Y. Xie, L. Carbone, C. Nobile, V. Grillo, S. D'Agostino, F. Della Sala, C. Giannini, D. Altamura, C. Oelsner, C. Krysch, P. D. Cozzoli, *ACS Nano*, **2013**, 7, 7352–7369
- A. Sommer, C. Cimpean, M. Kunz, C. Oelsner, H. J. Kupka, C. Krysch, *J. Phys. Chem. C*, **2011**, 115, 22781–22788
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- C. Rusu, H. Lanig, O. Othersen, C. Krysch, T. Clark, *J. Phys. Chem. B*, **2008**, 112, 8, 2445–2455
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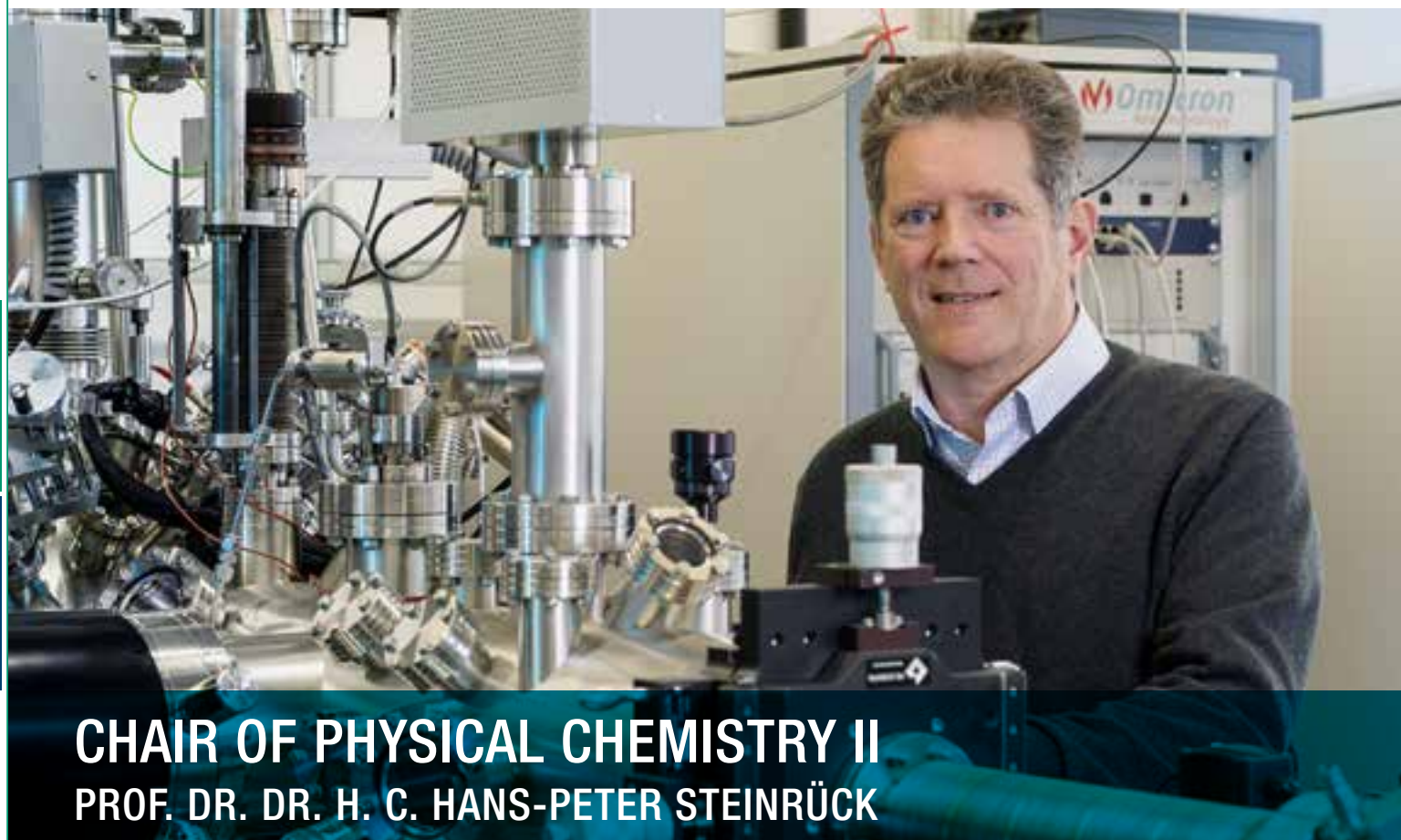
## SELECTED REVIEWS

- C. Cimpean, V. Groenewegen, V. Kuntermann, A. Sommer, C. Krysch, Ultrafast Exciton Relaxation Dynamics in Silicon Quantum Dots, *Laser & Photon. Rev.*, **2009**, 1

## SELECTED AWARDS

- 1989 Benningsen-Foerder (NRW) Award





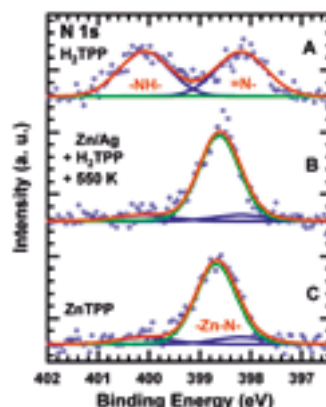
## CHAIR OF PHYSICAL CHEMISTRY II

### PROF. DR. DR. H. C. HANS-PETER STEINRÜCK

[hans-peter.steinrueck@fau.de](mailto:hans-peter.steinrueck@fau.de) • [www.chemie.fau.de/steinrueck](http://www.chemie.fau.de/steinrueck)

#### CURRICULUM VITAE

- Since 1998** University Full Professor, Chair of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 1994 – 1998** Associate Professor of Experimental Physics at the University of Würzburg, Germany
- 1993** Visiting Scientist at Rutgers University, USA
- 1992** Habilitation in Experimental Physics, Technical University of Munich, German
- 1985 – 1986** Postdoctoral Fellow, Department of Chemical Engineering, Stanford University, USA
- 1985** Dr. tech, Graz University of Technology, Austria
- 1983** Dipl.-Ing. in Technical Physics at Graz University of Technology, Austria



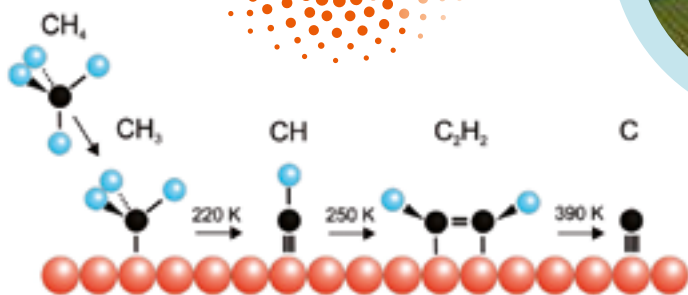
#### OBJECTIVES

The mission of the Chair of Physical Chemistry II is to provide an optimum of environment to perform surface and interface science at the highest possible level and to create an attractive and international competitive atmosphere for researchers at all stages of their career, from B.Sc., M.Sc. and PhD students to postdocs and junior group leaders. The research activities follow an interdisciplinary approach with numerous local, national and international cooperations with colleagues in physics, chemistry, chemical engineering, and materials science, which are documented in collaborative research projects and publications. Specific emphasis lays also on the education of undergraduate students, on lectures, seminars, and lab-courses.

#### SCIENTIFIC BACKGROUND

Surfaces are the outer boundary of any condensed material. They dominate the interaction with the environment and play a decisive role in numerous natural and technological processes, ranging from heterogeneous catalysis, sensor technology and nano-technology to modern material science. Our activities focus in the area of surface and interface science with main research interests in: 1) Development of new materials with novel electronic, geometric and chemical properties, 2) Investigation of elementary steps of surface reactions, and 3) Construction of advanced scientific apparatus. These studies aim at a fundamental physical and chemical understanding of the mechanisms and processes involved, at an atomic level. For these





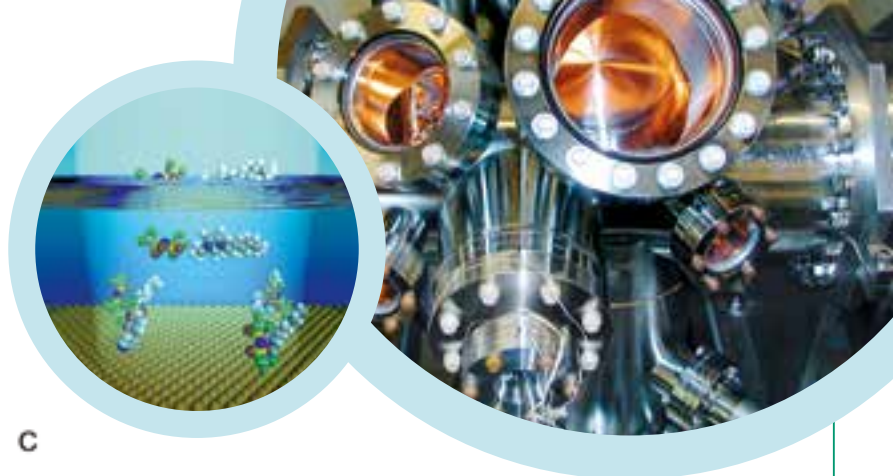
investigations a large variety of experimental methods is applied, including synchrotron radiation-based photoelectron spectroscopy, scanning electron and scanning tunneling microscopy, and molecular beam methods.

### RESEARCH HIGHLIGHTS

Our activities cover a number of different highlight topics: “*Surface Science with porphyrins*” pays specific attention to the synthesis of metallo-porphyrinoids by in-situ metallation on a surface, their formation of supramolecular networks, their internal conformation, their electronic interaction with the supporting substrates and the adsorption of small molecules at their metal center. “*Surface Science with Ionic Liquids*” addresses the systematic study of their surface composition, of enrichment effects and the chemical reactivity of dissolved transition metal complexes. “*Liquid alloy catalyst systems*” aim at a more efficient use of precious metals. The “*Chemical modification of graphene*” addresses different routes to functionalize graphene supported on metal substrates. Our “*In-situ studies of surface reactions*” aim at the investigation of processes in-situ on timescales down to 1 sec by high-resolution XPS or at pressures up to 1 mbar. And finally, “*Ultrathin metal, alloy and oxide films*” deal with the preparation of such systems and the systematic variation of their electronic, geometric, and chemical properties.

### PERSPECTIVES

Based on the achieved detailed understanding of simple model systems one of our future goals is to address more complex systems to bridge different gaps, which are present challenges in the science of solid / gas, liquid / gas and solid / liquid interfaces. The “*pressure gap*” concerns model conditions in ultrahigh vacuum systems vs. real world catalysis, the “*materials gap*” defect free single crystal surfaces vs. nanoparticles with facets, kinks and steps, and finally the “*communication gap*” stands for the difficulties one faces when new interdisciplinary collaborations are initiated. In addition, one major driving force is to continue our thorough investigations at the highest experimental level to obtain insight in the fundamental aspects of physical and chemical processes occurring at the surfaces and interfaces of solids and liquids.



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- N. Taccardi, M. Grabau, J. Debuschewitz, M. Distaso, M. Brandl, R. Hock, F. Maier, C. Papp, J. Erhard, C. Neiss, W. Peukert, A. Görling, H.-P. Steinrück, P. Wasserscheid, *Nat. Chem.*, **2017**, 9, 862–867
- D. Fantauzzi, S. Krick Calderón, J. E. Mueller, M. Grabau, C. Papp, H.-P. Steinrück, T. P. Senftle, A. C. T. van Duin, T. Jacob, *Angew. Chem. Int. Ed.*, **2017**, 56, 2594–2598
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- J. M. Gottfried, K. Flechtner, A. Kretschmann, T. Lukaszczuk, H.-P. Steinrück, *J. Am. Chem. Soc.*, **2006**, 128, 5644–5645

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- H.-P. Steinrück, P. Wasserscheid, Ionic Liquids in Catalysis, *Catalysis Lett.*, **2015**, 145, 380–397
- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, Liquid Organic Hydrogen Carriers: Surface Science Studies of Carbazole Derivatives, *Chem. Rec.*, **2014**, 14, 879–896
- H. Marbach, H.-P. Steinrück, Studying the dynamic behaviour of porphyrins as prototype functional molecules by scanning tunnelling microscopy close to room temperature, *Chem. Commun.*, **2014**, 50, 9034–9048
- C. Papp, H.-P. Steinrück, In-situ high-resolution X-ray photoelectron spectroscopy—Fundamental insights in surface reactions, *Surface Science Reports*, **2013**, 68, 446–487
- H.-P. Steinrück, Recent developments in the study of ionic liquid interfaces using X-ray photoelectron spectroscopy and potential future directions, *Phys. Chem. Chem. Phys.*, **2012**, 14, 5010–5029

### SELECTED AWARDS

- 2017 AVS Medard W. Welch Award, USA
- 2016 Fellow of the American Association for the Advancement of Science
- 2016 Member of the German National Academy of Sciences Leopoldina
- 2016 ERC Advanced Grant
- 2015 Doctor Honoris Causa, University of Szeged, Hungary
- 2015 Corresponding Member of Austrian Academy of Sciences
- 2013 Fellow of the American Physical Society
- 2012 Member of Academia Europaea-The Academy of Europe
- 2009 Guest Professor, University of Science and Technology of China



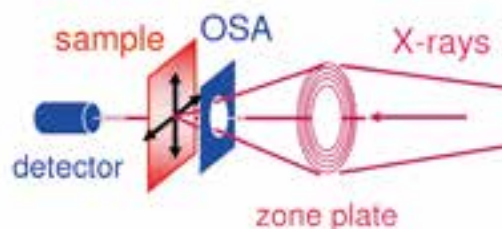
## PROFESSOR OF PHYSICAL CHEMISTRY

### PROF. DR. RAINER FINK

rainer.fink@fau.de • [www.chemie.fau.de/fink](http://www.chemie.fau.de/fink)

#### CURRICULUM VITAE

- Since 2002** University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 1993 – 2002** Researcher at the University of Würzburg (Prof. Umbach), Germany
- 1992 – 1993** Postdoctoral Fellow, Uppsala Universitet, Sweden
- 1992** PhD in Experimental Physics at the University of Konstanz (Prof. Schatz), Germany



#### OBJECTIVES

We aim for the spectroscopic and microscopic characterization of organic-based nanostructures, hybrid materials and thin films mainly using x-ray based analytical tools. The understanding of structure-property relationships is essential to improve organic electronic devices. High-resolution electron spectroscopy and x-ray microscopy offer insight into the electronic properties, electronic excitations, intra- and intermolecular interactions in controlled organic structures or molecules and molecular magnets or the nanoscopic structure of hybrid materials or keratin-based biomaterials.

#### SCIENTIFIC BACKGROUND

Ultrathin organic films are widely used in various fields, from, e.g., protective polymer films to active layers in organic electronic devices. Their electronic properties largely depend on the micro- and

nanostructure, which may be controlled by preparation conditions or interfacial interactions. We have explored the fundamental growth properties of organic thin films and their electronic structure from the submonolayer regime to thicker films. The impact of intermolecular interactions and the coupling to various substrate materials has been studied in detail. In particular, the initial growth process controls the formation of microcrystalline domains. High-resolution NEXAFS spectroscopy offers detailed insight into the intramolecular excitations and electronic relaxation effects when comparing the condensed and gas phases. In favourable cases, the coupling of core electron excitations to vibronic modes can be monitored. Structure-property relationships become particularly important in organic electronic devices like, e.g., organic field-effect transistors or bulk heterojunction solar cells. Soft x-ray spectroscopies may shine light

onto the chemical and electronic properties. Present soft x-ray microspectroscopes extend the superior spectroscopic fingerprint behaviour of NEXAFS to ultimate spatial resolutions and thus offer the chance to investigate more complex structures like multinary materials, polymer blends and hybrid or composite materials.

## RESEARCH HIGHLIGHTS

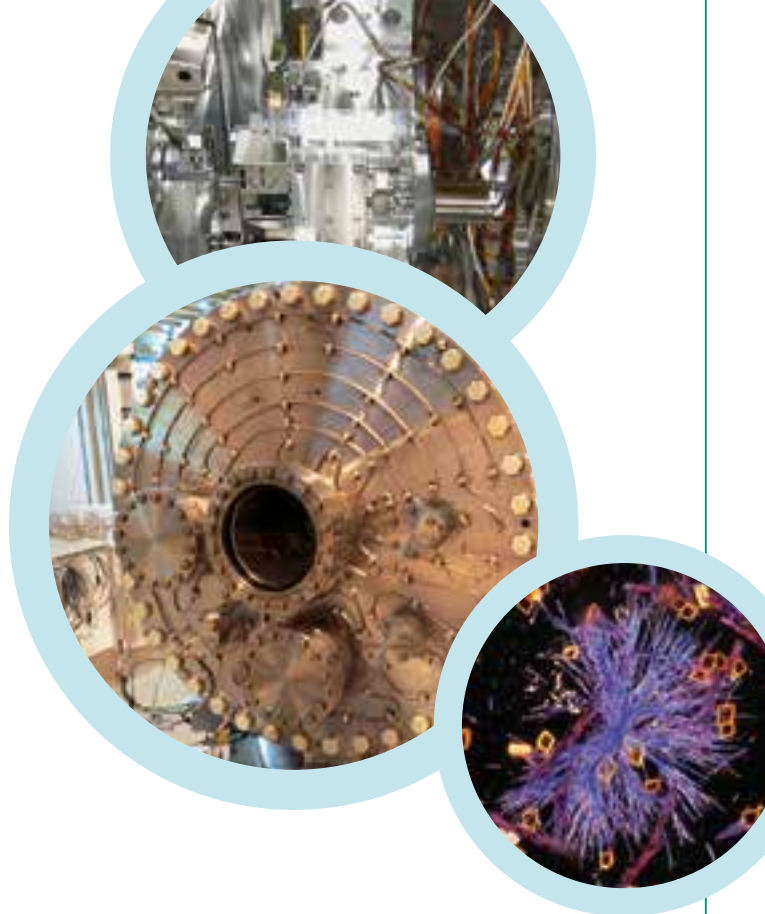
The delicate balance of lateral and vertical forces is crucial for the controlled growth of organic thin films on solid substrates. We were extending our long-standing experience in the field substrate-induced film growth on single-crystalline metal substrates to inert substrates like Si<sub>3</sub>N<sub>4</sub> and epitaxial MgO films on Ag(100). In these cases the influence of the substrate significantly reduces thus promoting 3D growth rather than ideal layer-by-layer growth modes. It turned out that MgO is extremely sensitive to intense soft x-ray or electron illumination. In particular in the presence of low partial pressures of water, unknown superstructures or nanostructures are formed.

Using scanning x-ray transmission microspectroscopy (STXM) a variety of different topics have been addressed and studied in detail. E.g., in spherical microparticles stabilized by a polyvinyl alcohol network may serve as gas micro-containers with potential applications in medical analysis and drug delivery. STXM could offer direct insight into the microbubbles to proof the gas enclosure. In some cases we were able to monitor the chemical changes within the shell thus enabling gas permeation. In addition, we analyzed the size and chemical modifications of thermoresponsive materials (e.g., hydrogels or phase-change materials).

Microspectroscopic thin film analysis focuses on the investigation of functional organic materials like, e.g., pentacene-based organic field-effect transistors. Using the local NEXAFS probe we were able to correlate the microstructure within the active channel of an OFET with the charge transport behaviour while the device is operated. Thus, we obtained detailed insight into the modification of the electronic levels in the on- and off-state of the device. Recent nano-spectroscopic studies on bulk-heterojunction (BHJ) solar cells allowed us to correlating the impact of NIR sensitizers to the nano-morphology and consequently the solar cell performances.

## PERSPECTIVES

There are few ongoing technological developments to improve the resolution in x-ray microspectroscopy. Recent improvements in Fresnel zone plate fabrication allows us to use x-ray optics with resolutions in the regime of 10 nm and thus opens a new ground for STXM analysis: In parallel coherent diffraction imaging is becoming an important tool in nanoanalysis. Implementation of such techniques into existing zone-plate scanning microscopes will provide access to the phase thus allowing more evolved image reconstruction techniques (ptychography). The availability of these novel tools will open new aspects in elemental or chemical imaging also in fields beyond fundamental sciences. We have started some new activities in the field of energy materials, cultural heritage specimens, keratin-based microfibers (human hair, wool, carpet fibers) or biodegradable functional materials.



Conventional preparation of organic thin films has shown significant drawbacks with respect to defect densities within the film. This is due to the diffusion-limited growth for deposition on solid substrates often leading to polycrystalline or microdomain films, specifically for vacuum deposited films. Recently, we have started to prepare extended single-crystalline organic films with crystal thicknesses of few monolayers only. We employ molecular self-organization at the liquid-liquid interface under well-controlled conditions. Again, the balance of lateral and vertical interactions is crucial to obtain single domain films on the size of 1 cm<sup>2</sup>. Significant reduction of defect densities lead to substantial improvement in charge-carrier mobilities in thus prepared OFETs.

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- R. Fink, Chr. Hub, G. Tzvetkov, Zone-plate based nanospectroscopy with soft x-rays at the SLS, *Acta Physica Polonica*, **2009**, A 115, 462 – 466
- J. Raabe, R. Fink, G. Tzvetkov, U. Flechsig, M. Böge, A. Jaggi, B. Sarafimov, C. Quitmann, M. Heuberger-Vernooij, T. Huthwelker, H. Ade, D. Kilcoyne, T. Tylliszczak, PolLux: A new Beamline for Soft X-Ray Spectromicroscopy at the SLS, *Rev. Sci. Instrum.*, **2008**, 79, 113704





## PROFESSOR OF PHYSICAL CHEMISTRY

### PROF. DR. JÖRG LIBUDA

joerg.libuda@fau.de • [www.chemie.fau.de/libuda](http://www.chemie.fau.de/libuda)

#### CURRICULUM VITAE

- Since 2005** University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 1996 – 2005** Group Leader, Department of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft (MPG), Berlin, Germany
- 2003** Habilitation, Humboldt University of Berlin, Germany
- 1998 – 1999** Postdoctoral Fellow, Department of Chemistry, Princeton University, USA
- 1996** PhD, Ruhr-University of Bochum, Germany

#### OBJECTIVES

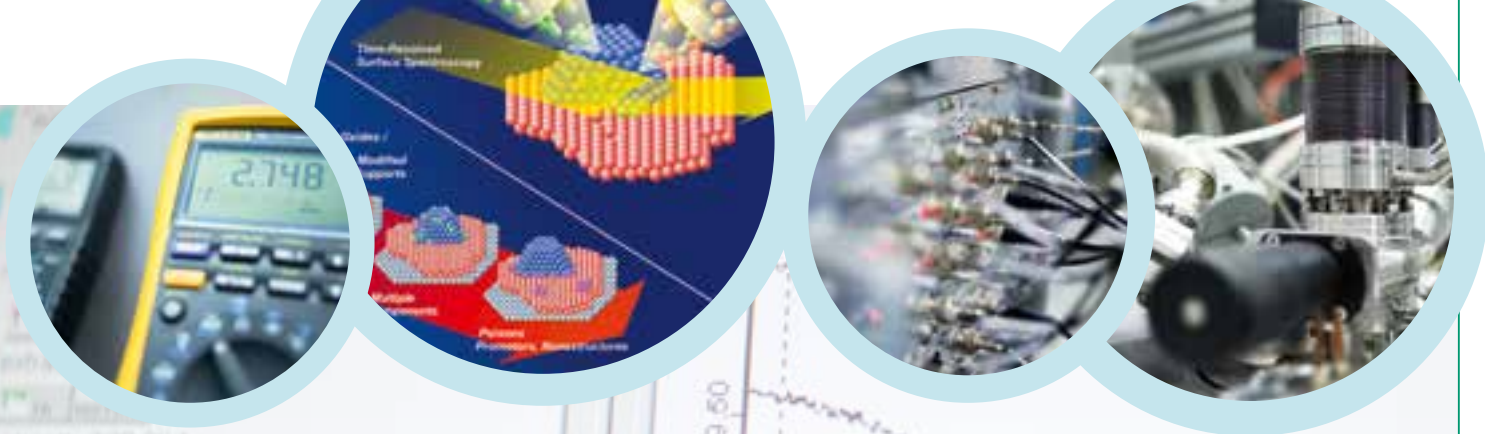
Chemical reactions and physical processes at complex surfaces play a pivotal role in many areas of today's technology. Towards a better understanding of the underlying physical and chemical phenomena at the microscopic level, we develop and investigate complex nanostructured model surfaces. Mechanisms, dynamics, and kinetics of chemical reactions on these models are probed using time-resolved in-situ und operando spectroscopies from ultrahigh vacuum up to atmospheric pressure and under electrochemical conditions. Thus, our work aims at linking fundamental surface science approaches to applied research.

#### SCIENTIFIC BACKGROUND

Heterogeneous catalysis, environmental and energy technology, materials science and nanotechnology: these are only few examples of central areas of 21<sup>st</sup> century technology, where surface and inter-

face reactions play a key role. A brief look at current research on related processes reveals, however, a quite surprising fact: The underlying chemistry is only poorly understood in most cases. This lack of knowledge is not just disappointing from a purely academic point of view. In fact, it also prevents any rational improvement and development in the corresponding fields.

The reasons for the limited insight into 'real life' surface and interface reactions become obvious if we have a closer look at the related chemical systems and environments. As an example, let us focus on the field of heterogeneous catalysis. Catalyst materials are highly complex multi-component mixtures with chemical properties sensitively depending on their particular nanostructure and composition. In catalyst development, these dependencies are vital, as they allow empirical optimization of catalytic performance. From a fundamental research point of view, however, the complexity of materials is fatal with respect to a microscopic level understanding. Here, our strategy



relies on the development of model systems, which allow us to simulate certain complex features of real systems under well-controlled conditions, simultaneously providing a maximum of structural and chemical control. Mechanistic and kinetic information is obtained on these model systems using state-of-the-art surface spectroscopies. This information can then be transferred to the real world application, where it may potentially inspire future improvements.

### RESEARCH HIGHLIGHTS

All current projects of our research group are embedded into interdisciplinary cooperations with research groups in chemistry, physics, theory, materials science, chemical engineering, or industry. In current projects in energy-related catalysis we investigate, for instance, electrochemical and heterogeneously catalyzed hydrogen storage and release with a special focus on a lower demand for critical materials such as noble metals. Together with partners from academia and industry we develop model systems to explore the fundamental surface chemistry of such materials using a surface science approach and transfer this knowledge to realistic materials and environments, i.e., ambient pressure and electrochemically controlled conditions. Here, we use not only in-house experiments, such as molecular beam techniques and time-resolved surface IR spectroscopy, but also synchrotron-radiation based methods. In the DFG Research Unit “funCOS”, an interdisciplinary team from chemistry, physics and engineering, we study the fundamental properties of organic thin films on oxide surfaces, systems that are used in molecular electronics, solar cells, or catalysis. Further projects aim at materials for energy conversion and storage, such as Liquid Organic Hydrogen Carriers, photoelectrochemical energy storage in organic molecules, and at novel concepts in catalysis, such as ionic-liquid-based model catalysis and material synthesis. For instance, we develop new ionic liquid model catalysts following a surface science approach. Such model systems provide insights into the interfacial chemistry of ionic liquid films at an unprecedented level of detail.

### PERSPECTIVES

The group is involved in several new activities, most of them emerging at the interface between fundamental sciences and engineering. A special focus is on the development of spectroscopic methods that directly link fundamental surface science and model catalysis to studies under realistic conditions and on real materials. To this aim a new facility for time-resolved in-situ and operando

spectroscopy has been set up within the Excellence Cluster Engineering of Advanced Materials. So-called operando methods combine measurements of catalytic activity with spectroscopic investigations performed at the same time. Currently, new spectroscopy facilities are developed to study atomically well-defined liquid-solid interfaces under electrochemically controlled conditions. In a unique fashion, these methods allow us to link scientific results obtained under ideal surface-science conditions to model studies on complex surfaces and, finally, to real-life catalysts. Such spectroscopic links close the often-cited gap between model studies and applied research and provide mechanistic insights that help to develop new catalytic systems at a knowledge-driven basis.

### SELECTED PUBLICATIONS

- T. Xu, T. Waehler, J. Vecchietti, A. Bonivardi, T. Bauer, J. Schwegler, P. S. Schulz, P. Wasserscheid and J. Libuda, Gluing ionic liquids to oxide surfaces: Chemical anchoring of functionalized ionic liquids by vapor deposition onto cobalt(II) oxide, *Angew. Chem. Int. Ed.*, **2017**, 56, 9072
- Y. Lykhach, S. M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvořák, V. Johánek, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolín, K. M. Neyman, J. Libuda, Counting electrons on catalyst nanoparticles, *Nat. Mater.*, **2016**, 15, 284
- A. Bruix, Y. Lykhach, I. Matolínová, A. Neitzel, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčíková, J. Mysliveček, K. C. Prince, S. Bruyère, V. Potin, F. Illas, V. Matolín, J. Libuda, K. M. Neyman, *Angew. Chem. Int. Ed.*, **2014**, 53, 10531–10535
- M. Kusche, F. Enzenberger, S. Bajus, H. Niedermeyer, A. Bösmann, A. Kaftan, M. Laurin, J. Libuda, P. Wasserscheid, *Angew. Chem. Int. Ed.*, **2013**, 52, 5028–5032
- G. N. Vayssilov, Y. Lykhach, A. Migani, T. Staudt, G. P. Petrova, N. Tsud, T. Skála, A. Bruix, F. Illas, K. C. Prince, V. Matolín, K. M. Neyman, J. Libuda, *Nat. Mater.*, **2011**, 10, 310–315

### SELECTED REVIEWS

- Y. Lykhach, A. Bruix, S. Fabris, V. Potin, I. Matolínová, V. Matolín, J. Libuda, K. M. Neyman, Oxide-based nanomaterials for fuel cell catalysis: the interplay between supported single Pt atoms and particles, *Catal. Sci. Technol.*, **2017**, 7, 4315
- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, Liquid Organic Hydrogen Carriers: Surface Science Studies of Carbazole Derivatives, *Chem. Rec.*, **2014**, 14, 879
- H.-P. Steinrück, J. Libuda, P. Wasserscheid, T. Cremer, C. Kolbeck, M. Laurin, F. Maier, M. Sobota, P. S. Schulz, M. Stark, Surface Science and Model Catalysis with Ionic Liquid-modified Materials, *Adv. Mater.*, **2011**, 23, 2571–2587
- J. Libuda, H.-J. Freund, Molecular Beam Experiments on Model Catalysts, *Surf. Sci. Rep.*, **2005**, 57, 157–298

### SELECTED AWARDS

- Fellow and Referee “Studienstiftung des Deutschen Volkes”
- 1996 Otto-Hahn-Medaille, Max-Planck-Gesellschaft (MPG)



**CHAIR OF THEORETICAL CHEMISTRY**  
**PROF. DR. ANDREAS GÖRLING**

andreas.goerling@fau.de • [www.chemie.fau.de/goerling](http://www.chemie.fau.de/goerling)

- ### CURRICULUM VITAE

**Since 2004** University Full Professor of Theoretical Chemistry and Director of the Computer Chemistry Center (CCC) at the University of Erlangen-Nürnberg, Germany

**2003 – 2004** Professor of Theoretical Chemistry, University of Bonn, Germany

**2001 – 2003** Associate Professor at the Chair of Theoretical Chemistry, Technical University of Munich (TUM), Germany

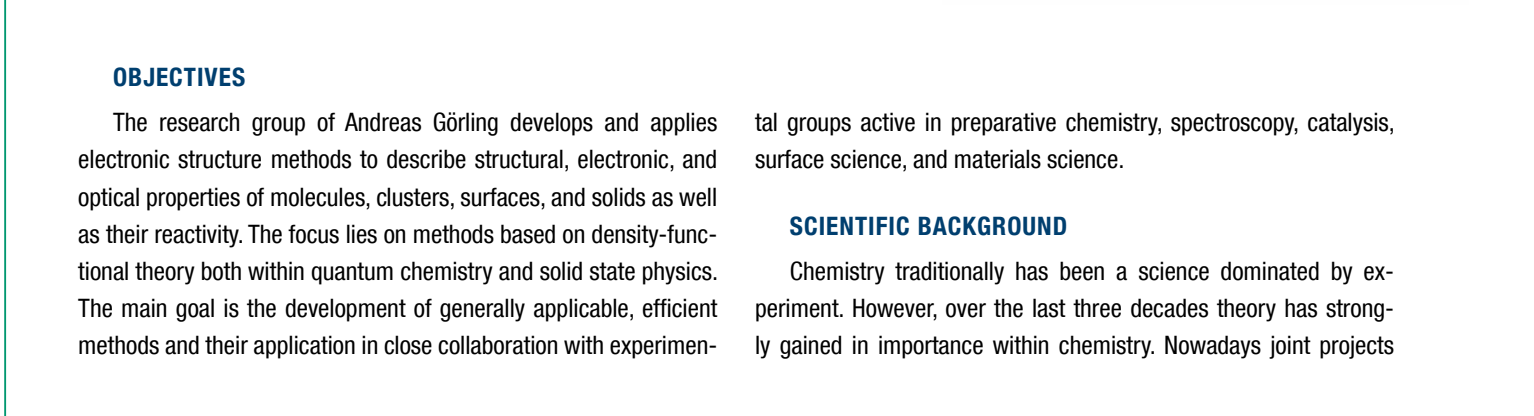
**1995 – 2000** Heisenberg Scholar of the Deutsche Forschungsgemeinschaft (DFG), Technical University of Munich (TUM), Germany

**1993 – 1995** Habilitation Scholar of the DFG, Technische Universität München and Tulane University, New Orleans, USA

**1991 – 1992** Postdoctoral Fellow, Tulane University, New Orleans, USA

**1990** PhD in Chemistry, Technical University of Munich (TUM) (Prof. Rösch), Germany

**1986** Diploma in Chemistry, Technical University of Munich (TUM), Germany



## OBJECTIVES

The research group of Andreas Görling develops and applies electronic structure methods to describe structural, electronic, and optical properties of molecules, clusters, surfaces, and solids as well as their reactivity. The focus lies on methods based on density-functional theory both within quantum chemistry and solid state physics. The main goal is the development of generally applicable, efficient methods and their application in close collaboration with experimen-

tal groups active in preparative chemistry, spectroscopy, catalysis, surface science, and materials science.

## SCIENTIFIC BACKGROUND

Chemistry traditionally has been a science dominated by experiment. However, over the last three decades theory has strongly gained in importance within chemistry. Nowadays joint projects

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as their reactivity. The focus lies on methods based on density-func-

Chemistry traditionally has been a science dominated by experiment. However, over the last three decades theory has strongly gained in importance within chemistry. Nowadays joint projects



by theoreticians and experimentalists have become the rule. Today theory not only helps interpreting and understanding experimental findings but makes predictions suggesting promising experiments or synthetic targets. The growing importance of electronic structure calculations results both from the availability of faster and faster computers and the development of more and more powerful electronic structure methods, in particular methods based on or related to density-functional theory. The activities of the group of Andreas Görling have to be seen in this context.

About half of the group focuses on the development of formal theory and new methods, including the implementation of the latter, both in homegrown computer codes and commercially available quantum chemistry packages. The other half of the group is concerned with applications of various electronic structure methods in joint projects with experimental groups. A characteristic of the group is that the scientific activities range from “paper and pencil” theory over the development and implementation of electronic structure methods to close collaborations with experimental partners.

### RESEARCH HIGHLIGHTS

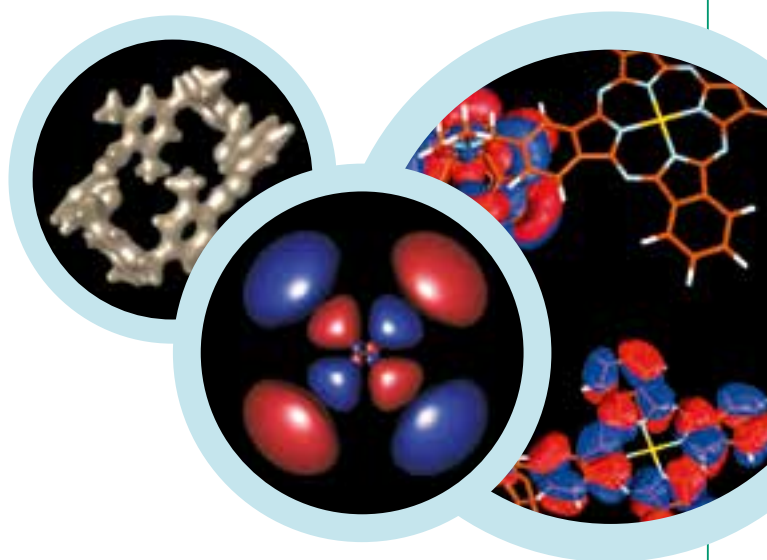
In recent years novel density-functional methods employing orbital-dependent functionals were developed, in particular, methods treating the electron correlation on the basis of the adiabatic-connection fluctuation-dissipation theorem. These methods do not suffer from the shortcomings of conventional density-functional methods and therefore, in contrast to the latter, can describe Van-der-Waals interactions and electronic structures characterized by static correlation which typically occur during the breaking and forming of bonds. The accuracy of the new density-functional methods is comparable to that of high-level, wave-function-based quantum chemistry methods while the required computational effort is distinctively lower. This opens up new exciting new perspectives for quantum chemistry, most importantly, the treatment of molecules or assemblies of molecules containing more than hundred atoms with unprecedented accuracy enabling predictions of their properties and reactivities with, so far, unmatched reliability.

Recent examples of applications of methods from theory in joint projects with experimental groups here in Erlangen comprise work on synthetic carbon allotropes in the framework of the collaborative research centre 953 and on the engineering of new materials within the excellence cluster EAM. Together with the group of Hans-Peter Steinrück of Physical Chemistry doping and chemical functionalization of graphene adsorbed on metal surfaces is investigated and collaborations with the group of Andreas Hirsch from Organic Chemistry range from the interpretation of Raman finger prints of functionalized graphene to the exploration of new two-dimensional materials like sheets of black phosphorous and antimonene. Within the research unit 1878 funded by the German Research Foundation functional molecules on complex oxide surfaces are investigated with various groups from chemistry and physics. In collaborations with the group of Peter Wasserscheid from Chemical Reaction Engineering novel catalytic concepts based on liquid metal mixtures, e.g., of gallium and palladium, are developed. The role of dispersion interactions on

efficiency and chemo-, regio-, and stereoselectivity of organocatalysts is investigated with the group of Svetlana Tsogoeva from Organic Chemistry.

### PERSPECTIVES

In the future the interplay between method development and applications shall become even closer. The new methods developed in recent years will be further developed and optimized and will be made available to the quantum chemistry community in widely used computer packages. In this way, the arsenal of available methods for investigating questions in chemistry and materials science is going to be enlarged. The work on novel functional materials will remain a research focus of the group, in the future concentrating in particular on two-dimensional materials and interfaces.



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- G. Abellán, C. Neiss, A. Görling, F. Hauke, A. Hirsch, et al., *Angew. Chem. Int., Ed.*, **2017**, 56, 15267
- N. Taccardi, F. Maier, C. Papp, C. Neiss, W. Peukert, A. Görling, H.-P. Steinrück, P. Wasserscheid, et al., *Nat. Chem.*, **2017**, 9, 862
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- P. Bleiziffer, A. Heßelmann, A. Görling, *J. Chem. Phys.*, **2012**, 136, 134102
- D. Malko, F. Viñes, C. Neiss, A. Görling, *Phys. Rev. Lett.*, **2012**, 108, 086804
- A. Heßelmann, A. Görling, *Phys. Rev. Lett.*, **2011**, 106, 093001

### SELECTED REVIEWS

- A. Heßelmann, A. Görling, Random-phase approximation correlation methods for molecules and solids, *Mol. Phys.*, **2011**, 109, 2473–2500
- A. Görling, Exact-exchange Methods and Perturbation Theory along the Adiabatic Connection, in: M. Marques, C. A. Ullrich, F. Nogueira, A. Rubio, K. Burke, E. K. U. Gross, *Lecture Notes in Physics 706*, Springer, Heidelberg, **2006**, 137
- A. Görling, Orbital- and state-dependent functionals in density-functional theory, *J. Chem. Phys.*, **2005**, 123, 062203

### SELECTED AWARDS

- 1995–2000 Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (DFG)



# PROFESSOR OF THEORETICAL CHEMISTRY

## PROF. DR. DIRK ZAHN

[dirk.zahn@fau.de](mailto:dirk.zahn@fau.de) • [www.chemie.fau.de/zahn](http://www.chemie.fau.de/zahn)

### CURRICULUM VITAE

- Since 2010** University Professor of Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany  
**2008 – 2010** Heisenberg Fellow, Visiting Professor in Cagliari, Italy and Istanbul, Turkey  
**2002 – 2008** Habilitation at the Max Planck Institute for Chemical Physics of Solids, Dresden, Germany  
**2000 – 2002** Postdoctoral Fellow at the Max Planck Institute for Solid State Research, Stuttgart, Germany and the Swiss Federal Institute of Technology (ETH), Zürich, Switzerland  
**1997 – 2000** PhD in Theoretical Biochemistry at the Technische Universität Darmstadt, Germany

### OBJECTIVES

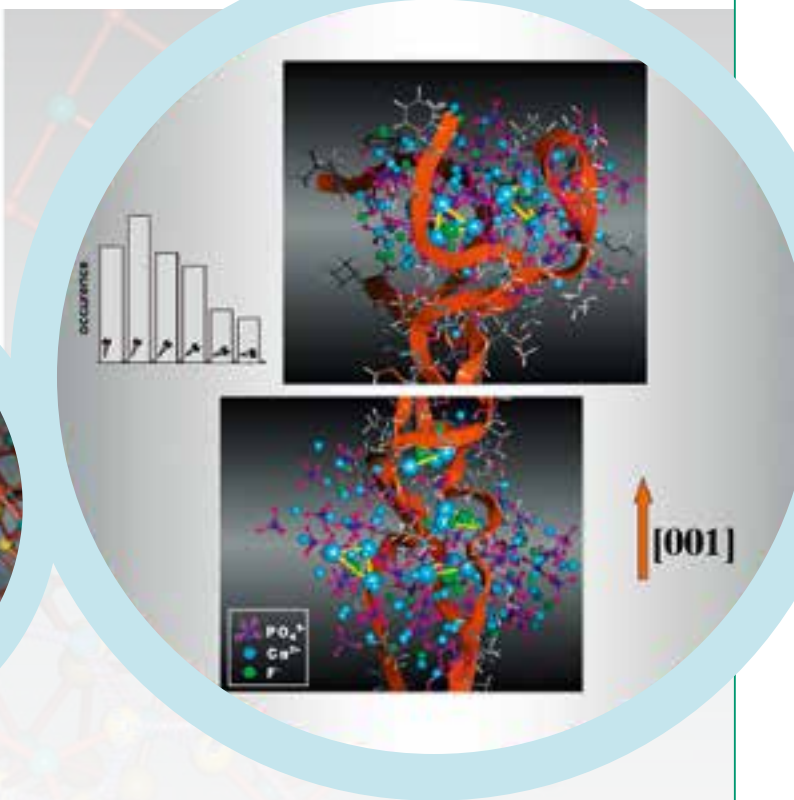
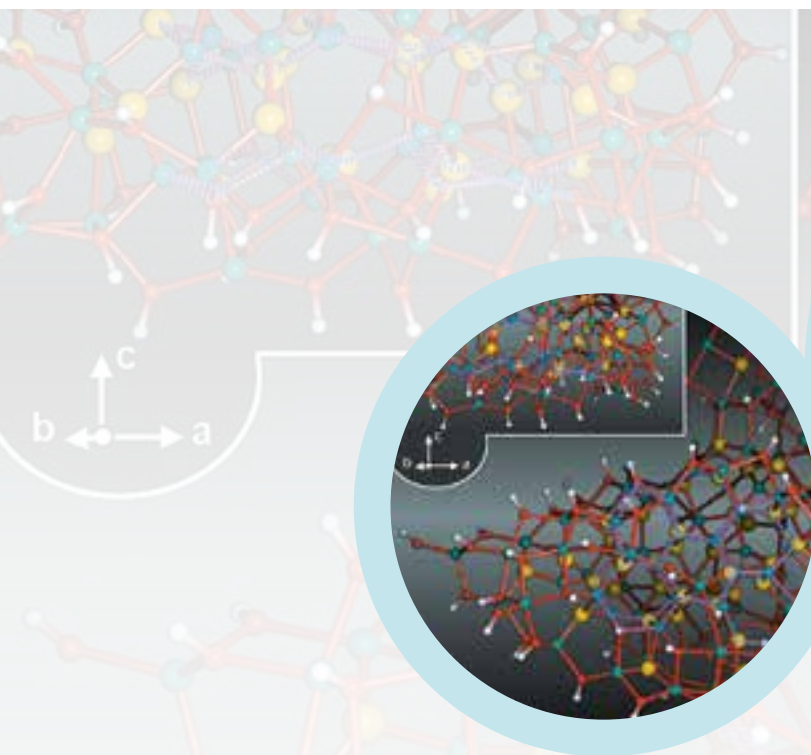
The aim of our group is the development and application of static and molecular dynamics simulations for the investigation of the mechanisms of reactions, nucleation events and self-organization processes. The addressed topics range from materials science, solid state chemistry up to biophysics and general physical chemistry.

### SCIENTIFIC BACKGROUND

The time-length scale problem inherent to complex systems represents the key obstacle to the direct simulation of many interesting processes. By development and application of powerful algorithms to tackle these limitations to atomistic simulations, we paved the road to detailed mechanistic investigations of nucleation, self-organization and reactions. On the basis of realistic simulation scenarios we establish increasingly close connections to the experiments.

### RESEARCH HIGHLIGHTS

Using novel molecular dynamics strategies, we uncovered mechanisms of ion aggregation and nanocrystal formation and rationalized the structure and properties of (nano)composite materials. Crystal nucleation and growth is of fundamental interest in physics, chemistry, and materials science, but also in a specific discipline of biology – the investigation of biominerals. While nucleation processes and materials properties are well characterized at the macroscopic and mesoscopic scale by a wealth of experimental evidence, in particular for understanding mechanisms at the atomic level of detail, computer simulations have proven to be a very powerful tool. An important part of our work is the development of efficient methods to allow the study of realistic crystal nucleation scenarios with a direct relation to solid state and materials chemistry. The aim of our molecular dynamics simulation studies is 1) to explore the nucleati-



on mechanisms of nanocrystalline matter. Starting from the association of single ions, accessible insights range from the mechanisms of motif formation, ripening reactions and the self-organization of nanocrystals to interactions with growth-controlling additive molecules and the formation of hybrid materials. On this basis, 2) reliable building rules for scale-up models are derived. By bridging length scales from aggregates counting a few hundreds of ions to models of up to millions of atoms we 3) pave the way to the investigation of materials properties.

Thus, by bridging fundamental physical chemistry and materials science, a bottom-to-top approach is pursued to open a new perspective to the profound understanding of complex nanomaterials and the characterization of its peculiar properties from computer simulation.

Moreover, we explore the mechanisms of self-assembled monolayer formation and their interplay with the nature of the substrate surface and the solvent used. On this basis, we aim at molecular scale understanding to tailor SAMs in favor of desired properties to promote application as optical or electronic device, protective coating, lubrication, or template for further compound association.

## PERSPECTIVES

We wish to boost bottom-to-top strategies for nanomaterial syntheses by mechanistic understanding elaborated from atomistic simulations. Along this line, we explore nanocrystal growth, the self-organization of adsorbate molecules and the formation of SAMs, composites, and complex systems mimicking devices. Our work is inspired from close cooperation to experiments, both from academic and industry partners.

## SELECTED PUBLICATIONS

- H. Dietrich, T. Schmaltz, M. Halik, D. Zahn, *Phys. Chem. Chem. Phys.*, **2017**, 19, 5137–5144
- H. Dietrich, S. Scheiner, L. Portilla, D. Zahn, M. Halik, *Advanced Materials*, **2015**, 27, 8023–8027
- P. Ectors, P. Duchstein, D. Zahn, *Cryst. Growth & Design*, **2014**, 14, 2972–2976
- D. Zahn, E. Bitzek, *PLOS one*, **2014**, 9, e93309
- T. Milek, D. Zahn, *Nanoletters*, **2014**, 14, 4913–4917

## SELECTED REVIEWS

- J. Anwar, D. Zahn, “Polymorphic Phase Transitions: Macroscopic Theory and Molecular Simulation”, *Advanced Drug Delivery Reviews*, **2017**, 117, 47–70
- T. Milek, P. Duchstein, D. Zahn, Molekulardynamik: Mit Simulationen Nanokristallen und -kompositen auf der Spur, *Nachr. Chem.*, **2012**, 3, 868–871
- D. Zahn, Tackling time-reversibility in transition path sampling molecular dynamics simulations, *Mol. Sim.*, **2012**, 38, 211–217
- D. Zahn, Modeling martensitic transformations in crystalline solids: validity and redesign of geometric approaches, *Z. Krist.*, **2011**, 226, 568–575
- D. Zahn, Molecular Dynamics Simulation of Ionic Conductors: Perspectives and Limitations, *J. Mol. Model.*, **2011**, 17, 1531–1535
- J. Anwar, D. Zahn, Uncovering Molecular Processes in Crystal Nucleation using Molecular Simulation, *Angew. Chem., Int. Ed.*, **2011**, 50, 1996–2013
- T. Milek, P. Duchstein, G. Seifert, D. Zahn, Motif Reconstruction in Clusters and Layers: Benchmarks for the Kawska-Zahn Approach to model Crystal Formation, *Chem. Phys. Chem.*, **2010**, 11, 847–852

## SELECTED AWARDS

- 2008 Heisenberg Fellowship
- Visiting professorship awards (Italy, Turkey)





## CHAIR OF MEDICINAL CHEMISTRY

### PROF. DR. PETER GMEINER

[peter.gmeiner@fau.de](mailto:peter.gmeiner@fau.de) • [www.chemie.fau.de/gmeiner](http://www.chemie.fau.de/gmeiner)

#### CURRICULUM VITAE

- Since 1999** University Full Professor, Chair of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany  
**1994 – 1996** Professor of Medicinal Chemistry at the University of Bonn, Germany  
**1988 – 1994** Research Associate at the Ludwig-Maximilians-Universität München, Germany  
**1987 – 1988** Postdoc at the University of California in Berkeley, USA

#### OBJECTIVES

At the aim of discovering novel molecular probes and drug candidates, Peter Gmeiner's group investigates design, chemical synthesis, and pharmacological properties selective ligands for G protein-coupled receptors. In this context, radioligand binding studies, X-ray crystal structures and functional assays reveal the structural origins of subtype selectivity, intrinsic activity and biased signalling. Within these topics, the Gmeiner laboratory has proven substantial experience in the design, organic synthesis, and biological investigation of bioactive molecules and contributes to highly attractive developments in CNS-active drugs.

#### SCIENTIFIC BACKGROUND

Prof. Dr. Peter Gmeiner received his PhD in 1986 from the University of Munich. He was a Postdoc at the University of California in Berkeley, USA. He subsequently returned to Munich as a research associate. In 1992, he was appointed at the University of Bonn as a

Professor of Pharmaceutical Chemistry declining an offer for a professorship at the University of Heidelberg, at the same time. Dated of October 1996, he has been chaired Full Professor of Pharmaceutical Chemistry at the University of Erlangen-Nürnberg. In 2008, Peter Gmeiner has been elected as the chairman of the Pharmaceutical/Medicinal Chemistry Section of the German Pharmaceutical Society (DPHG). Peter Gmeiner has a track record of more than 200 publications in peer-reviewed scientific journals including patents and patent applications. He serves as referee for the German Research Foundation (DFG), the Alexander von Humboldt-Foundation and the DAAD and for more than 20 top ranked journals in the fields of Chemistry and Pharmacology. He is an Editorial and International Advisory Board Member of scientific journals including *Bioorganic & Medicinal Chemistry*, *Bioorganic & Medicinal Chemistry Letters*, and *ChemMedChem*. Peter Gmeiner's research spans the design, organic synthesis and pharmacological investigation of bioactive molecules.

Prof. Peter Gmeiner is the spokesman of the Research Training Group "Medicinal Chemistry of Selective GPCR Ligands" (GRK 1910).

## RESEARCH HIGHLIGHTS

G-Protein coupled receptors (GPCRs) are of particular interest as pharmaceutical target proteins in Medicinal Chemistry since a large number of diseases can be treated by selective GPCR agonists or antagonists. Peter Gmeiner's group investigates design, chemical synthesis and pharmacological properties of subtype-selective GPCR ligands. Using an integrative approach, the group develops molecular probes to understand, control and engineer receptor-ligand binding, selectivity and function. The Gmeiner research group investigates allosterically regulated target proteins including the dopamine receptor subtypes D2long, D2short, D3 and D4 as valuable model systems. On the course of these investigations, we found the first family of receptor ligands that selectively display (neutral)-antagonist properties at the dopamine D4 receptor. Behavioral pharmacological investigations indicated atypical antipsychotic activities for the azaindole derivative FAUC 213. Heterocyclic carboxamides of the type FAUC 346 and FAUC 365 as analogs of the lead compound BP 897 were developed in the Gmeiner Laboratory as valuable compounds for the treatment of cocaine abuse. In vivo investigations that were performed at the National Institute of Drug Abuse (NIDA) in Bethesda, USA, revealed diagnostic biological properties in animal models. When we explored the binding site crevice of the dopamine receptor, novel atypical arene bioisosteres could be designed, which had not been investigated in drug discovery, yet. As an example, metallocene and paracyclophane derived bioisosteres showed excellent ligand binding properties.

## PERSPECTIVES

Although G-protein coupled receptors (GPCRs) have been studied extensively in the past, our understanding of their function at the molecular level is still incomplete. It has been shown that GPCRs mediate diverse signal-transduction pathways by similar mechanisms by binding a variety of ligands and G-proteins. Their interaction with agonists leads to a low-affinity conformation of the active state that is thought to facilitate G-protein binding. Only in the presence of both agonist and G-protein is the high-affinity receptor state formed, which promotes signal transduction. The  $\beta$ 2-adrenergic receptor ( $\beta$ 2AR), which represents an important target for cardiac and asthma drugs, is an extensively studied model system for the large superfamily of G-protein coupled receptors (GPCRs). To overcome relatively rapid association and dissociation rates of commercial  $\beta$ 2AR agonists, our strategy depends on a combination on a covalent  $\beta$ 2AR agonist incorporating a  $\beta$ 2-adrenergic agonist core and a reactive chemical group that could be targeted to a specific residue on the receptor. Employing the structure of the carazolol-bound  $\beta$ 2AR as a template, a flexible linker was added to bridge these two components. Thus, the covalent attachment would not inhibit binding of the agonist core or conformational flexibility of the transmembrane heli-



ces. The covalent  $\beta$ 2AR-agonist complex formed efficiently, and was able to activate a heterotrimeric G protein. A covalent agonist-bound  $\beta$ 2AR-T4L fusion protein could be crystallized and determined for its structure. Applying our newly developed methodology, we could determine active-state crystal structures of the muscarinic M2 receptor and the  $\beta$ 2AR in presence of a covalent adrenaline analog, in collaboration with Prof. Brian Kobilka at the Department of Molecular Physiology, Stanford University. Our current projects aim to exploit the covalent ligand strategy to the discovery of highly innovative GPCR-ligand complexes in multiple activation states. Taking advantage of such structural information, we aim to develop highly specific allosteric ligands, biased agonists and bivalent modulators.

## SELECTED PUBLICATIONS

- D. Weichert, A.C. Kruse, A. Manglik, C. Hiller, C. Zhang, H. Hübner, B. K. Kobilka, P. Gmeiner, *Proc. Natl. Acad. Sci. USA*, **2014**, 111, 10744–10748
- D. Möller, R.C. Kling, M. Skultety, K. Leuner, H. Hübner, P. Gmeiner, *J. Med. Chem.*, **2014**, 57, 4861–4875
- A. C. Kruse, A. M. Ring, A. Manglik, J. Hu, K. Hu, K. Eitel, H. Hübner, E. Pardon, C. Valant, P. M. Sexton, A. Christopoulos, C. C. Felder, P. Gmeiner, J. Steyaert, W. I. Weis, K. C. Garcia, J. Wess, B. K. Kobilka, *Nature*, **2013**, 504, 101–106
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- D. M. Rosenbaum, C. Zhang, J. A. Lyons, R. Holl, D. Aragao, D. H. Arlow, S. G. F. Rasmussen, H.-J. Choi, B. T. DeVree, R. K. Sunahara, P. S. Chae, S.H. Gellman, R.O. Dror, D.E. Shaw, W.I. Weis, M. Caffrey, P. Gmeiner, B. K. Kobilka, *Nature*, **2011**, 469, 236–240
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## SELECTED REVIEWS

- S. Löber, H. Hübner, N. Tschammer, P. Gmeiner, Recent advances in the search for D<sub>3</sub>- and D<sub>4</sub>-selective drugs: probes, models and candidates, *Trends Pharmacol. Sci.*, **2011**, 32, 148–157
- F. Boeckler, P. Gmeiner, The Structural Evolution of Dopamine D3 Receptor Ligands—Structure-Activity Relationships and Selected Neuropharmacological Aspects., *Pharmacology & Therapeutics*, **2006**, 112, 281–333

## SELECTED AWARDS

- Johann-Wolfgang-Döbereiner Prize of the DPhG
- Phoenix Pharmazie Wissenschaftspreis



## PROFESSOR OF MEDICINAL CHEMISTRY

### PROF. DR. JUTTA EICHLER

jutta.eichler@fau.de • [www.chemie.fau.de/eichler](http://www.chemie.fau.de/eichler)

#### CURRICULUM VITAE

**Since 2008** Professor of Medicinal Chemistry, University of Erlangen-Nürnberg, Germany  
**2004** Habilitation in Bioorganic Chemistry, Technical University of Braunschweig, Germany  
**2000 – 2008** Group Leader, Helmholtz Centre for Infection Research, Braunschweig, Germany  
**1991 – 1998** Postdoctoral Fellow, Research Scientist, Assistant Member, Torrey Pines Institute for Molecular Studies, San Diego, USA  
**1991** PhD, Humboldt-University, Berlin, Germany

#### OBJECTIVES

To probe and modulate protein function through controlled interference with the underlying molecular interactions. The focus of our research is on the exploration of protein-protein interactions using synthetic binding site mimics, as well as the use of these mimetic peptides as inhibitors for novel therapeutic approaches.

#### SCIENTIFIC BACKGROUND

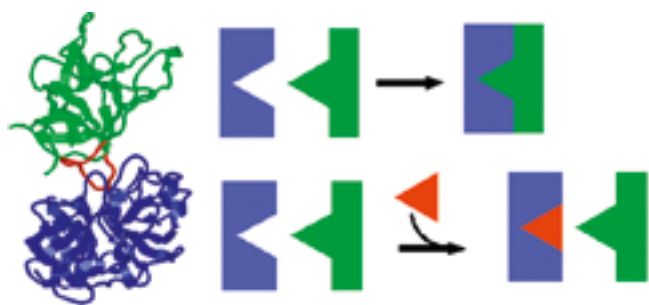
Essentially all biological processes are based on specific binding events, which are initiated by molecular recognition between bio-macromolecules. The design and generation of molecules, which can mimic the binding and / or functional sites of proteins, represents a promising strategy for the exploration an understanding of protein structure and function. In addition to this basic significance, such mimetic molecules are also useful tools for a range of biomedical applications, particularly the development of inhibitors of therapeutic

relevant protein-protein interactions. Synthetic peptides are a promising type of molecules for protein binding site mimics, as they can be generated as exact copies of protein fragments, as well as in diverse chemical modification, which includes the incorporation of building blocks other than the proteinogenic amino acids. These variations not only increase the chemical diversity presented by synthetic peptides, but also their metabolic stability, making them better drug candidates.

#### RESEARCH HIGHLIGHTS

Entry of the AIDS virus HIV-1 into its host cells is mediated by a precise cascade of molecular interactions between viral proteins and cellular receptors. Attachment of the HIV-1 envelope glycoprotein gp120 to the coreceptors CXCR4 and CCR5, respectively is a pivotal element of this entry process. Recently, we have designed and gen-





erated a peptide that presents parts of the extracellular domain of CXCR4, which belongs to the family of GPCRs. The functionality of this CXCR4 mimetic peptide was demonstrated by its affinity to HIV-1 gp120, and, more importantly, by its ability to discriminate between gp120 from CXCR4- and CCR5- using HIV-1 in binding assays involving recombinant proteins, as well as in cellular infection assays. Apart from their potential biomedical applications, such molecules are useful tools for the exploration of HIV-1 tropism at the molecular level. Furthermore, we could show that the interaction of gp120 with CXCR4 can be functionally mimicked by peptides presenting the binding sites of the two proteins for each other, i.e. the V3 loop of gp120 and the three extracellular loops of CXCR4.

Recently, we have extended the scope of using assembled peptides for the synthetic mimicry of discontinuous protein binding sites, to antibody paratopes, which directly contact the respective antigen. Such a paratope mimetic peptide of the ant-HIV-1 antibody mAb b12 was found to selectively bind to the antigen, i.e. HIV-1 gp120, as well as to inhibit infection of cells with the virus.

### PERSPECTIVE

Our ongoing and future research plans include the design and generation of hybrid molecules that target two or more protein-protein-interactions simultaneously, as well as probing the concept of mimicking protein-protein interactions by peptide-peptide interactions in the context of other proteins. Furthermore, we will address the relationship of functional and structural mimicry, i.e. the question whether protein binding site mimics are able to adopt structures that resemble their arrangement within the structural context of the protein they are derived from, and whether such structural analogy correlates with the affinity to the respective ligand. The goal is to understand the structural features that govern the affinity of these mimicry, which will in turn guide the design of improved molecules.

### SELECTED PUBLICATIONS

- C. Haußner, D. Damm, S. Nirschl, A. Rohrhofer, B. Schmidt, J. Eichler, *ChemBioChem*, **2017**, 18, 647–653
- A. Groß, R. Brox, D. Damm, N. Tschammer, B. Schmidt, J. Eichler, *Bioorg.Med.Chem.*, **2015**, 23, 4050–4055
- A. Groß, K. Rödel, B. Kneidl, N. Donhauser, M. Mössl, E. Lump, J. Münch, B. Schmidt, J. Eichler, *ChemBioChem*, **2015**, 16, 446–454
- U. Kafurke, A. Erijman, Y. Aizner, J.M. Shifman, J. Eichler, *J.Peptide Sci.*, **2015**, 21, 723–730
- A. Berthelmann, J. Lach, M. A. Gräwert, M. Groll, J. Eichler, *Org.Biomol. Chem.*, **2014**, 12, 2606–2614
- K. Möbius, R. Dürr, C. Haußner, U. Dietrich, J. Eichler, *Chem.Eur.J.*, **2012**, 18, 8292–8295

### SELECTED REVIEWS

- C. Haußner, J. Lach, J. Eichler, Synthetic antibody mimics for the inhibition of protein—ligand interactions. *Curr.Opin.Chem.Biol.*, **2018**, 40, 72–77
- A. Groß, C. Hashimoto, H. Sticht, J. Eichler, Synthetic Peptides as Protein Mimics. *Front.Bioeng.Biotechnol.*, **2016**, 3, 211
- J. Eichler, Peptides as protein binding site mimetics. *Curr.Opin.Chem.Biol.*, **2008**, 12, 707–713

### SELECTED AWARDS

- 2001 BioFuture Award of the German Federal Department of Education and Research (BMBF)



## PROFESSOR OF MEDICINAL CHEMISTRY

### PROF. DR. MARKUS HEINRICH

[markus.heinrich@fau.de](mailto:markus.heinrich@fau.de) • [www.chemie.fau.de/heinrich](http://www.chemie.fau.de/heinrich)

#### CURRICULUM VITAE

- Since 2009** University Professor of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany  
**2005 – 2009** Habilitation, Technical University of Munich (TUM), Germany  
**2003 – 2005** Postdoctoral Fellow, Ecole Polytechnique, Palaiseau, France  
**2000 – 2003** PhD in Chemistry, Ludwig-Maximilians-Universität München (LMU), Germany  
**1995 – 2000** Diploma in Chemistry, Ludwig-Maximilians-Universität München (LMU), Germany

#### OBJECTIVES

Our group is interested in the development of new radical reactions and their application in the fields of medicinal chemistry, radiochemical labelling and imaging, environmental chemistry, agrochemistry and natural product synthesis.

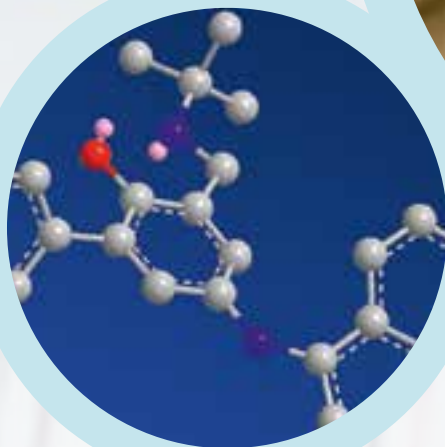
We therefore focus on the development of radical reactions which can be conducted under very mild and simple reaction conditions with solvents such as water. To maintain a wide and general applicability, our aim is to use only non-toxic metals or metal-free conditions.

#### SCIENTIFIC BACKGROUND

The applicability of organic radical chemistry is still restricted by the fact that even newly developed reactions depend on the use of toxic ingredients. In addition, radical chemistry is widely believed to be non-selective and the reaction course to be difficult to control. Not surprisingly, only very few radical reactions can be found among the industrial processes used for the preparation of pharmaceutical substances. Against this background, the synthetic potential of radical reactions appears to be by far not exploited.

#### RESEARCH HIGHLIGHTS

In the past five years we have been able to show that reactions proceeding via aryl radicals possess a far greater potential in organic synthesis than was known before. The radicals were generated under well-defined reaction conditions which enable them to undergo selective addition reactions to various substrates. In a first step new methodologies for the intermolecular carboamination and carbhydroxylation of olefins could be developed. Later we found that improved protocols where the use of water as solvent plays a key role, even allow the functionalization of aromatic substrates. With these



new synthetic opportunities in hands several important products became accessible in fewer steps and far more efficiently than before. Applications include the treatment of chronic obstructive pulmonary disease (COPD) and of infections caused by the human cytomegalovirus (HCMV).

### PERSPECTIVES

Our future research is aimed at the discovery of new, ideally metal-free, radical reactions possessing a broad applicability in organic and medicinal chemistry. In addition we are currently investigating the combination of our synthetic methods with the important issue of waste reduction. So far unknown synthetic transformations are going to be evaluated with respect to their potential use in combinatorial syntheses of compound libraries. Finally, biological testing will be performed for the elucidation of structure-activity relationships. In this way we hope to open up new, efficient and environmentally benign ways of access to important chemical products, especially pharmaceuticals.

### SELECTED PUBLICATIONS

- M. C. D. Fürst, E. Gans, M. J. Böck, M. R. Heinrich, *Chem. Eur. J.*, **2017**, 23, 15312–15315
- N. Hegmann, L. Prusko, M. R. Heinrich, *Org. Lett.*, **2017**, 19, 2222–2225
- S. Kindt, K. Wicht, M. R. Heinrich, *Angew. Chem. Int. Ed.*, **2016**, 55, 8744 – 8747
- R. Lasch, S. K. Fehler, M. R. Heinrich, *Org. Lett.*, **2016**, 18, 1586–1589
- A. L. Bartuschat, K. Wicht, M. R. Heinrich, *Angew. Chem. Int. Ed.*, **2015**, 54, 10294–10298
- S. K. Fehler, G. Pratsch, M. R. Heinrich, *Angew. Chem. Int. Ed.*, **2014**, 53, 11361–11365
- C. de Salas, M. R. Heinrich, *Green Chem.*, **2014**, 16, 2982–2987

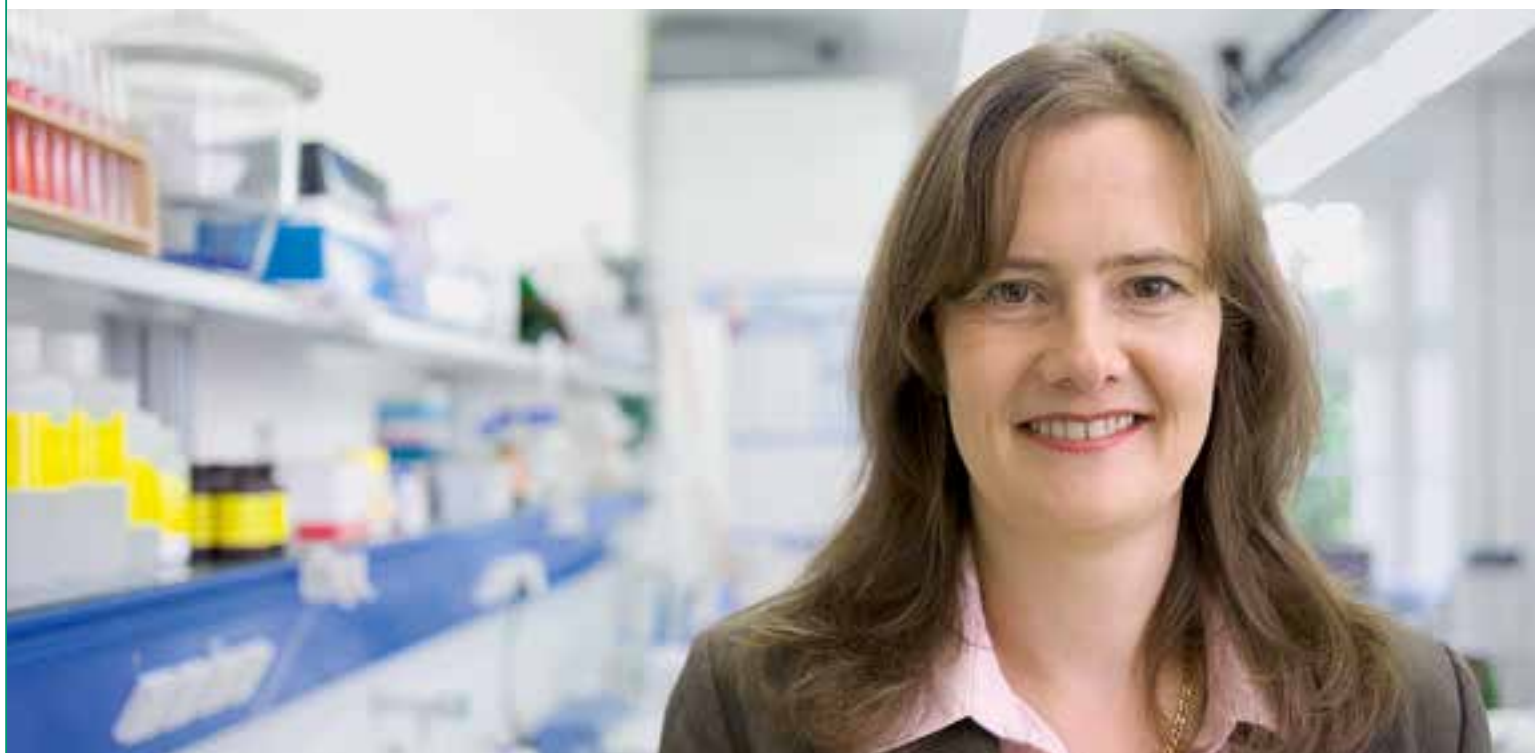
### SELECTED REVIEWS

- S. Kindt, M. R. Heinrich, *Synthesis*, **2016**, 48, 1597–1606

### SELECTED AWARDS

- 2008 ADUC Prize of the Year





## CHAIR OF FOOD CHEMISTRY

### PROF. DR. MONIKA PISCHETSRIEDER

monika.pischetsrieder@fau.de • [www.chemie.fau.de/pischetsrieder](http://www.chemie.fau.de/pischetsrieder)

#### CURRICULUM VITAE

- Since 2004** University Full Professor, Chair of Food Chemistry at the University of Erlangen-Nürnberg, Germany  
**1999 – 2004** Associate Professor at the University of Erlangen-Nürnberg, Germany  
**1997 – 2000** Visiting Assistant Professor at the Columbia University, New York, USA  
**1995 – 1999** Assistant Professor at the Ludwig-Maximilian-Universität München (LMU), Germany  
**1994 – 1995** Postdoc at the Case Western University, Cleveland, USA  
**1994** PhD, Ludwig-Maximilian-Universität München (LMU), Germany

#### OBJECTIVES

The goal of our research is to understand how chemistry and physiology interact in nutrition.

#### SCIENTIFIC BACKGROUND

As a food chemist, I am convinced that we need to combine profound knowledge in chemistry as well as physiology in order to understand how food interacts with the human organism. Therefore, I worked in a chemistry lab for my PhD before joining work groups interested in the molecular basis of diseases as postdoctoral fellow and visiting assistant professor. This experience taught me that the major challenge in food chemistry is the complexity arising from the interaction of a diverse and heterogeneous chemical system with a diverse and heterogeneous biological system. As a consequence, systematic approaches are required on the chemical as well as bio-

logical interface to understand the diversity of physiological reactions caused by food components. For a food chemist, thermally processed food is particularly fascinating as well as challenging, because the complex natural composition of a food item is considerably multiplied by a network of thermally induced reactions among a multi-component system. In this context, the development and application of novel untargeted and highly sensitive analytical techniques are a prerequisite to fully comprehend the chemical composition of a food item. On the long run, the understanding how complex food systems interact with the human organism will catalyze the development of novel food products with custom tailored functionality.

#### RESEARCH HIGHLIGHTS

There are several approaches to face the challenge of the chemical complexity of food in physiological reactions. With the aim to

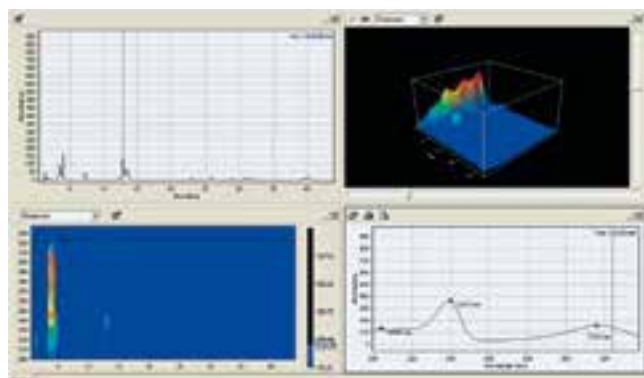


evaluate the sedative effects of plant foods, for example, activity guided fractionation was applied to identify eugenol as the main GABAA receptor modulator in clove extracts. Using a synthesized substructure library as an alternative approach, aminoreductones were determined as major immunomodulating compounds in roasted coffee. Virtual screening of a food component data base led to the identification of malt-derived hordenine as a biased dopamine D2 receptor agonist, which is an important target in food reward. Furthermore, non-targeted proteome analysis opened an insight into the low molecular weight peptidome of milk leading to the identification of novel bioactive peptides and to the development of marker peptides to ensure food authenticity. Taken together, the combination of complementary cutting edge analytical approaches is the basis for the identification of novel principles explaining the bioactivity of our food.

Among possible bioactivities, the interaction of food components with neurofunction is of particular focus in my group, which is studied in interdisciplinary collaborations with the goal to elucidate, for example, the molecular basis of food reward.

## PERSPECTIVES

During the last years, we were able to gain a lot of information on the chemical composition of our nutrition. The major future challenge will be to link this information to the complex physiological and biological consequences. Similar to the chemical interface, novel systematic and non-targeted approaches will be required to understand the diversity of physiological reactions to food.



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- T. Sommer, H. Hübner, A. El Kerdawy, P. Gmeiner, M. Pischetsrieder, T. Clark, *Sci. Rep.*, **2017**, 7, 44201
- S. Bartenbacher, C. Östreicher, M. Pischetsrieder, *Mol. Nutr. Food Res.*, **2017**, 61, 9, 1600655, doi 10.1002/mnfr.201600655
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- T. Hoch, S. Kreitz, S. Gaffling, M. Pischetsrieder, A. Hess, *Sci. Rep.*, **2015**, 5, 10041; doi: 10.1038/srep10041
- F. Baum, M. Fedorova, R. Hoffmann, M. Pischetsrieder, *J. Proteome Res.*, **2013**, 12, 5447–5462
- S. Mittelmaier, M. Pischetsrieder, *Anal. Chem.*, **2011**, 83, 9660–9668

## SELECTED REVIEWS

- M. Hellwig, S. Gensberger-Reigl, T. Henle, M. Pischetsrieder, Food-derived 1,2-dicarbonyl compounds and their role in diseases *Semin Cancer Biol.*, **2017**, doi 10.1016/j.semcancer.2017.11.014
- M. Pischetsrieder, L. Atzenbeck, S. Gensberger-Reigl, I. Weigel, Chemistry and clinical relevance of carbohydrate degradation in drugs *Drug Discov. Today*, **2016**, 21, 1620–1631
- M. Pischetsrieder, T. Henle, Glycation products in infant formulas—chemical, analytical, and physiological aspects *Amino Acids*, **2012**, 42, 1111–1118

## SELECTED AWARDS

- 2007 Forpion Research Award
- 2007 Cofresco Research Prize
- 1996 Bayerischer Habilitationsförderpreis 1996



## CHAIR OF AROMA AND SMELL RESEARCH

### PROF. DR. ANDREA BÜTTNER

[andrea.buettner@fau.de](mailto:andrea.buettner@fau.de) • [www.chemie.fau.de/buettner](http://www.chemie.fau.de/buettner)

#### CURRICULUM VITAE

- Since 2017** University Full Professor, Chair of Aroma and Smell Research at the University of Erlangen-Nürnberg, Germany
- Since 2017** Deputy Director of the Fraunhofer Institute for Process Engineering and Packaging IVV, Freising, Germany
- 2012 – 2017** University Professor of Aroma Research at the University of Erlangen-Nürnberg, Germany
- Since 2007** Head of Department of Sensory Analytics, Fraunhofer Institute for Process Engineering and Packaging IVV, Freising, Germany
- 2007 – 2012** Assistant Professor and Head of a BMBF Junior Research Group at the University of Erlangen-Nürnberg, Germany
- 2006** Habilitation at Technical University of Munich (TUM), Germany
- 2002 – 2006** Internship for Excellent Junior Researchers (HWP II) at the Technical University of Munich (TUM), Germany and of the German Research Community at the German Research Center for Food Chemistry (DFA), Garching, Germany
- 1999 – 2002** Postdoctoral Fellow at DFA, Garching, Germany and the Institute for Food Chemistry, TUM, Germany
- 1999** PhD in Food Chemistry, Technical University of Munich (TUM), Germany

#### OBJECTIVES

The Büttner research group undertakes to investigate topics relating to the analysis and characterisation of aromas and smells, as well as non-odorous volatiles encountered in everyday life. Identification of novel substances and a characterisation of their smell properties based on structure-odour activity considerations are key aspects of this work. Novel smells are created and strategies are developed for the avoidance of unwanted smells based on a combined chemo-analytical and human-sensory decoding of the underlying substances. We elucidate the formation and liberation pathways of odorants and develop techniques for controlling such processes, both in foods as well as non-food materials.

Our odour research encompasses the entire chemo-analytical side of odorant characterisation using experimental tools such as high resolution two-dimensional gas chromatography-mass spectrometry coupled to olfactometry (HR-2D-GC-MS/O), online mass spectrometric gas phase analysis, e.g., in breath aroma monitoring, and stable-isotope dilution assays (SIDA) analysis for quantification of trace odour compounds; furthermore, we endeavour to monitor, characterise, and positively influence the human responses to odour exposure / perception, both on a physiological and / or psychological-behavioural basis.

Consequently, our studies are focussed on investigating the underlying processes in human odorant perception and how these are



rated, with an aim to broaden our understanding of behavioural responses that are associated with acceptance, preference or rejection of smells or smell-associated materials and situations.

## SCIENTIFIC BACKGROUND

Odour exposure, for instance in food aromas or material or environmental emissions, is one facet of the diverse sensory factors that may strongly impact humans during their everyday life, albeit often being perceived quite unconsciously, which has led to the sensation of smell to be widely rated as being of comparatively lower relevance than other sensations, e.g., sound or vision.

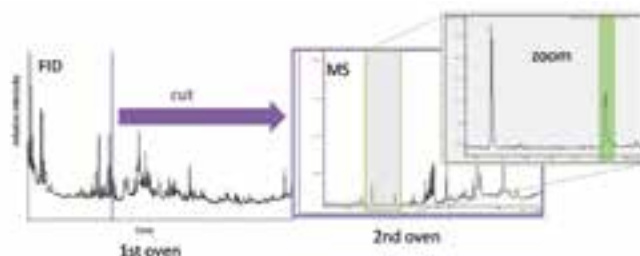
On the other hand, smells play a crucial role in shaping our lives. From birth we learn to interact with our environment using our sense of smell. Evolutionary processes have engendered a multi-faceted communication that is supported—even dominated—by olfaction.

Today, humans are increasingly exposed to smells that were not encountered by our ancestors. These are ubiquitous in our present-day environment and are met in all aspects of daily life, with sources ranging from manmade materials, industry, cars, household products, etc.; the list is practically endless. Surprisingly, odorous molecules responsible for modern smells are often unknown, as is their influence on perception, physiology and wellbeing. This is especially true for smells that are encountered in everyday living and working situations. In particular, humans are exposed to a whole host of smells, e.g., whilst commuting, during periods at work or school, or when conducting other physical activities, all commonly in indoor environments.

## RESEARCH HIGHLIGHTS

A comprehensive treatment of modern smells and their impact on human life currently does not exist. The two research groups of Prof. Büttner at FAU and Fraunhofer IVV align the senso-chemo-analytical characterisation of everyday smells encountered by mankind with the elucidation of perceptual, hedonic, behavioural and physiological responses of humans to such odours at different stages of life.

In view of this, our groups investigate physiological and psychological effects of odorants on humans, specifically in relation to foods but also non-food materials such as polymers and plastic materials and other materials that humans encounter in every-day life. Some of our recent studies have dealt with the characterisation of odorants by sensory and chemo-analytical techniques such as HR-GC-MS/O and SIDA. Thereby, we have reported for the first time on specific extremely potent odorants that could be identified as sources of common odour nuisances in daily life. Structure-odour activity relationship studies have targeted diverse substance groups such as alkylated, halogenated and methoxylated phenols, homologous enones and di-enones as well as their corresponding alcohols, to name but a few. Characterisation of uptake and metabolism processes within the human body has been achieved in *in vivo* as well as *in vitro* studies, and is the basis for investigating other physiological effects of odorants *in vivo* and *in vitro* such as the activation of brain receptor systems involved in sedative and anxiolytic processes.



Moreover, the immediate as well as the post-oral or post-inhalation human-physiological and behavioural responses to odorants are monitored, for example, by biofeedback parameters such as electroencephalography (EEG), heart rate, breathing patterns, as well as mimic analysis. Unconscious processing and response of humans to odorant exposure is thereby another important topic of our joint research groups, as is the individual odour rating based on inter-individual differences in olfactory skills and personal experience.

## PERSPECTIVES

- Characterisation of odorants and volatiles relevant to human food, non-food materials and the environment
- Resorption, transfer and metabolism processes of odorants and volatiles in humans
- Physiological and psychological / behavioural responses of humans from odorant exposure

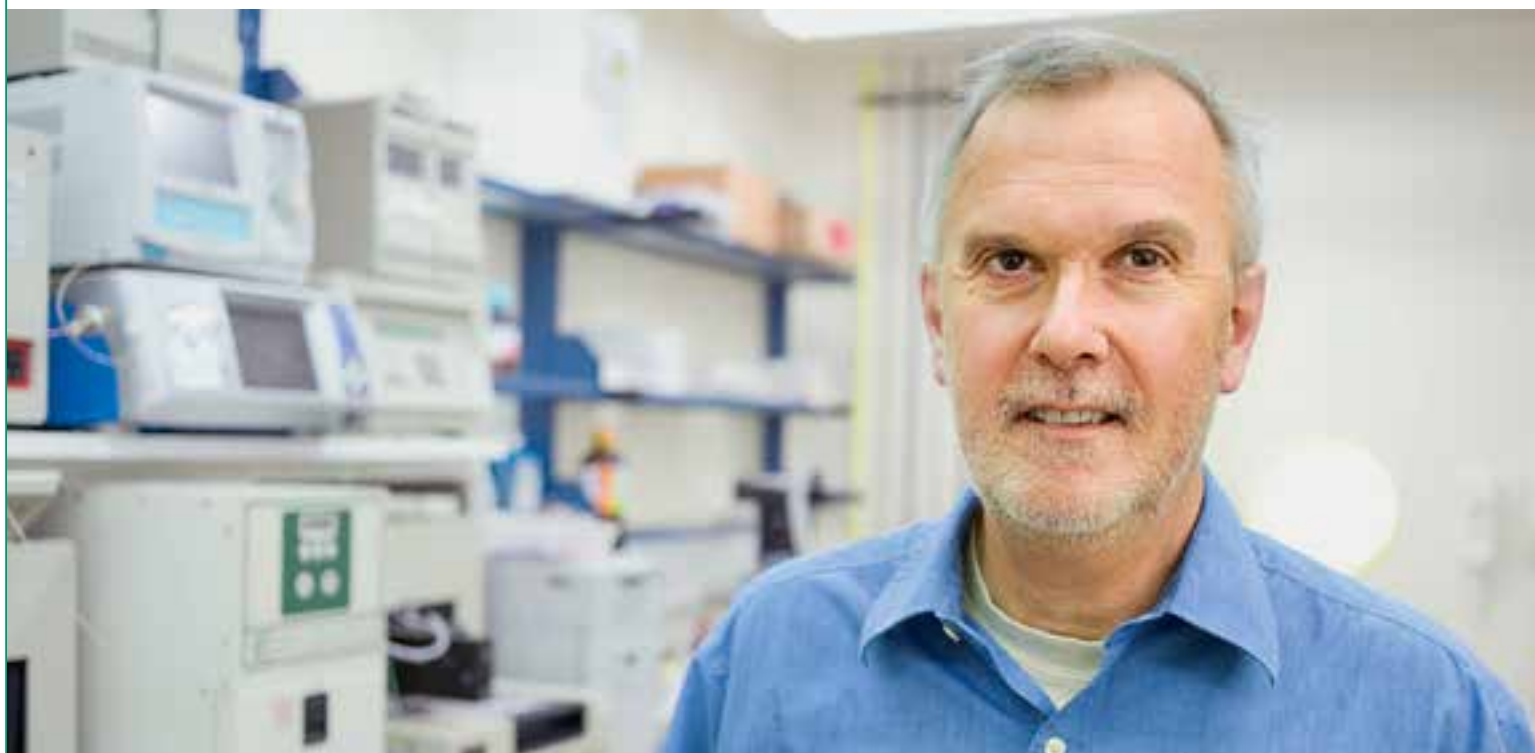


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- M. Strangl, T. Fell, M. Schlummer, A. Maeurer, A. Büttner, *J. Cleaner Prod.*, **2017**, 40, 1500–1507
- F. Juhlke, K. Lorber, M. Wagenstaller, A. Büttner, *Food Chem. section*, **2017**, doi: 10.3389/fchem.2017.00120
- P. Denk, C. Velasco-Schön, A. Büttner, *Anal. Bioanal. Chem.*, **2017**, 409, 5249–5258
- A. Heinlein, M. Metzger, H. Walles, A. Büttner, *Food Funct.*, **2014**, 3, 318–335
- C. Siefarth, Y. Serfert, S. Drusch, A. Büttner, *Foods*, **2014**, 3, 30–65
- K. Lorber, P. Schieberle, A. Büttner, *J. Agric. Food Chem.*, **2014**, 62, 1025–31
- M. Wagenstaller, A. Büttner, *Metabolites*, **2013**, 3, 637–657
- C. Hartmann, A. Triller, M. Spehr, R. Ditttrich, H. Hatt, A. Büttner, *ChemplusChem*, **2013**, 78, 695–702
- F. Kirsch, K. Horst, W. Röhrig, M. Rychlik, A. Büttner, *Metabolomics*, **2013**, 9, 483–496
- A. Kessler, C. Villmann, H. Sahin, M. Pischetsrieder, A. Büttner, *Flavour Fragr. J.*, **2012**, 27, 297–303

## SELECTED AWARDS

- 2017 AGFD Fellow Award, Agricultural and Food Chemistry Division, American Chemical Society
- 2013 Nutricia Wissenschaftspreis
- 2012 Danone Innovation Prize
- 2011 Young Investigator Award Food and Agricultural Division, American Chemical Society (ACS)
- 2010 Kurt-Tüffel Award for Young Scientists, Society of Food Chemistry (LChG), German Chemical Society (GDCh)
- 2004 Firmenich Flavor and Fragrance Science Award
- 1999 Weurman Flavour Best Poster-Award



## CHAIR OF PHARMACEUTICS

### PROF. GEOFFREY LEE PHD

geoff.lee@fau.de • [www.chemie.fau.de/lee](http://www.chemie.fau.de/lee)

#### CURRICULUM VITAE

- Since 1993** University Full Professor, Chair of Pharmaceutical Technology at the University of Erlangen-Nürnberg, Germany
- 1986 – 1993** Professor of Pharmaceutical Technology at the University of Heidelberg, Germany
- 1984 – 1986** Assistant Professor, College of Pharmacy, University of Illinois, Chicago, USA
- 1983 – 1984** Alexander-von-Humboldt Stipendiat, University of Regensburg, Germany
- 1980 – 1983** Postdoctoral Research Fellow, University of Southern California, Los Angeles and University of North Carolina, Chapel Hill, USA

#### OBJECTIVES

The ultimate goal in pharmaceuticals is easy to declare: let's deliver a drug to its molecular site of action in the right dose at the right time. Achieving this goal is quite another matter. We specialize in all aspects of the development, manufacture, and pharmacokinetic behaviour of classic and more modern drug delivery systems. Our goal is to ensure that they perform as required to give the optimum therapeutic effect.

#### SCIENTIFIC BACKGROUND

My PhD research work was only marginally related to pharmaceuticals—I worked on the colloidal stability of emulsions supervised by Tharwat Tadros in London. It was in Los Angeles where I first became involved in the transdermal delivery of drugs. I gained much expertise in the *in vitro* measurement of drug permeation rate through excised membranes of human skin. When I started in Hei-

delberg, I expanded this research area greatly to include a detailed study of how the barrier property of human skin is related to its morphology at the cellular and molecular levels. After moving to Erlangen I developed a further major research area in the process engineering of proteins for use in drug products. The major thrust is to detail the damaging effects of operational processes on the molecular structure of proteins. The operations are those involved in the processes of spray-drying and freeze-drying and include atomization, droplet drying and particle formation and particle collection. In the past couple of years a further research interest has developed. This is the design and preparation of nanoparticulate structures that show inertial cavitation in a low-energy ultrasonic field. The use of nanoparticles as drug delivery systems has become a big issue in pharmaceuticals research; the design of sonosensitive polymeric or inorganic nanoparticles is novel and promising, but highly challenging.

## RESEARCH HIGHLIGHTS

I manage three research groups.

**1. Biologic Particles:** microparticles containing biological molecules such as proteins or diagnostic reagents are designed, manufactured and characterized. The production processes are spray-drying, spray freeze-drying and cryopelletization with which we have extensive expertise. For each biomolecule a suitable formulation is developed and processing conditions identified but produce microparticles having the required properties. Of strong interest (also for industry) is the use of spray-drying to produce flowable, storage-stable protein particles as an alternative to freeze-drying of bulk. The particle formation process and the kinetic changes occurring to a protein—unfolding, aggregation, inactivation—are researched using single droplet acoustic levitation. The second current interest is the use of cryopelletization to produce large microparticles ( $> 1000\ \mu\text{m}$  in diameter) as carriers for diagnostic agents.

**2. Thin Films and Membranes:** this means transdermal drug delivery. The thin films aspect involves research into thin self-adhesive polymeric films whose drug release rate is controlled by the saturation solubility of the drug within the polymer. By reducing saturation solubility in the polymer, the drug release and permeation rate through an adjacent skin membrane can be enhanced. This has great potential applications to allow reduced drug loading of such transdermal films. The preparation of ultrathin polymer films ( $< 20\ \mu\text{m}$ ) is a particular challenge and is required to allow measurement of saturation solubility without supersaturation. A major research effort is the design of a fully-synthetic membrane which can simulate the barrier property of human stratum corneum (SC). This membrane must have a high tortuosity of up to 1000 to simulate the effects of the internal morphology of the SC on macroscopic diffusion rate. Our membranes are prepared from ceramic colloidal dispersions that are freeze-dried in such a way that directional freezing occurs to produce and long chimney-like pores. Once cross-linked and filled with lipid this directional pore structure should achieve our goal.

**3. Nanostructures:** polymeric and inorganic highly-rugged nanoparticles have the potential for inertial cavitation when treated with an ultrasonic pressure wave. The challenge is to produce stealth-type nanoparticles of the correct size (around  $100\ \text{nm}$ ) that have the correct surface morphology for gas entrapment. Two morphologies are being attempted: the 'Grand Canyon' model based on brittle fracture; and the 'hub cap' model based on microcollapse of a highly porous particle. Both are being developed using freeze-drying technologies. This whole research area runs in cooperation with Biomedical Engineering in Oxford.

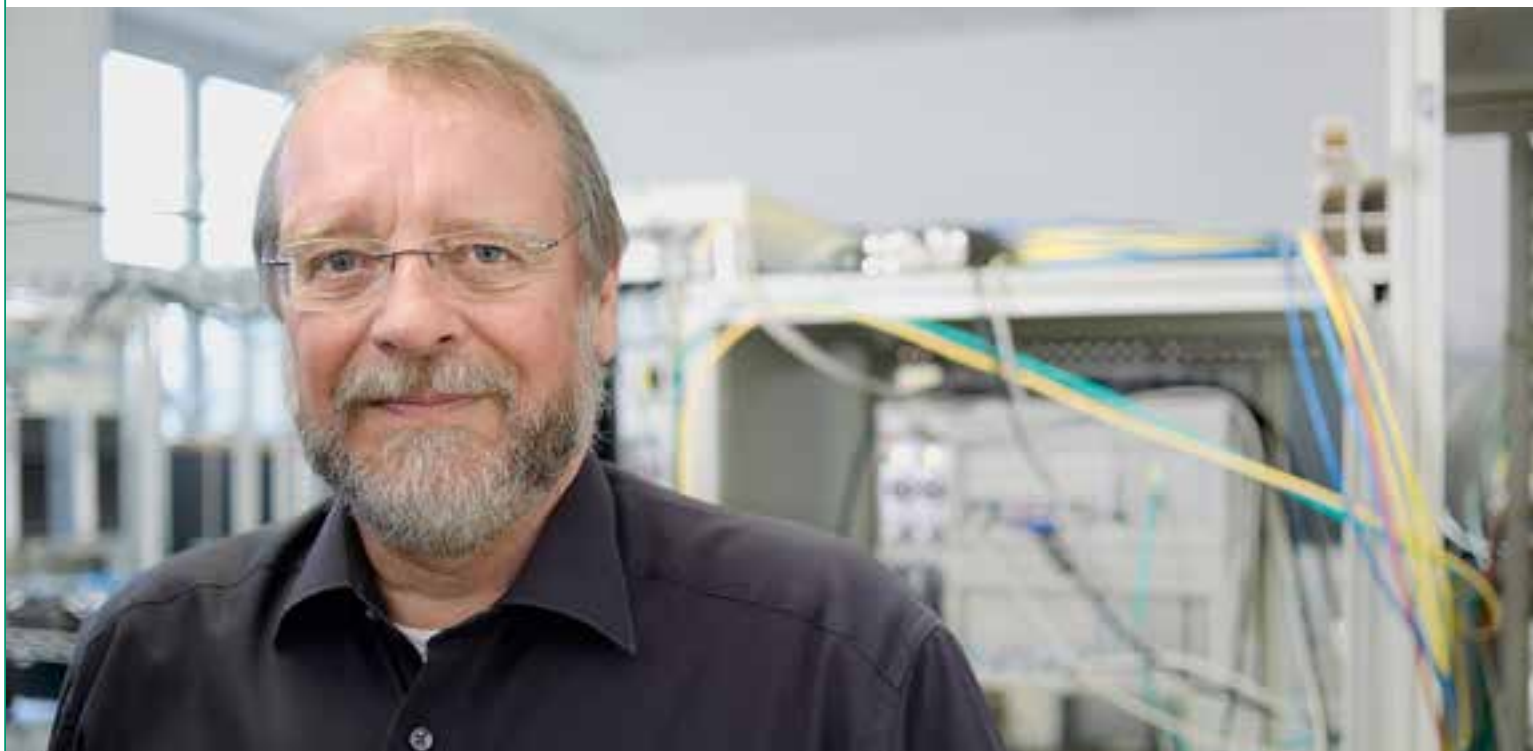
## PERSPECTIVES

The biologic particles group will become more centered on the acoustic levitator to examine the kinetics of drying and particle formation. This has many potential applications, not only in the field of pharmaceuticals but also in other areas as adhesives technology. Thin films and membranes group will concentrate on developing the fully synthetic surrogate for human SC based on high membrane tortuosity. The nanostructures group has potential to become a major research thrust.

## SELECTED PUBLICATIONS

- S. Großberger, T. Frey, G. Lee, *Chem. Eng. Sci.*, **2017**, 167, 154–160
- S. Großberger, T. Frey, G. Lee., *Materials*, **2017**, 10, 409
- G. Straller, G. Lee, *Int. J. Pharm.*, **2017**, 532, 444–449
- N. Keil, G. Lee, *Coll. & Polymer Sci.*, **2016**, 294, 1921–1928
- J. Schaefer, G. Lee, Making large, *Pharm. Devel. Technol.*, **2016**, 21, 7, 803–811
- A. Kunst, G. Lee, *J. Pharm. Sci.*, **2016**, 105, 4, 1496–1500
- S. Ullrich, S. Seyferth, G. Lee, *Int. J. Pharm.*, **2015**, 495, 52–57
- J. Schaefer, G. Lee, *Powder Technology*, **2015**, 277, 231–236





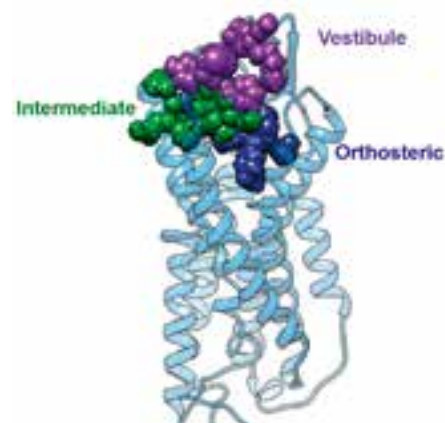
# PROFESSOR OF COMPUTATIONAL CHEMISTRY

## APL. PROF. TIM CLARK PHD

tim.clark@fau.de • [www.chemie.fau.de/clark](http://www.chemie.fau.de/clark)

### CURRICULUM VITAE

- 2006 – 2016** Professor of Computational Chemistry at the University of Portsmouth, Great Britain
- Since 1993** Technical Director, Computer Chemistry Center at the University of Erlangen-Nürnberg, Germany
- 1977 – 1993** Academic Councilor of the Institute of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
- 1976 – 1977** NATO Fellow at the University of Erlangen-Nürnberg, Germany
- 1975 – 1976** NATO Fellow at Princeton University, USA
- 1973 – 1975** Imperial Chemical Industries Fellow at Queen's University, Belfast, Great Britain



### OBJECTIVES

Our aim is to develop and use methods to simulate real systems, both technical and biological in order to understand their structure, function and properties. A broad spectrum of theoretical techniques, from classical force fields to high-level quantum mechanics, is used for this purpose. Topics of special interest are peptide hormones and G-protein coupled receptors, simulating molecular electronic devices and the theory of non-covalent interactions. The methods developed are designed to bridge the gap between classical and quantum mechanical modeling techniques on the atomistic and mesoscales and to calculating the electronic properties of extremely large (100,000 atom) systems with semiempirical molecular orbital theory.

### SCIENTIFIC BACKGROUND

Computational chemistry, as distinct from the more traditional theoretical chemistry, is primarily concerned with modeling and simulating real systems in order to understand their behavior, calculate data that are not available experimentally and, more recently to predict properties and behavior before experiments are performed. The techniques used range from seemingly simple force fields (mechanical models of molecules) to extremely compute-intensive levels of ab initio molecular orbital (MO) or density functional theory (DFT). As our interest is centered on biological and nanotechnological systems, we usually deal with large, often flexible molecular aggregates. We must therefore consider the dynamics of the system by performing

molecular dynamics (MD) simulations at quite “cheap” levels of theory before collecting “snapshots” from the simulations to calculate not only the instantaneous properties of the complex system, but also its macroscopic properties as the sum of those of the individual snapshots. Thus, modeling complex systems of “soft matter” involves not only calculating the properties correctly (the Hamiltonian), but also making sure that the structures calculated are really representative for the macroscopic system at real temperatures (the sampling).

## RESEARCH HIGHLIGHTS

Research highlights in computational chemistry almost always involve predictions that are later confirmed by experiment or theoretical models that lead to a better understanding of experimental results. Traditionally, computational chemistry techniques have been used most in the life sciences but modeling new materials and molecular electronic devices is becoming more important. Our work on G-protein coupled receptors and their peptide-hormone ligands, for instance, has revealed new binding sites and modes of action and provided details of the conformations of peptide hormones such as vasopressin in solution. Simulating electronic devices not only allows us to support experimentalists in developing prototypes, but also leads to new understanding of the bonding in electroactive organic aggregates. Simulating self-assembled monolayer field-effect transistors, for instance, led to the discovery of a new type of interstitial electron trap between  $C_{60}$  fullerenes. In order to be able to simulate the electronic properties of devices on the nanometer scale, we have developed a massively parallel semiempirical MO program that is capable of calculating 100,000 or more atoms. Finally, detailed high-level *ab initio* calculations first led to a complete understanding of halogen bonding as a subset of the more general  $\sigma$ -hole bonding and later revealed other directional non-covalent interactions such as anisotropic dispersion.

## PERSPECTIVES

Computational techniques are limited only by the capacity of the hardware and the imagination of the researcher. Strangely enough, the former is often less limiting than the latter. It is therefore important to recognize the immense power of modern computers and to develop new techniques to use them to the full to investigate chemical, technical and biological questions. Experimentalists are increasingly working with molecules, particles and aggregates that are small enough to be simulated completely, even by quantum mechanical calculations, using a combination of modern hard- and software. The dual aspects of sampling and the Hamiltonian outlined above will play an ever increasing role as modeling and simulation begin to be able to treat complete nanoscale devices. There are already many areas of the chemistry of molecules in which high level quantum mechanical calculations can be considered more accurate than experiment. Extending these areas and developing techniques to treat ever more complex macromolecules, micelles, vesicles, membranes, self-assembled monolayers and even complete photocells or electronic devices is the aim of modern computational chemistry. Modeling



and simulation has been called the “third pillar of science” alongside experiment and theory. Modern computer capabilities are now making direct comparisons between nanoscale experiments and simulations possible.

## SELECTED PUBLICATIONS

- M. Kriebel, D. Sharapa, and T. Clark, *J. Chem. Theor. Comput.*, **2017**, 13, 6308–6316 (DOI: 10.1021/acs.jctc.7b00568)
- T. Clark, *J. Mol. Model.*, **2017**, 23, 297 (DOI: 10.1007/s00894-017-3473-y)
- T. Schmaltz, B. Gothe, A. Krause, S. Leitherer, H.-G. Steinrück, M. Thoss, T. Clark and M. Halik, *ACS Nano*, **2017**, 11, 8747–8757 (DOI: 10.1021/acsnano.7b02394)
- N. Saleh, P. Ibrahim, G. Saladino, F. L. Gervasio and T. Clark, *J. Chem. Inf. Model.*, **2017**, 57, 1210–1217 (DOI: 10.1021/acs.jcim.6b00772)
- N. Saleh, G. Saladino, F. L. Gervasio and T. Clark, *Chem. Sci.*, **2017**, 8, 4019–4026 (DOI: 10.1039/C6SC04647A)
- B. Basel, J. Zirzmeier, C. Hetzer, B. Phelan, M. Krzyaniak, R. Reddy, P. Coto, N. Horwitz, R. Young, F. White, F. Hampel, T. Clark, M. Thoss, R. R. Tykwinski, M. Wasielewski and D. M. Guldi, *Nat. Commun.*, **2017**, 8, 15171 (DOI: 10.1038/ncomms15171)

## SELECTED REVIEWS

- P. Politzer, J. S. Murray, T. Clark and G. Resnati, The  $\sigma$ -Hole Revisited, *PhysChemChemPhys*, **2017**, 19, 32166–32178 (DOI: 10.1039/C7CP06793C)
- T. Clark, Odd-Electron Bonds, *ChemPhysChem*, **2017**, 18, 2766–2771 (DOI: 10.1002/cphc.201700417R1)
- T. Clark, G-Protein coupled receptors: answers from simulations, *Beilstein J. Org. Chem.*, **2017**, 13 1071–1078 (DOI:10.3762/bjoc.13.106)
- T. Clark, Halogen Bonds and  $\sigma$ -Holes, *Faraday Disc. “Halogen Bonding in Supramolecular and Solid State Chemistry”*, **2017**, 203, 9–27 (DOI: 10.1039/C7FD00058H)
- T. Clark, Simulating charge transport in flexible systems, *Perspectives in Science*, **2015**, 6, 58–65 (DOI: 10.1016/j.pisc.2015.06.003)
- P. Politzer, J. S. Murray and T. Clark, Sigma-Hole Bonding: A Physical Interpretation, in *Halogen Bonding I: Impact on Materials Chemistry and Life Sciences* (P. Metrangola and G. Resnati, Eds), *Topics in Current Chemistry*, **2015**, 358, 19–42 (DOI: 10.1007/128\_2014\_568)
- T. Clark, J. J. P. Stewart, MNDO-like Semiempirical Molecular Orbital Theory and its Application to Large Systems, *Computational Methods for Large Systems*, **2011**, Chapter 8
- P. Politzer, J. S. Murray, T. Clark, Halogen bonding: an electrostatically-driven highly directional noncovalent interaction, *Phys. Chem. Chem. Phys.*, **2010**, 12, 7748–7757

## SELECTED AWARDS

- 2009 Klaus-Wilhelm-von-der-Lieth-Medaille of the Molecular Graphics and Modelling Society



## PROFESSOR OF MOLECULAR NANOSTRUCTURES (ICMM)

### PROF. DR. FRANZISKA GRÖHN

franziska.groehn@fau.de • [www.chemie.fau.de/groehn](http://www.chemie.fau.de/groehn)

#### CURRICULUM VITAE

- Since 2009** University Professor of Molecular Nanostructures at the Interdisciplinary Center for Molecular Materials (ICMM), University of Erlangen-Nürnberg, Germany
- 2001 – 2009** Group leader at the Max Planck Institute for Polymer Research, Mainz, and Institute of Physical Chemistry, University of Mainz, Germany
- 1998 – 2000** Postdoctoral fellow at National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA
- 1998** PhD from Max Planck Institute of Colloids and Interfaces and University of Potsdam, Germany

#### OBJECTIVES

The goal of the Gröhn Group is to develop new concepts for the formation of nanostructures through self-assembly. In particular, we establish routes for the design of functional and responsive supramolecular nanoparticles and organic-inorganic hybrid materials. Exciting potential lies in applications such as solar energy conversion, smart materials and drug carriers. Understanding physical chemical fundamentals of self-assembly, particle formation and detailed nanostructure characterization are essential to fulfilling this goal.

#### SCIENTIFIC BACKGROUND

With regard to the world's decreasing energy resources, developing strategies to exploit solar energy becomes increasingly important. Supramolecular nanoscale architectures exhibit a variety of fascinating natural structures and functions in systems such as

cell membranes, DNA-protein complexes and photosystems. Hence, self-assembling building blocks is highly promising in terms of creating functional units with tailored properties. The capability of rearrangement can be exploited to build switchable units and adaptive structures.

Another specialty of natural systems is organic-inorganic hybrid nanostructures that create unique material properties, for example, the stability and lightness of sea shells or shark teeth. This is one motivation for the synthesis of hybrid structures by polymer templating, which also leads to inorganic nanoparticles with special optical, electrical or magnetic properties.

A major key to such structures is to develop a fundamental understanding of the underlying principles of self-assembly and particle formation. Organic synthesis of desired building blocks plays a role



in our group, as well as the characterization of nanoscale structures by a combination of methods such as scattering and imaging techniques, spectroscopy and thermodynamic investigations.

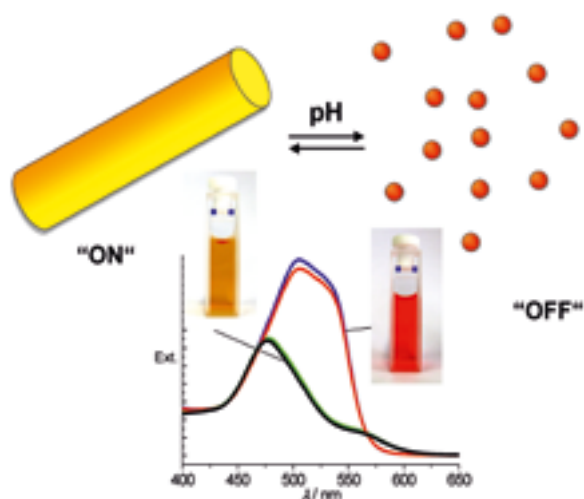
## RESEARCH HIGHLIGHTS

Recent highlights in the Gröhn Group include the formation of novel light switchable particles, organic-inorganic hybrid systems and assemblies for photocatalysis. Recently, we established electrostatic self-assembly as a new concept for the formation of versatile supramolecular assemblies; we have built well-defined polymer nano-objects with a variety of architectures from spheres and cylinders to vesicles and networks. Macroions interconnect with structural multivalent counterions by combining different interactions and effects, e.g., ionic forces,  $\pi$ - $\pi$  stacking and geometric factors. For example, hollow capsules with 250 nm diameter and 20 nm wall thickness spontaneously form from 5 nm sized dendrimeric building blocks and trivalent ionic dye molecules. They can be filled with peptides that can then be released through a pH change. Such pH responsive carriers are of interest for tumor research.

One approach toward solar energy conversion is to take advantage of photocatalysis. We have developed a new type of photocatalytically active self-assembled structure: Porphyrin-polyelectrolyte nanoscale assemblies exhibit tunable optical properties, including strong fluorescence and up to 20-fold higher photocatalytic activity than the corresponding porphyrins alone. Supramolecular catalysts based on polyelectrolytes and inorganic nanoparticles can exhibit expressed selectivity or even allow catalytic reactions in solution that are not possible with the building blocks alone.

A different approach toward an active material system is to transfer light energy into mechanical energy; we have shown how light energy can be converted into nanoscale size and shape changes. This route is particularly promising for applications in drug delivery and nanosensors. Various light-switchability concepts have been developed to create photoresponsive nano-objects in solution.

The key to a targeted structure design is elucidating structure-directing effects: We have revealed that a defined aggregation number results from the interplay of attractive and repulsive interaction and is encoded in the total free energy change  $\Delta G$ . Regarding the particle shape, the central point is the enthalpy/entropy balance. Assembly



thermodynamics encode nanoscale size and shape, while thermodynamics are encoded in molecular properties. We have determined a general relationship between molecular structure, enthalpy/entropy balance and assembly.

## PERSPECTIVES

With these concepts of self-assembly combining different non-covalent interaction forces, we have opened routes to creating versatile nanostructures. A future focus will be on building complex functional nano-objects, nanostructured surfaces and materials, particularly for light—chemical and light—mechanical and light—electrical energy conversion. A variety of functional building blocks can be introduced to build novel composite nanoparticles with targeted properties. Foundation is the insight into the physical chemistry of structure formation and functionality, for which we develop time-resolved scattering setups. Organic and organic-inorganic hybrid structures will be designed for catalysis, medicine and optical devices. It is expected that multi-force self-assembly will lead to striking novel functional nanoparticles and structures.

## SELECTED PUBLICATIONS

- A. Kutz, G. Mariani, R. Schweins, C. Streb, F. Gröhn, *Nanoscale*, **2018**, 10, 914
- G. Mariani, D. Moldenhauer, R. Schweins, F. Gröhn, *J. Am. Chem. Sci.*, **2016**, 138, 1280
- C. Cardenas-Daw, Carlos, F. Gröhn, *J. Am. Chem. Soc.*, **2015**, 137, 8660
- J. Düring, A. Hölzer, U. Kolb, R. Branscheid, F. Gröhn, *Angew. Chem. Int. Ed.*, **2013**, 52, 8742
- I. Willerich, F. Gröhn, *Angew. Chem. Int. Ed.*, **2010**, 49, 8104

## SELECTED REVIEWS

- F. Gröhn, Soft Matter Nanoparticles with Various Shapes and Functionalities Can Form through Electrostatic Self-Assembly, *Soft Matter*, **2010**, 6, 4296–4302

## SELECTED AWARDS

- 2006 Transatlantic Frontiers of Chemistry
- 2004 Reimund-Stadler Award, German Chemical Society
- 1989 International Chemistry Olympiad

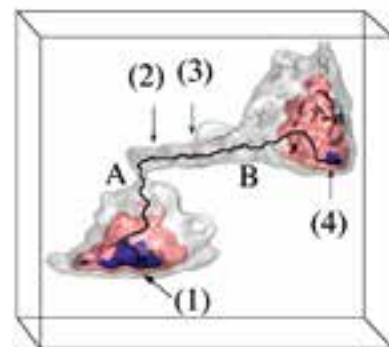


## PROFESSOR OF COMPUTATIONAL CHEMISTRY (ICMM) PROF. DR. BERND MEYER

bernd.meyer@fau.de • [www.chemie.fau.de/bmeyer](http://www.chemie.fau.de/bmeyer)

### CURRICULUM VITAE

- Since 2007** University Professor of Computational Chemistry at the Interdisciplinary Center for Molecular Materials (ICMM) and the Computer Chemistry Center (CCC) at the University of Erlangen-Nürnberg, Germany
- 2007** Visiting Scientist at the University of Oxford, Great Britain
- 2006** Habilitation in Theoretical Chemistry
- 2004 – 2007** Head of a Junior Research Group at the Ruhr-University of Bochum, Germany
- 2000 – 2004** Research Associate at the Ruhr-University of Bochum, Germany
- 1999 – 2000** Postdoc at Rutgers University, New Jersey, USA
- 1998** PhD in Physics at the Max Planck Institute for Metals Research, Stuttgart, Germany



### OBJECTIVES

The aim of our research is to achieve a better understanding of chemical processes at surfaces and interfaces. Using atomistic computer simulations we study how molecules interact with surfaces and how the physical and chemical properties of surfaces are modified by adsorbates. In particular, we focus on identifying relevant surface structures forming under reaction conditions, and we elucidate mechanisms of chemical reactions on surfaces in order to gain new insights into surface functionalization, solid / liquid interfaces, heterogeneous catalysis and the growth mechanism of molecular networks, coatings and nanostructures.

### SCIENTIFIC BACKGROUND

The chemical interaction and bonding of molecules to surfaces plays an important role in the functionalization of nanomaterials, for example in dye-sensitized solar cells or in molecular electronics. Nanoparticles are usually protected by a shell of organic molecules. This ligand shell can also be utilized to tune their optical and electronic properties. While we know the position of each atom within the molecules, the precise atomic structure of such organic / inorganic interfaces is basically unknown. Heterogeneous catalysis is based on the ability of surfaces to form and break chemical bonds to reactant molecules from the surrounding liquid or gas phase. Often adsorbates



also profoundly modify the structural and electronic properties of surfaces. This is utilized, for example, in sensors, but it also takes place when materials corrode. Finally, an understanding of the chemical and mechanical properties of coatings, which are used to protect materials or to make them more wear resistant, is of fundamental interest.

## RESEARCH HIGHLIGHTS

In the past years, our main focus has been on studying oxide surfaces, processes in heterogeneous catalysis and chemical properties of graphene. By using atomistic density-functional theory calculations we provided new insights into the very peculiar surface chemistry of indium oxide, a material which is frequently used for transparent electrodes. In a reducing environment  $\text{In}_2\text{O}_3(111)$  forms a highly ordered layer of indium ad-atoms instead of oxygen vacancies as other oxides, whereas a highly regular and stable pattern of hydroxyl groups is formed upon contact with water. For the example of methanol adsorption on rutile  $\text{TiO}_2(110)$  we showed that surface re-relaxations can induce strong substrate-mediated interactions between the molecules, which lead to rather complex arrangements of the adsorbates.

In heterogeneous catalysis we obtained a fundamental understanding of the so-called 'strong metal-support interactions' in Cu/ZnO catalysts, which are used for hydrogenation reactions, for example methanol synthesis from syngas. Accelerated *ab initio* molecular dynamics (AIMD) simulations revealed a subtle interplay between the reduction state of ZnO, the stability of reaction intermediates and the activation barriers of elementary reaction steps, which leads to an extensive free energy landscape and a complex reaction network for the hydrogenation of CO to methanol. In another project we provided a detailed analysis why some binary Ni-based compounds are excellent catalysts for the hydrogen evolution reaction in electrochemical water splitting.

Finally, to give an example of our studies on graphene chemistry, by using AIMD simulations we showed that the friction of intercalated sulfuric acid molecules in graphite strongly depends on the stacking and the oxidation state of the graphite layers. These results provide an atomistic understanding why only certain graphites form proper intercalates that can be delaminated into high-quality graphene in a scalable process.

## PERSPECTIVES

Most of our past studies were related to the chemical interaction of molecules from the gas phase with surfaces. In the future we will focus more on chemical processes at reactive solid / liquid interfaces. This requires the calculation of free energies by enhances molecular dynamics sampling techniques such as metadynamics. To overcome the limited time and length scales in *ab initio* molecular dynamics simulations we will continue our development of a more approximate, semiempirical method, which is based on a parameterization of the electronic structure problem (density-functional-based tight-binding). In our approach, this parameterization is derived directly from first-principles calculations without fitting.



## SELECTED PUBLICATIONS

- S. Seiler, C.E. Halbig, F. Grote, P. Rietsch, F. Börrnert, U. Kaiser, B. Meyer, S. Eigler, *Nat. Commun.*, **2018**, 9, 836
- M. Wagner, P. Lackner, S. Seiler, A. Brunsch, R. Bliem, S. Gerold, Z. Wang, J. Osiecki, K. Schulte, L.A. Boatner, M. Schmid, B. Meyer, U. Diebold, *ACS Nano*, **2017**, 11, 11531–11541
- M. Lepper, J. Köbl, T. Schmitt, M. Gurrath, A. de Siervo, M.A. Schneider, H.-P. Steinrück, B. Meyer, H. Marbach, W. Hieringer, *Chem. Commun.*, **2017**, 53, 8207–8210
- M. Ledendecker, H. Schlott, M. Antonietti, B. Meyer, M. Shalom, *Adv. Energy Mater.*, **2017**, 7, 1601735
- R.A. Schäfer, K. Weber, F. Hauke, V. Krstic, B. Meyer, A. Hirsch, *Angew. Chem. Int. Ed.*, **2017**, 55, 14858–14862
- D. Silber, P.M. Kowalski, F. Traeger, M. Buchholz, F. Bebensee, B. Meyer, Ch. Wöll, *Nat. Commun.*, **2016**, 7, 12888
- B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, *Nature*, **2014**, 505, 533–537
- L. Martinez-Suarez, J. Frenzel, D. Marx, B. Meyer, *Phys. Rev. Lett.*, **2013**, 110, 086108

## SELECTED REVIEWS

- J. Frenzel, J. Kiss, N.N. Nair, B. Meyer, D. Marx, Methanol Synthesis on ZnO from Molecular Dynamics, *Phys. Stat. Sol. B*, **2013**, 250, 1174–1190





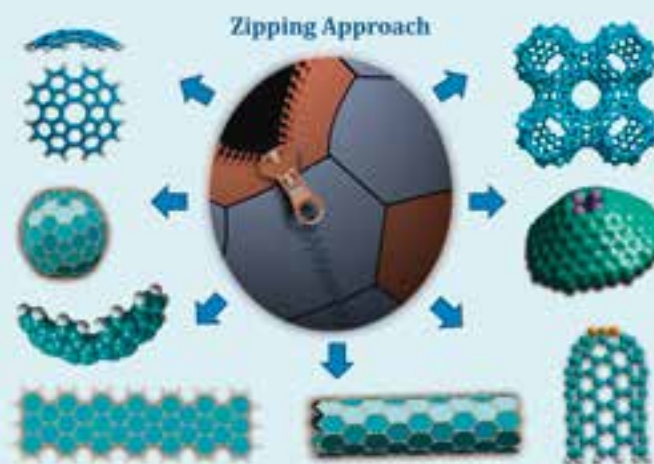
## ORGANIC CHEMISTRY

### PD DR. KONSTANTIN AMSHAROV

konstantin.amsharov@fau.de  
www.chemie.fau.de/amsharov

#### CURRICULUM VITAE

- Since 2014** Junior group leader, Organic Chemistry, University of Erlangen-Nürnberg, Germany
- 2012** Habilitation, Organic Chemistry, University of Stuttgart, Germany
- 2005 – 2013** Postdoctoral Fellow, Max Planck Institute FKF, Stuttgart, Germany
- 2002 – 2004** Postdoctoral Fellow, Institute of Macromolecular Compounds, Russian Academy of Science, St. Petersburg, Russia
- 1999 – 2002** PhD, Polymer Chemistry, Institute of Macromolecular Compounds, Russian Academy of Science, St. Petersburg, Russia
- 1994 – 1999** Chemistry studies, St. Petersburg State University, St. Petersburg, Russia



#### OBJECTIVES AND PERSPECTIVES

Our research group has its main focus on the rational synthesis of atomically-precise carbon-based nano-architectures including the rational synthesis of non-classical fullerenes, buckybolls, graphene nanoribbons, nanographenes and carbon nanotubes. Our synthetic strategy is based on the synthesis of the precursor molecules—polycyclic aromatic hydrocarbons, containing the carbon framework required for the formation of the target nanostructure. The respective precursor molecule can be “rolled up” to the desired carbon nanostructure via intramolecular Aryl-Aryl domino-coupling. The characteristic feature of the approach is a zipper mechanism of cyclization by which the regioselectivity of each condensation step is unambiguously predefined by the specially “designed” precursor structure. Our main goal is to find and to develop alternative synthetic approaches suitable for preparative production of various carbon allotrope in isomerically pure form.

#### SELECTED PUBLICATIONS

- A.K. Steiner, K. Amsharov, *Angew. Chem. Int. Ed.*, **2017**, 56, 147-32-14736
- J.F. Greisch, K. Amsharov, J. Weippert, P. Weis, A. Böttcher, M.M. Kappes, *J. Am. Chem. Soc.*, **2016**, 138(35), 11254 – 11263
- J.R. Sanchez-Valencia, T. Dienel, O. Gröning, I. Shorubalko, A. Mueller, M. Jansen, K. Amsharov, P. Ruffieux, R. Fasel, *Nature*, **2014**, 512, 61 – 64
- K. Amsharov, M. Kabdulov, M. Jansen, *Angew. Chem. Int. Ed.*, **2012**, 51, 4594 – 4597
- K. Amsharov, N. Abdurakhmanova, S. Stepanow, S. Rauschenbach, M. Jansen, K. Kern, *Angew. Chem. Int. Ed.*, **2010**, 49, 9392 – 9396

#### SELECTED AWARDS

- 2013 Heisenberg Stipendium (DFG)



## THEORETICAL CHEMISTRY

### PD DR. ANDREAS HESSELMANN

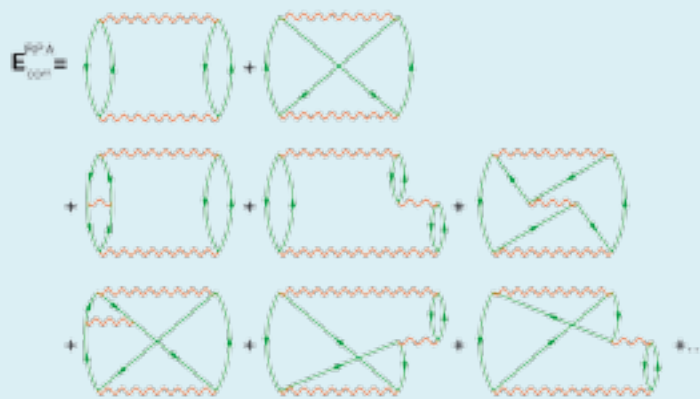
andreas.hesselmann@fau.de  
www.chemie.fau.de/hesselmann

#### CURRICULUM VITAE

<b>Since 2012</b>	Lecturer (PD) at the University of Erlangen-Nürnberg, Germany
<b>2012</b>	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Göring), Germany
<b>2006</b>	Postdoctoral Fellow, Theoretical Chemistry, University of Erlangen-Nürnberg, Germany
<b>2005</b>	Postdoctoral Fellow, University of Århus (Prof. Jørgensen), Denmark
<b>2004</b>	Postdoctoral Fellow, University of Duisburg-Essen (Prof. Jansen), Germany
<b>2003</b>	PhD, Theoretical Chemistry, Heinrich-Heine University of Düsseldorf, Germany

#### RESEARCH HIGHLIGHTS

We are working on the development of generally applicable new density functionals that are based on wave-function methods but in which the favourable scaling behaviour of standard DFT is conserved. This will require the combination of the method with fast numerical algorithms to extend the applicability to large systems. A first step in this direction has already been made by introducing a new orbital-dependent exchange-correlation functional derived from the fluctuation-dissipation formula with exact Kohn-Sham exchange.



Density-functional theory methods are also employed to describe intramolecular correlation effects in the framework of the intermolecular Symmetry-Adapted Perturbation Theory (SAPT). This method, termed DFT-SAPT, enables a decomposition of intermolecular interaction energies into distinct physically interpretable terms like electrostatics, induction, dispersion and exchange repulsion types of interaction. In this way, in contrast to the commonly used supermolecular methods that are used to describe intermolecular interactions with quantum chemistry methods, the intermolecular perturbation theory also allows a characterisation and deeper understanding of the bonding in intermolecular complexes.

#### FUTURE PERSPECTIVE

The structures and stabilities of large molecules depend strongly on the underlying inter- and intramolecular forces between noncovalently bonded groups. While intramolecular interactions determine the predominant conformations of a molecule, intermolecular interactions between a solute with a solvent environment can greatly influence the structures and properties of a molecule relative to the gas phase. Therefore, we are planning to derive theoretical methods which allow to quantify the different energy contributions in complex embedded systems in order to be able to describe the influence of solvent effects on the molecular structure.

#### SELECTED PUBLICATIONS

- O. R. Meitei, A. Heßelmann, *J. Comp. Chem.*, **2017**, 25, 2500
- C. Esterhuysen, A. Heßelmann, T. Clark, *Chem. Phys. Chem.*, **2017**, 18, 772
- A. Heßelmann, *J. Chem. Theory Comput.*, **2015**, 11, 1607
- A. Heßelmann, T. Korona, *J. Chem. Phys.*, **2014**, 141, 094107
- A. Heßelmann, A. Göring, *Mol. Phys.*, **2010**, 108, 359
- A. Heßelmann, A. Göring, *Phys. Rev. Lett.*, **2009**, 102, 233003
- A. Heßelmann, G. Jansen, *M. Schütz, J. Am. Chem. Soc.*, **2006**, 128, 11730
- A. Heßelmann, G. Jansen, *M. Schütz, J. Chem. Phys.*, **2005**, 122, 014103

#### SELECTED REVIEWS

- A. Heßelmann, „Intermolecular interaction energies from Kohn-Sham Random Phase Approximation correlation methods“, in: *Non-covalent Interactions in Quantum Chemistry and Physics*, Ed.: Alberto Otero de la Roza und Gino DiLabio, Elsevier, **2017**

#### SELECTED AWARDS

- 2004 Gottschalk-Diederich-Baedeker Award



## THEORETICAL CHEMISTRY

### PD DR. WOLFGANG HIERINGER

wolfgang.hieringer@fau.de  
www.chemie.fau.de/hieringer

#### CURRICULUM VITAE

Since 2010	Lecturer (PD), Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany
2010	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg, Germany
2004 – 2010	Habilitand, Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Görling), Germany
2003 – 2004	Postdoctoral Fellow, Theoretical Chemistry at the Technical University of Munich (TUM), Germany
2002 – 2003	Postdoctoral Fellow, Theoretical Chemistry at the Universität Bonn, Germany
2000 – 2002	Postdoctoral Fellow, Theoretical Chemistry at the Vrije Universiteit Amsterdam (Prof. Baerends), NL
2000	PhD in Inorganic Chemistry, Technical University of Munich (TUM) (Prof. W. A. Herrmann), Germany
1997	Diploma Degree in Chemistry, Technical University of Munich (TUM), Germany

#### RESEARCH HIGHLIGHTS

In our research we use quantum chemical methods, in particular density functional theory, to theoretically study complex problems in catalysis, surface science, and photophysics, with a special focus on systems containing transition metals. Recent examples deal with the

theoretical investigation of large metalloporphyrin molecules at surfaces, surface-bound organometallic coordination polymers or nanostructures. We have been able to identify, for the first time, the surface analogue of the so-called *trans* effect, which has been known before only in the field of coordination chemistry. We have elucidated the mechanism of the homogeneous ruthenium-catalyzed water-gas shift reaction and other reactions in ionic liquid solution, and contributed to the characterization of one of the very first U(II) complexes known to date. We also work on spectroscopic techniques such as core-level spectroscopy. Recently, we have developed new density-functional methods to both accurately and efficiently describe excitations of core-electrons in large molecules, followed by successful applications in surface science. Many of our projects involve collaborations with experimentally working groups of various disciplines.

#### FUTURE PERSPECTIVE

Our goal is to design novel functional transition metal systems with unprecedented catalytic, electronic, or optical properties using modern theoretical methods. To this end, we mainly use accurate quantum chemical methods, but we will also combine them with more efficient force-field techniques to treat environmental effects. We will furthermore continue to develop computer programs which provide the necessary functionality to achieve our goals.

#### SELECTED PUBLICATIONS

- M. Lepper, J. Köbl, T. Schmitt, M. Gurrath, A. de Siervo, M. A. Schneider, H.-P. Steinrück, B. Meyer, H. Marbach, W. Hieringer, *Chem. Commun.*, **2017**, 53, 8207–8210
- M. Chen, J. Shang, Y. Wang, K. Wu, J. Kuttner, G. Hilt, W. Hieringer, J. M. Gottfried, *ACS Nano*, **2017**, 11, 134–143
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- S. La Pierre, A. Scheurer, F. W. Heinemann, W. Hieringer, K. Meyer, *Angew. Chem. Int. Ed.*, **2014**, 53, 7158–7162
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- H. Schulz, A. Görling, W. Hieringer, *Inorg. Chem.*, **2013**, 52, 4786–4794
- Q. Fan, C. Wang, Y. Han, J. Zhu, W. Hieringer, J. Kuttner, G. Hilt, J. M. Gottfried, *Angew. Chem. Int. Ed.*, **2013**, 52, 4668–4672
- W. Hieringer, K. Flechtner, A. Kretschmann, K. Seufert, W. Auwärter, J. V. Barth, A. Görling, H.-P. Steinrück, J. M. Gottfried, *J. Am. Chem. Soc.*, **2011**, 133, 6206–6222

#### SELECTED AWARDS

- 2011 Starting Grant of the Cluster of Excellence “Engineering of Advanced Materials”
- 2003 Marie Curie Reintegration Grant of the European Commission
- 2000 Marie Curie Individual Fellowship of the European Commission





## INORGANIC CHEMISTRY

### PD DR. MARAT M. KHUSNIYAROV

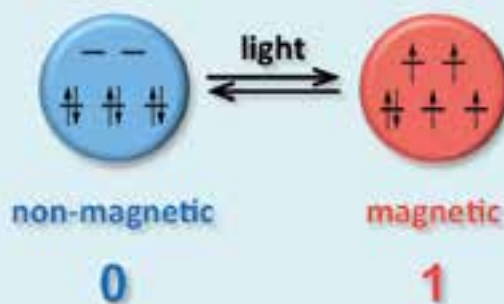
marat.khusniyarov@fau.de  
www.chemie.fau.de/khusniyarov

#### CURRICULUM VITAE

- Since 2016** Lecturer (PD), University of Erlangen-Nürnberg, Germany
- 2016** Habilitation in Inorganic Chemistry, University of Erlangen-Nürnberg (Prof. K. Meyer), Germany
- 2009 – 2016** Junior group leader, Inorganic Chemistry, University of Erlangen-Nürnberg, Germany
- 2006 – 2009** Postdoctoral Fellow, Max Planck Institute for Bioinorganic Chemistry, Mülheim an der Ruhr, Germany
- 2002 – 2006** PhD in Inorganic Chemistry, Philipps University of Marburg, Germany
- 1997 – 2002** Study of Chemistry, Department of Natural Science, Novosibirsk State University, Russia

#### RESEARCH HIGHLIGHTS

Modern coordination chemistry is at the heart of our research. We develop, synthesize, and investigate the properties of unique metal complexes in the context of particular applications including molecular switches, molecular sensors, and functional materials. We are not limited to the synthesis of coordination compounds and preparation of materials, but also use a broad range of physical and spectroscopic methods, photochemistry, and ab initio quantum chemical calculations to confirm the desired functionality.



We developed a unique class of magnetic molecular switches based on spin-crossover iron(II) complexes featuring photoactive ligands. These complexes can be reversibly and efficiently switched between non-magnetic “0” and magnetic “1” states with light at room temperature. The unprecedented photoswitching at molecular level was achieved in solutions and in the solid state, followed by very recent results on photoswitchable thin films.

We brought two novel concepts to the field of molecular magnetism: Coordination-Induced Valence Tautomerism (CIVT) and Ligand-Driven Light-Induced Valence Tautomerism (LD-LIVT). Those allow for chemical and unprecedented photochemical switching of valence tautomeric metal complexes and associated magnetic properties at room temperature.

#### FUTURE PERSPECTIVE

We will bring the developed molecular switches to various surfaces to achieve the control at the ultimate single-molecule level, which will allow to construct magnetic molecular memory and magnetic molecular sensors. Responsive contrast agents for magnetic resonance imaging will be developed on the base of spin-crossover metal complexes. Finally, we aim to develop unique photoswitchable catalysts for the copolymerization of olefins.

#### SELECTED PUBLICATIONS AND REVIEWS

- L. Poggini, M. Milek, G. Lodi, A. Naim, G. Poneti, L. Squillantini, A. Magnani, F. Totti, P. Rosa, M. M. Khusniyarov, M. Mannini, *Materials Horizons*, **2018**, DOI: 10.1039/C7MH01042G
- M. Mörtel, A. Witt, F. W. Heinemann, S. Bochmann, J. Bachmann, M. M. Khusniyarov, *Inorg. Chem.*, **2017**, 56, 13174–13186
- M. M. Khusniyarov, *Chem. Eur. J.*, **2016**, 22, 15178–15191
- B. Rösner, M. Milek, A. Witt, B. Gobaut, P. Torelli, R. H. Fink, M. M. Khusniyarov, *Angew. Chem. Int. Ed.*, **2015**, 54, 12976–12980
- A. Witt, F. W. Heinemann, M. M. Khusniyarov, *Chem. Sci.*, **2015**, 6, 4599–4609
- A. Witt, F. W. Heinemann, S. Sproules, M. M. Khusniyarov, *Chem. Eur. J.*, **2014**, 20, 11149–11162
- M. Milek, F. W. Heinemann, M. M. Khusniyarov, *Inorg. Chem.*, **2013**, 52, 11585–11592

#### SELECTED AWARDS

- 2016 “Emerging Talents Initiative” Grant, FAU Erlangen-Nürnberg, Germany
- 2014 Temporary position for principal investigator, German Research Foundation, Germany
- 2009 Liebig Fellowship, Fonds der Chemischen Industrie, Germany
- 2006 Postdoctoral Fellowship, Max Planck Society, Germany
- 2002 Diploma in Chemistry with honors, Novosibirsk State University, Russia



## ORGANIC CHEMISTRY

### PD DR. MILAN KIVALA

[milan.kivala@fau.de](mailto:milan.kivala@fau.de)

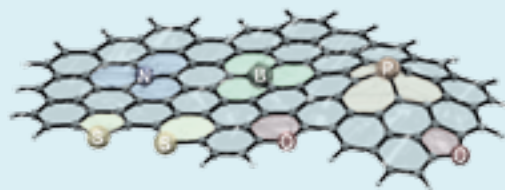
[www.chemie.fau.de/kivala](http://www.chemie.fau.de/kivala)

#### CURRICULUM VITAE

<b>Since 2017</b>	Stand-in Professor, Organic Chemistry, University of Erlangen-Nürnberg, Germany
<b>2016</b>	Habilitation in Organic Chemistry, University of Erlangen-Nürnberg (Prof. Tykwinski), Germany
<b>2011–2016</b>	Junior group leader, Organic Chemistry, University of Erlangen-Nürnberg, Germany
<b>2009–2011</b>	Postdoctoral Fellow, Max Planck Institute for Polymer Research (Prof. Müllen), Mainz, Germany
<b>2008–2009</b>	Postdoctoral Fellow, ETH Zürich (Prof. Diederich), Switzerland
<b>2004–2008</b>	PhD, Organic Chemistry, ETH Zürich (Prof. Diederich), Switzerland
<b>1998–2003</b>	Chemistry studies, University of Chemistry and Technology, Prague, Czech Republic

#### RESEARCH HIGHLIGHTS

The focal point of our research program is the synthesis and study of heteroatom-doped polycyclic aromatic hydrocarbons (PAHs) with the aim to i) investigate the influence of interior heteroatoms on their fundamental characteristics and ii) apply the resulting compounds as active materials in organic optoelectronic devices. We use various rationally designed low-molecular building blocks that



are transformed into unprecedented  $\pi$ -conjugated heteroatom-rich architectures in newly developed synthetic protocols. While our research program is clearly synthesis-driven, fundamental understanding and function of the resulting compounds are essential for us.

#### FUTURE PERSPECTIVE

The long-term objective of this project is the fabrication of very large heteroatom-doped  $\pi$ -conjugated scaffolds which should not only act as defined molecular fragments of heteroatom-doped carbon allotropes but also display fascinating chemistry and unprecedented properties. While pursuing this goal, we expect that many intriguing discoveries will be made. This project is situated at the interface between organic chemistry, physical organic chemistry, and materials science. In other words, the compounds prepared within this research will become the subject of interdisciplinary collaborative investigations.

#### SELECTED PUBLICATIONS

- Z. Yang, J. Gebhardt, T. A. Schaub, T. Sander, J. Schönamsgruber, H. Soni, A. Görling, M. Kivala, S. Maier, *Nanoscale*, **2018**, 10, 3769–3776
- B. D. Gliemann, V. Strauss, J. F. Hitzengerger, P. O. Dral, F. Hampel, J.-P. Gisselbrecht, T. Drewello, W. Thiel, D. M. Guldi, M. Kivala, *Chem. Eur. J.*, **2017**, 23, 12353–12362
- T. A. Schaub, S. M. Brülls, P. O. Dral, F. Hampel, H. Maid, M. Kivala, *Chem. Eur. J.*, **2017**, 23, 6988–6992
- A. Roth, T. A. Schaub, U. Meinhardt, D. Thiel, J. Storch, V. Cirkva, P. Jakubik, D. M. Guldi, M. Kivala, *Chem. Sci.*, **2017**, 8, 3494–3499
- C. Steiner, J. Gebhardt, M. Ammon, Z. Yang, A. Heidenreich, N. Hammer, A. Görling, M. Kivala, S. Maier, *Nat. Commun.*, **2017**, 8, 14765
- T. A. Schaub, E. M. Zolnhofer, D. P. Halter, T. E. Shubina, F. Hampel, K. Meyer, M. Kivala, *Angew. Chem. Int. Ed.*, **2016**, 55, 13597–13601
- C. Steiner, B. D. Gliemann, U. Meinhardt, M. Gurrath, B. Meyer, M. Kivala, S. Maier, *J. Phys. Chem. C*, **2015**, 119, 25945–25955
- A. T. Haedler, K. Kreger, A. Issac, M. Kivala, N. Hammer, J. Köhler, H.-W. Schmidt, R. Hildner, *Nature*, **2015**, 523, 196–199
- N. Hammer, T. E. Shubina, J.-P. Gisselbrecht, F. Hampel, M. Kivala, *J. Org. Chem.*, **2015**, 80, 2418–2424
- P. O. Dral, M. Kivala, T. Clark, *J. Org. Chem.*, **2013**, 78, 1894–1902

#### SELECTED REVIEWS

- N. Hammer, T. A. Schaub, U. Meinhardt, M. Kivala, *Chem. Rec.*, **2015**, 15, 1119–1131

#### SELECTED AWARDS

- 2017 Emmy-Noether-Habilitationspreis des Universitätsbundes Erlangen-Nürnberg e.V.
- 2017 Forschungspreis der Dr. Otto Röhm Gedächtnisstiftung
- 2014 EAM Starting Grant, DFG Exzellenzcluster 'Engineering of Advanced Materials'
- 2012 Fonds der Chemischen Industrie Grant
- 2010–2012 Humboldt Fellowship for Postdoctoral Researchers
- 2009–2010 Swiss National Science Foundation Fellowship
- 2009 ETH Medal
- 2003 Honor Award of Josef Hlávka



## MEDICINAL CHEMISTRY

### PD DR. HARALD LANIG

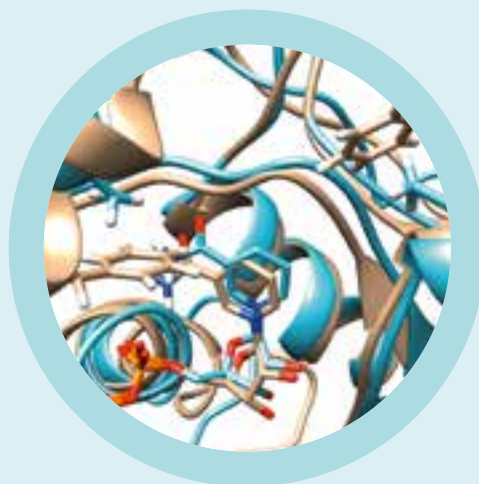
harald.lanig@fau.de  
www.chemistry.nat.fau.eu/lanig

#### CURRICULUM VITAE

- Since 2013** Managing Director of the Central Institute for Scientific Computing (ZISC)
- Since 2012** Lecturer (PD) at the University of Erlangen-Nürnberg, Germany
- 2012** Habilitation in Medicinal Chemistry, University of Erlangen-Nürnberg (Prof. Gmeiner), Germany
- 2005 – 2012** Postdoctoral Fellow, Medicinal Chemistry, University of Erlangen-Nürnberg, Germany
- 2000 – 2005** Research Assistant, Pharmacy and Food Chemistry, University of Erlangen-Nürnberg, Germany
- 1995 – 1999** Postdoctoral Fellow, Organic Chemistry, Computer Chemistry Center, University of Erlangen-Nürnberg, Germany
- 1994** PhD in Physical Chemistry, University of Würzburg, Germany

#### RESEARCH HIGHLIGHTS

My general interest focuses on the exploration of structure and dynamics of proteins and DNA with classical simulation methods. I am applying Molecular Dynamics, Comparative Modeling and Molecular Docking techniques to understand how chemical signals are processed, transduced, and converted into protein structural changes.



es. For example, the activation of G-Protein Coupled Receptors and Tetracycline Repressor variants, structure and dynamics of Collagen type II model systems, Orphan Nuclear Receptors, enzymes like the Prolyl Hydroxylase PHD2 and Progesterone 5 $\beta$ -Reductases have been investigated by modelling and simulation techniques.

#### FUTURE PERSPECTIVE

Based on my experience in modelling and simulation of protein structures and dynamics, I am focusing on proteins which are able to interact with oligonucleotides (transcription factors) to understand how the interaction with DNA changes its principal properties. Furthermore, I am developing structural models for Fibulin-4, a large calcium binding glycoprotein that has an important role in development and integrity of extracellular matrices and already a single mutation may cause severe diseases. In all current and future projects, I am emphasizing the collaboration with experimentalists for a successful synergy with theory in an iterative way.

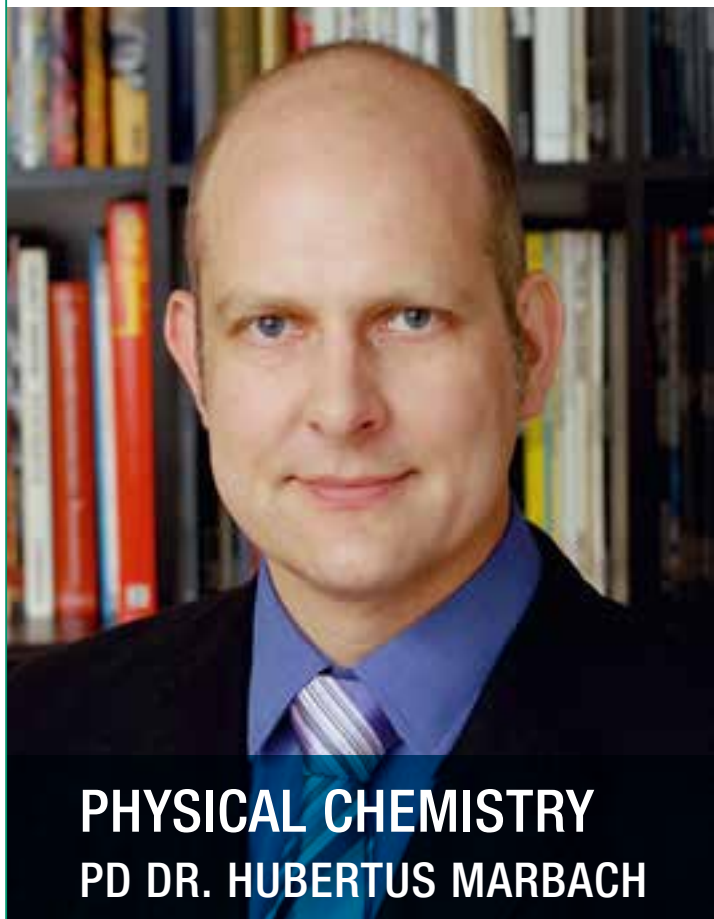
#### SELECTED PUBLICATIONS

- T. Sasaki, H. Lanig, K. von der Mark, *Matrix Biology*, **2016**, 132–149
- J. Petersen, H. Lanig, J. Munkert, P. Bauer, F. Müller-Uri, W. Kreis, *J. Biomol. Struct. Dynam.*, **2015**, 1667–1680
- R. C. Kling, N. Tschammer, H. Lanig, T. Clark, P. Gmeiner, *PLoS One*, **2014**, 9, e100069
- C. R. Wick, H. Lanig, C. M. Jäger, N. Burzlaff, T. Clark, *Eur. J. Inorg. Chem.*, **2012**, 4973–4985
- F. Haberl, H. Lanig, T. Clark, *Proteins*, **2009**, 77, 857–866
- U. Böiers, H. Lanig, B. Sehnert, R. Holmdahl, H. Burkhardt, *Eur. J. Immunol.*, **2008**, 38, 2784–2795
- H. Lanig, T. Clark, M. G. Hicks, C. Kettner, Proceedings of the International Beilstein Workshop, **2008**
- K. von der Mark, H. von der Mark, E. Pöschl, H. Lanig, T. Sasaki, R. Deutzmann, *J. Mol. Biol.*, **2007**, 371, 1188–1203
- F. Boeckler, H. Lanig, P. Gmeiner, *J. Med. Chem.*, **2005**, 48, 694–709

#### SELECTED AWARDS

- Members of the German Pharmaceutical Society and the Royal Society of Chemistry
- Chairman of the Molecular Graphics and Modelling Society—German Section
- Grant from the Bavarian Ministry of Science and Research
- Grants from Federal Ministry of Education and Research and Fonds der Chemischen Industrie





## PHYSICAL CHEMISTRY

### PD DR. HUBERTUS MARBACH

hubertus.marbach@fau.de  
www.chemie.fau.de/marbach

#### CURRICULUM VITAE

- 2014 – 2017** Stand-in Professor, Experimental Physics, University of Erlangen-Nürnberg, Germany
- Since 2010** Lecturer (PD), Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 2010** Habilitation in Physical Chemistry at the University of Erlangen-Nürnberg (Prof. Steinrück), Germany
- 2004 – 2009** Postdoctoral Fellow, Physical Chemistry at the University of Erlangen-Nürnberg (Prof. Steinrück), Germany
- 2002 – 2004** Postdoctoral Fellow at the Surface Science Center, University of Pittsburgh (Prof. Yates, Prof. Levy), PA, USA
- 2002** PhD in Physical Chemistry and Electrochemistry, University of Hannover (Prof. Imbihl), Germany
- 1997** Diploma Degree in Physics, University of Dortmund, Germany

#### RESEARCH HIGHLIGHTS

The generation and investigation of nanostructures on surfaces is in the center of my current research activities. In my working group we follow different routes to fabricate tailor-made nanoscaled struc-

tures. The first (bottom-up) approach is based on the self-assembly of molecules or atoms on surfaces. In this context the geometric and electronic structure of porphyrin derivatives as prototype examples for functional molecules has been intensively studied on different substrates. In particular, we systematically explored temperature dependent processes which allow for determining the energetics of the corresponding molecular processes close to room temperature (e.g., diffusion, metalation reaction, conformational switching). In our second (top-down) approach a highly focused electron beam is used to locally dissociate adsorbed precursor molecules (electron beam induced deposition, EBID) or to directly modify the properties of the substrate with lithographical control. For both projects we target the understanding of the fundamental physical and chemical processes on an atomic level based on microscopic and spectromicroscopic investigations. Our main methods are scanning tunneling microscopy and spectroscopy, scanning electron microscopy, local Auger electron spectroscopy and atomic force microscopy in an ultra high vacuum environment.

#### FUTURE PERSPECTIVE

In the future we will target the combination of the two projects described above. Structures fabricated with the electron beam techniques will serve as templates for the local anchoring and/or functionalization of large organic molecules, i.e., in particular porphyrins.

Other future research activities will include:

- further investigation of fundamental aspects of electron induced processes
- further exploration of the controlled conformational switching of individual porphyrin molecules close to room temperature

#### SELECTED PUBLICATIONS

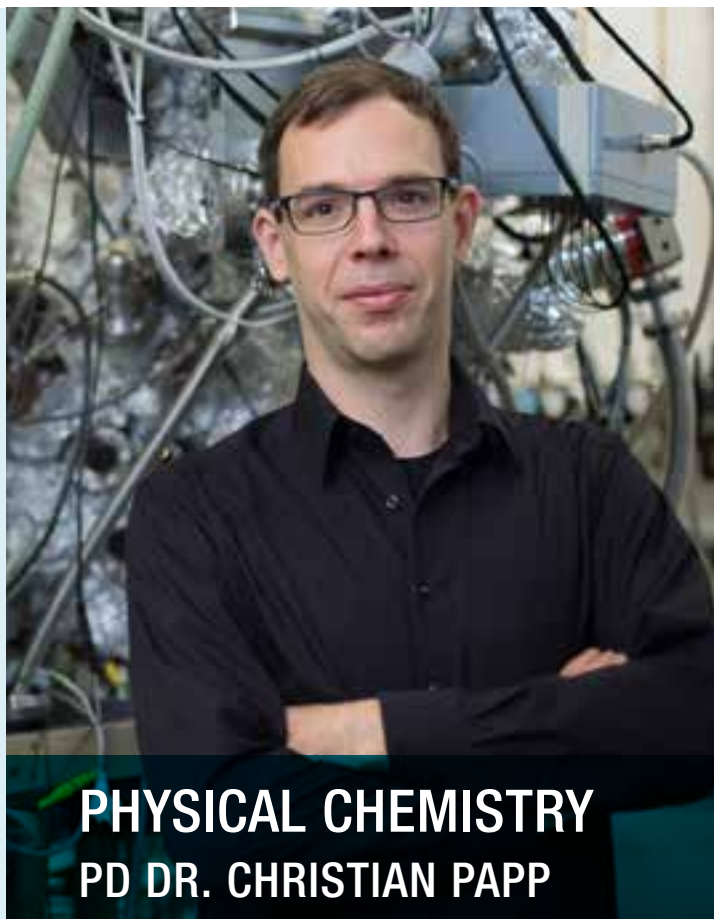
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- S. Ditzel, M. Stark, M. Drost, F. Buchner, H.-P. Steinrück, H. Marbach, *Angew. Chem. Int. Ed.*, **2012**, 51, 10898–10901
- M.-M. Walz, M. Schirmer, F. Vollnhals, T. Lukasczyk, H.-P. Steinrück, H. Marbach, *Angew. Chem. Int. Ed.*, **2010**, 49, 4669–4673
- T. Lukasczyk, M. Schirmer, H.-P. Steinrück, H. Marbach, *Small*, **2008**, 4, 841–844

#### SELECTED REVIEWS

- H. Marbach, Surface mediated in situ metalation reactions of porphyrins at the solid vacuum interface, *Acc. Chem. Res.*, **2015**, 48, 2649–2658
- H. Marbach, Electron beam induced surface activation: a method for the lithographic fabrication of nanostructures via catalytic processes, *Appl. Phys. A*, **2014**, 117, 987–995
- H. Marbach and H.-P. Steinrück, Studying the dynamic behaviour of porphyrins as prototype functional molecules by scanning tunnelling microscopy close to room temperature, *Chem. Commun.*, **2014**, 50, 10225–10228

#### SELECTED AWARDS

- 2015 PCCP Hot Topic Prize, Bunsen Tagung, Bochum
- 2010 PCCP Hot Topic Prize, Bunsen Tagung, Bielefeld
- 2008 PCCP Hot Topic Prize, Bunsen Tagung, Saarbrücken



## PHYSICAL CHEMISTRY

### PD DR. CHRISTIAN PAPP

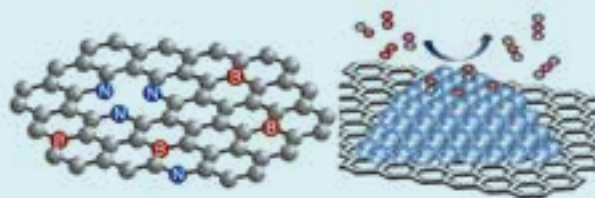
christian.papp@fau.de  
www.chemie.fau.de/papp

#### CURRICULUM VITAE

- Since 2015** Lecturer (PD), Physical Chemistry at the University of Erlangen-Nürnberg, Germany
- 2011 – 2014** Habilitation, Department of Chemistry and Pharmacy, Universität Erlangen-Nürnberg, Germany
- Since 9/2009** Group leader of the surface and in-situ spectroscopy group
- 2008 – 2009** Postdoctoral fellow (Feodor Lynen grant), Materials Science Division, Lawrence Berkeley National Laboratory and Physics Department, University of California, Davis (Charles S. Fadley)
- 2007** Postdoctoral work, Chair of Physical Chemistry, Universität Erlangen-Nürnberg
- 2007** PhD in Physical Chemistry at the University of Erlangen-Nürnberg, Germany

#### RESEARCH HIGHLIGHTS

His research is focused on the fundamental understanding of surface processes on the atomic and molecular level. The systems studied range from the reaction of atoms and small molecules such as sulfur, and CO to the more complex surface reactions of Liquid Organic Hydrogen Carriers (LOHCs), which are a potential solution of chemical hydrogen storage. He studies the formation and properties of



chemically modified graphene, including nitrogen- and boron-doped graphene as well as single-sided graphane. Model catalytic studies of the reactivity of nanocluster arrays on a graphene template lead to new quantitative insights in the chemistry on carbon-supported clusters, elucidating the adsorption properties, the reactivity as well as poisoning mechanisms. A further project is the investigation of surface reactions with XPS at near ambient pressures, with ionic liquids and model catalysts. His studies are conducted with in situ XPS at the synchrotron facility BESSY II of the Helmholtz-Zentrum Berlin, and in the lab in Erlangen.

#### FUTURE PERSPECTIVE

In the future we target to further expand our fundamental knowledge on the surface chemistry on surfaces ranging flat surfaces to nanoclusters for the catalysis of small molecules to LOHCs and other novel energy storage applications. Graphene and other novel supported 2D materials will be synthesized and functionalized with the aim to obtain a fundamental understanding of their reactivity and to get chemical handle to tune their physicochemical properties. A further new route in our studies are liquid metal alloys used as heterogeneous catalysts.

#### SELECTED PUBLICATIONS

- F. Späth, J. Gebhardt, F. Düll, U. Bauer, P. Bachmann, C. Gleichweit, A. Görling, H. P. Steinrück, and C. Papp, *2D Materials*, **2017**, 4, 35026
- N. Taccardi, M. Grabau, J. Debuschewitz, M. Distaso, M. Brandl, R. Hock, F. Rietzler, F. Maier, C. Papp, J. Erhard, C. Neiss, A. Görling, H.-P. Steinrück, and P. Wasserscheid, *Nat. Chem.*, **2017**, 9, 862
- D. Fantauzzi, S. Krick Calderón, J. E. Mueller, M. Grabau, C. Papp, H.-P. Steinrück, T. P. Senftle, A. C. T. van Duin, and T. Jacob, *Angew. Chem. Int. Ed.*, **2017**, 56, 2594
- I. Niedermaier, M. Bahlmann, C. Papp, C. Kolbeck, W. Wei, S. Krick-Calderón, M. Grabau, P. Schulz, P. Wasserscheid, H.-P. Steinrück, and F. Maier, *J. Am. Chem. Soc.*, **2014**, 136, 436
- C. Gleichweit, M. Amende, S. Schernich, W. Zhao, M. P. A. Lorenz, O. Höfert, N. Brückner, P. Wasserscheid, J. Libuda, H.-P. Steinrück, and C. Papp, *ChemSusChem*, **2013**, 6, 974
- J. Englert, C. Dotzer, G. Yuang, M. Schmid, C. Papp, J. M. Gottfried, H.-P. Steinrück, E. Spieker, F. Hauke, and A. Hirsch, *Nat. Chem.*, **2011**, 3, 279

#### SELECTED REVIEWS

- C. Papp, *Catalysis Letters*, **2017**, 147, 2
- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, *The Chemical Record*, **2014**, 14, 879
- C. Papp, H.-P. Steinrück, *Surface Science Reports*, **2013**, 68, 446

#### SELECTED AWARDS

- 2015 Emmy-Noether-Habilitationspreis des Universitätsbundes Erlangen-Nürnberg
- 2015 Dozentenpreis of the Fonds der Chemischen Industrie



## COMPUTATIONAL CHEMISTRY

PD DR. TATYANA SHUBINA

tatyana.shubina@fau.de  
www.chemie.fau.de/shubina

### CURRICULUM VITAE

<b>Since 2018</b>	Group leader, Computational Material Chemistry, University of Erlangen-Nürnberg, Germany
<b>2018</b>	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Clark), Germany
<b>2012 – 2017</b>	Junior group leader, Theoretical Chemistry, University of Erlangen-Nürnberg, Germany
<b>2007 – 2011</b>	Postdoctoral Fellow, Computer Chemistry Center, University of Erlangen-Nürnberg, Germany
<b>2005 – 2006</b>	Humboldt Fellow, Computer Chemistry Center, University of Erlangen-Nürnberg, Germany
<b>2003</b>	PhD in Organic Chemistry at the National Technical University of Ukraine (KPI), Ukraine

### RESEARCH HIGHLIGHTS

Since 1996 my research interests have been focusing on solving various problems in the field of chemistry with the help of computers, specifically application of computational chemistry. It has become an indispensable tool that is nowadays commonly used together with state-of-the-art experimental techniques. It can be applied successfully to study mechanisms of reactions, to gain an insight into the structures and properties of sometimes-elusive species that cannot

be detected by experimental methods, to predict new compounds or new drugs—to name but a few areas.

Over the past five decades, our ability to treat material properties at a fundamental, quantum level has improved tremendously, in large part because the advance of computer power has allowed us to attack far more complex and larger problems. Today it is possible, for instance, to calculate the unit cell dimensions of a crystalline solid from first principles with a reliability in the range of a few percent. Once the geometry has been determined, a range of properties, such as electronic, optical and magnetic can also be calculated with a high degree of reliability. We can also look in detail into properties and reactivity of, for example, enzymes—molecules that are responsible for a vast number of processes in all living organisms, as opposed to simple 5–10 atom molecules, say 10–15 years ago.

Since I joined the Computer Chemistry Center in Erlangen in 2005, I have carried out various projects—in collaboration with our collaborators-experimentalists—focusing on studying properties, formation, reactivity and application of porphyrins and related systems, as well as electron-transfer (ET) reactions (significant to biological processes and solar cell devices).

### FUTURE PERSPECTIVE

While such methods can be extremely helpful at the R&D stage performed at the research lab, however, presently they cannot be applied at the industrial level outside the pharmaceutical industry.

There is an obvious room for improvement that can come from introduction of machine learning, automation and robotization in chemistry and chemical technology. Currently, the machine learning approach for predicting chemical reactions outcome is largely untapped area; not to mention that lots of data and knowledge that can be used is wasted—because failed experiments are never reported. The existing sophisticated synthesis machines are spending disproportionate amount of time only on selected chemical transformations and do their work in the same batch-by-batch manner as humans. Automation of synthesis is done only for key steps along the chemical reaction pathway and requires on/off human involvement for non-automated parts. Fully automated continuous synthesis done by machines is still missing.

Since 2015, I have become very interested in new emerging fields and technologies, such as blockchain and IoT and their application in chemistry. Consequently, my research interests and activities had shifted towards those topics, including software development. Our research projects are focused on: application of machine learning and artificial intelligence in chemistry and wrapping up data security and ownership with blockchain.

### SELECTED PUBLICATIONS AND REVIEWS

- R. Lippert, T.E. Shubina, S. Vojnovic, A. Pavic, J. Veselinovic, J. Nikodinovic-Runic, N. Stankovic, I. Ivanović-Burmazović, *J. Inorg. Biochem.*, **2017**, 171, 76
- T.A. Schaub, E.M. Zolnhofer, D.P. Halter, T.E. Shubina, F. Hampel, K. Meyer, M. Kivala, *Angew. Chem. Int. Ed.*, **2016**, 55, 13597
- S. Hematian, I. Kenkel, T.E. Shubina, M. Dürr, J. Liu, M. Siegler, I. Ivanović-Burmazović, K. Karlin, *J. Am. Chem. Soc.*, **2015**, 137, 6602





**PHYSICAL CHEMISTRY**  
**DR. OLE LYTKEN**

ole.lytken@fau.de  
www.chemie.fau.de/lytken

#### CURRICULUM VITAE

- Since 2011** Junior group leader, Physical Chemistry, University of Erlangen-Nürnberg, Germany
- 2009 – 2011** Postdotoral Fellow, Physical Chemistry, University of Erlangen-Nürnberg, Germany
- 2006 – 2008** Postdotoral Fellow, University of Washington, Seattle, USA
- 2005** PhD, Chemical Engineering, Technical University of Denmark, Lyngby, Denmark

#### OBJECTIVES AND PERSPECTIVES

Our focus is the reactions of large organic molecules, such as porphyrins, with single-crystal surfaces. We study the reactions both in ultrahigh vacuum but also in the liquid phase, using monochromatized and synchrotron-radiation X-ray photoelectron spectroscopy combined with mass spectrometry. Our goal is a fundamental understanding of the reactions occurring on the surfaces.

#### SELECTED PUBLICATIONS AND REVIEWS

- J. Köbl, T. Wang, C. Wang, M. Drost, F. Tu, Q. Xu, H. Ju, D. Wechsler, M. Franke, H. Pan, H. Marbach, H.-P. Steinrück, J. Zhu, O. Lytken, *Chemistry Select*, **2016**, 1, 6103
- M. Franke, F. Marchini, N. Jux, H.-P. Steinrück, O. Lytken, F. Williams, *Chem. Eur. J.*, **2016**, 22, 8520
- M. Röckert, M. Franke, Q. Tariq, N. Jux, M. Stark, A. Kaftan, S. Ditze, H. Marbach, M. Laurin, J. Libuda, H.-P. Steinrück and O. Lytken, *J. Phys. Chem. C*, **2014**, 118, 26729
- M. Röckert, S. Ditze, M. Stark, J. Xiao, H.-P. Steinrück, H. Marbach, O. Lytken, *J. Phys. Chem. C*, **2014**, 118, 1661
- O. Lytken, W. Lew, C.T. Campbell, *Chem. Soc. Rev.*, **2008**, 37, 2172
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- F. Abild-Pedersen, O. Lytken, J. Engbæk, G. Nielsen, I. Chorkendorff, J. K. Nørskov, *Surf. Sci.*, **2005**, 590, 127
- O. Lytken, H. N. Waltenburg, I. Chorkendorff, *Surf. Sci.*, **2003**, 543, 207



**ORGANIC CHEMISTRY**  
**DR. GONZALO ABELLÁN**

gonzalo.abellan@fau.de  
www.chemie.fau.de/abellan

#### CURRICULUM VITAE

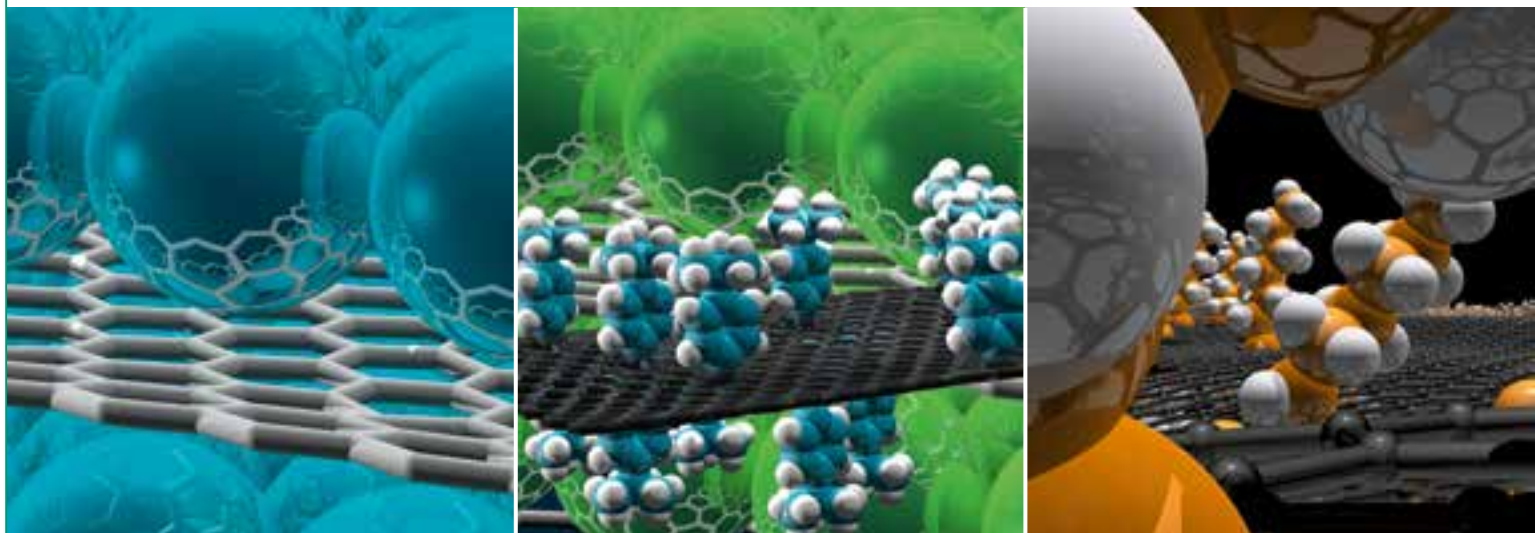
- Since 2017** Junior Group Leader, Organic Chemistry, University of Erlangen-Nürnberg, Germany
- 2016 – 2017** Senior Research Associate, Central Institute for New Materials and Processes, University of Erlangen-Nürnberg, Germany
- 2014 – 2016** Marie Curie Postdoctoral Research Fellow, Organic Chemistry, University of Erlangen-Nürnberg, Germany
- 2014** PhD in Nanoscience and Nanotechnology, Institute of Molecular Science (ICMol), University of Valencia, Spain

#### OBJECTIVES AND PERSPECTIVES

The key point of my research program is exploring the chemistry of novel elemental bidimensional (2D) materials beyond graphene. I aim to develop the chemical functionalization of 2D black phosphorus, antimony, arsenic and bismuth, and use them as building blocks for the development of complex hybrid heterostructures. I am also committed to the applications of these materials in energy storage, catalysis and electronics. To achieve these goals I count on a multi-disciplinary team of international collaborators.

#### SELECTED PUBLICATIONS AND REVIEWS

- G. Abellán, P. Ares, S. Wild, E. Nuin, C. Neiss, D. Rodríguez-San Miguel, P. Segovia, E. G. Michel, A. Görling, F. Hauke, J. Gómez-Herrero, A. Hirsch, F. Zamora, *Angew. Chem. Int. Ed.*, **2017**, 56, 14389
- G. Abellán, S. Wild, V. Lloret, N. Scheuschner, R. Gillen, U. Mundloch, J. Maultzsch, M. Varela, F. Hauke, A. Hirsch, *J. Am. Chem. Soc.*, **2017**, 139, 10432 – 10440
- G. Abellán, M. Schirowski, K. Edlthammer, M. Fickert, K. Werbach, H. Peterlik, F. Hauke, A. Hirsch, *J. Am. Chem. Soc.*, **2017**, 139, 5175 – 5182
- G. Abellán, C. Neiss, V. Lloret, S. Wild, J. C. Chacón-Torres, K. Werbach, F. Fedi, H. Shiozawa, A. Görling, H. Peterlik, T. Pichler, F. Hauke, A. Hirsch, *Angew. Chem. Int. Ed.*, **2017**, 56, 15267 – 15273
- G. Abellán, V. Lloret, U. Mundloch, M. Marcia, C. Neiss, A. Görling, M. Varela, F. Hauke, A. Hirsch, *Angew. Chem. Int. Ed.*, **2016**, 55, 14557
- C. Gibaja, D. Rodríguez-San-Miguel, P. Ares, J. Gómez-Herrero, M. Varela, R. Gillen, J. Maultzsch, F. Hauke, A. Hirsch, G. Abellán, F. Zamora, *Angew. Chem. Int. Ed.*, **2016**, 55, 14345



## COLLABORATIVE RESEARCH CENTRE SFB 953: “SYNTHETIC CARBON ALLOTROPES”



Synthetic carbon allotropes such as fullerenes, carbon nanotubes and graphene currently represent one of the most promising materials families with enormous potential for high-performance applications in the fields of nanoelectronics, optoelectronics, hydrogen storage, sensors and reinforcements of polymers based on their unprecedented electronic, optical, mechanical and chemical properties.

The scientific interest of the SFB 953 “Synthetic Carbon Allotropes” is devoted to fundamental chemical and physical questions such as controlled allotrope doping with heteroatoms, development of synthesis protocols for novel carbon allotrope systems, sorting and separation of carbon nanotubes, investigation of the intrinsic chemical reactivity, and the development of carbon based architectures and devices.

Hence tremendous interdisciplinary efforts are required that systematically combine the expertise of chemists, physicists, engineers, and theoreticians, together with the contributions of high-end analytical instrumentation. The Friedrich-Alexander University of Erlangen-Nürnberg hosts probably the largest and most productive pioneering community in Europe or even worldwide at the forefront of carbon allotrope research. SFB 953 therefore constitutes the ideal forum to advance the field of synthetic carbon allotropes towards the desired goal of creating new materials for high-performance applications.

SFB 953 is structured according to three research areas and two central projects. Research area A (Synthesis and Functionalization) provides the materials basis of the SFB. Chemical functionalization of existing synthetic carbon allotropes and development of new carbon modifications both lie at the forefront of this effort. The next level within the process chain is the systematic investigation of physical and materials properties and the development of concepts for device fabrication. This is guaranteed by the close interaction with Research Area B (Electronic, Optical and Structural Properties) and the two scientific central projects (Z Projects) on high-resolution electron microscopy and tandem mass spectrometry. This highly integrated and interdisciplinary approach of the SFB also necessitates a close connection with Research Area C (Theory). Both classical and quantum mechanical calculations provide the basis for an in-depth understanding of reaction mechanisms, stability as well as electronic, optical, structural and mechanical properties of synthetic carbon allotropes and their derivatives. Moreover, theory will provide some of the most valuable design principles for the exploration of hitherto unknown forms of carbon.

### CONTACT

Speaker: *Prof. Dr. Andreas Hirsch*

Vice-Speaker: *Prof. Dr. Heiko B. Weber*

Administrative Coordinator: *Dr. Frank Hauke*

sfb953@fau.de, [www.sfb953.fau.de](http://www.sfb953.fau.de)







## RESEARCH TRAINING GROUP GRK 1910: “MEDICINAL CHEMISTRY OF SELECTIVE GPCR LIGANDS”

Approximately 30 % of the drugs on the market exert their biological activities upon binding to G-protein coupled receptors (GPCRs). Severe diseases are frequently associated with dysfunctions of GPCRs.

The Research Training Group, located at FAU and at the University of Regensburg, Germany, aims to explore the ligand induced control of monoaminergic and peptidergic GPCRs. In addition to the elucidation of molecular mechanisms, we attempt to contribute to a rational development of functionally selective GPCR drugs for the treatment of chronic inflammatory, cardiovascular and CNS diseases and for diagnostic purposes. The research program is strongly interdisciplinary, covering computer assisted design of selective ligands, chemical synthesis of target compounds, the investigation of ligand-receptor interactions and the elaboration of functional selectivity by analysis of ligand-specific signaling. The

program specific qualification profile integrates chemical, radiopharmaceutical, pharmacological, molecular biological, bioanalytical and biochemical aspects of drug research. The main issues of the qualification programs are retreats, workshops, seminars and online seminars, dealing with and promoting the core research idea. All graduates will get the opportunity to work for 3–4 months in the research laboratory of a collaborator abroad to acquire new knowledge, apply modern methods and techniques and to gain international experience even before the completion of the doctorate.

### CONTACT

*Prof. Dr. Peter Gmeiner*  
peter.gmeiner@fau.de  
www.grk1910.de

## RESEARCH UNIT FOR 1878: “funCOS — FUNCTIONAL MOLECULAR STRUCTURES ON COMPLEX OXIDE SURFACES”



The DFG Research Unit “funCOS — Functional Molecular Structures on Complex Oxide Surfaces” (FOR 1878) was established in 2013. It comprises a total of 13 groups and project leaders at FAU from the Departments of Chemistry and Pharmacy, the Department of Physics, and the Department of Materials Science, as well as 2 external groups at the Paris Lodron University of Salzburg, Austria. funCOS aims at a fundamental understanding of molecular films and ordered structures bound to oxide surfaces. Such systems are at the heart of emerging technologies, with potential fields of application including molecular electronics, solar energy conversion, and catalysis. In spite of the potential of these technologies, the current understanding of molecule oxide interfaces is poor at the atomic level. Whereas the surface science approach to functional organic molecules on metals

has provided a wealth of knowledge on bonding mechanisms and structure formation, organic oxide interfaces have remained largely unexplored; a situation which we denotes as the ‘materials gap’ in organic thin film science. funCOS aims at closing this gap and at providing the fundamental knowledge basis required for the design of tailor-made interfaces. Eventually this knowledge should enable us to perform ‘functional landscaping’ of molecular films on oxides at the nanoscale.

### CONTACT

*Prof. Dr. Jörg Libuda*  
joerg.libuda@fau.de  
www.funcos.fau.de





## CLUSTER OF EXCELLENCE ENGINEERING OF ADVANCED MATERIALS (EAM)

### FROM MOLECULES TO MATERIALS

Advanced materials with properties tailored on the molecular scale and mesoscale are expected to stimulate evolutionary advances and revolutionary breakthroughs in emerging key technologies such as information and communications technology, catalysis, energy and transportation. The Cluster of Excellence “Engineering of Advanced Materials—Hierarchical Structure Formation for Functional Devices”—or EAM—is the only interdisciplinary research collaboration of its type in Germany to focus on materials science and processes.

The vision of the Cluster is to bridge the gap between fundamental research and real-world applications of modern high-performance materials in key scientific and engineering areas. Bridging the gap between materials design at the molecular level and macroscopic properties (“from molecules to materials to functions”) requires novel forms of interdisciplinary cooperation. At the Cluster 200 researchers from 9 disciplines (Applied Mathematics, Chemical Engineering, Chemistry, Computer Science, Electrical Engineering, Materials Science and Engineering, Medicine, Mechanical Engineering, and Physics) collaborate in 90 projects, from basic research in physics and chemistry as well as many areas of applications such as chemical and electrical engineering and materials science.

### RESEARCH AREAS

Cross-sectional topics are explored in three interdisciplinary centers:

- Functional Particle Systems
- Nanoanalysis and Microscopy
- Multiscale Modeling and Simulation

EAM focuses on four fields of application which are organized in value chains that represent hierarchical material classes with increasing complexity:

- Engineering of nanoelectronic materials
- Engineering of photonic and optical materials
- Engineering of catalytic materials
- Engineering of lightweight materials

### INTERDISCIPLINARY NETWORK OF PARTNERS

The Cluster of Excellence was established at the University of Erlangen-Nürnberg in November 2007 within the framework of the Excellence Initiative. The funding by DFG amounts to 80 million Euros for ten years with additional substantial support by the University and the state of Bavaria. EAM is based on existing and visible excellences within the University of Erlangen-Nürnberg as well as on the expertise of the Max Planck Institute for the Science of Light, the Fraunhofer Institute for Integrated Circuits (IIS) and Fraunhofer Institute for Integrated Systems and Device Technology (IISB), New Materials Fürth GmbH, Bavarian Center for Applied Energy Research (ZAE), and other notable academic and industrial research partners.



**ENGINEERING  
OF ADVANCED  
MATERIALS**

### CONTACT

Cluster Coordinator: *Prof. Dr. Wolfgang Peukert*  
Cluster Co-Coordinator: *Prof. Dr. Peter Wasserscheid*  
eam-administration@fau.de  
www.eam.fau.de







## COMPUTER CHEMISTRY CENTER (CCC)

The Computer-Chemie-Centrum (CCC) was founded in 1993 as a central facility of the Faculty of Natural Sciences II (Chemistry, Pharmacy and Biology) and was later integrated into the Department of Chemistry and Pharmacy. CCC houses three research groups, those of Prof. Dr. T. Clark (CCC / Organic Chemistry), Prof. Dr. B. Meyer (Interdisciplinary Center for Molecular Materials, ICMM) and Prof. Dr. D. Zahn (Theoretical Chemistry) with a total of approximately 50 researchers.

The research topics treated at CCC range from protein and DNA simulations and computational drug design through to simulation and design of new materials. Together, the three groups in CCC use a spectrum of calculational techniques from classical molecular dynamics and semiempirical molecular orbital theory to density-functional theory and high-level *ab initio* calculations.

Groups from CCC are involved in both SFB 953 and the Excellence Cluster Engineering of Advanced Materials. CCC offers teaching in modeling and simulation and computational drug design as well as more traditional subjects.

Prof. Dr. A. Görling is the Chairman of the Kollegiale Leitung of CCC and Prof. Dr. T. Clark is its Technical Director.

### CONTACT

*Apl. Prof. Tim Clark PhD*  
tim.clark@fau.de  
www.chemie.fau.de/ccs



## EMIL FISCHER CENTER (EFC)

The Emil Fischer Center serves as a platform for interdisciplinary research between work groups from pharmaceutical sciences, food chemistry, chemistry, and molecular medicine.

The goal of the Emil Fischer Center is to focus, to crosslink and to support the scientific work on bioactive molecules, target proteins and bioanalytics. The main topics are the identification of target proteins, target protein formulation and modulation, ligand-protein interactions and target proteins in signal transduction. The intention behind this research is to bridge chemistry and biomedical sciences leading to the development of novel therapeutic strategies and to understand the interaction of new bioactive small molecules with their target proteins and physiological function.

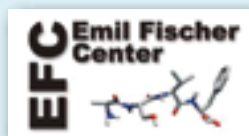
The Emil Fischer Center operates the Core Unit for Bioanalytics, where the scientific and technical competence on targeted and non-targeted metabolome analysis as well as targeted proteome analysis is focused. The bioanalytical expertise covers further techniques of molecular biology and functional assays.

Furthermore, the Emil Fischer Center coordinates the interdisciplinary education of students in the field of pharmacy, food chemistry and molecular medicine. Excellent post graduates are trained by the Emil Fischer Graduate School, which is operated by the Emil Fischer Center.

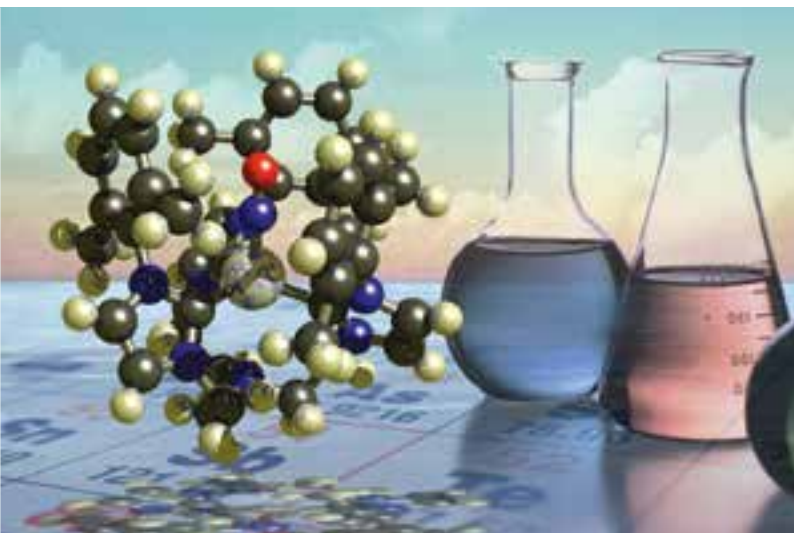
Research at the Emil Fischer Center and the Emil Fischer Graduate School is supported by several organizations and research collaborations, such as the DFG graduate program 1910 as well as the BMBF, EU, Elite Network of Bavaria, and the Bayerische Forschungsförderung.

### CONTACT

*Prof. Dr. Monika Pischetsrieder*  
monika.pischetsrieder@fau.de  
www.efc.fau.de







## ERLANGEN CATALYSIS RESOURCE CENTER (ECRC)

With the inauguration of ECRC in 2008, the University brings together scientists with a strong expertise in „catalysis“ from various fields such as chemical engineering, synthetic organic and inorganic chemistry, physical chemistry and theoretical chemistry. 14 research groups from the Department of Chemistry and Pharmacy (DCP) and the Department of Chemical and Biological Engineering (CBI) participate in the center representing an active and highly interdisciplinary community of chemists and engineers working in the fields of homogenous, heterogeneous and biocatalysis as well as chemical reaction engineering and surface science. ECRC represents a center for the integrated investigation of complex catalytic materials and processes aiming at the combination of catalyst and process design. Research within the center is currently focusing on:

- the design of novel catalysts for sustainable processes and energy applications,
- the use of a large number of spectroscopic techniques to study catalysts under working („operando“) conditions,
- the development of new reactor concepts,
- process intensification.

Moreover, ECRC is part of the interdisciplinary undergraduate and graduate education in catalysis. Particular emphasis is placed on the integration of (undergraduate) students into state-of-the-art catalysis research at an early stage of their education.

ECRC is managed by an executive board elected by the members of the center which presently consists of two scientists from CBI (Prof. Dr. P. Wasserscheid and Prof. Dr. K. E. Wirth) and two scientists from DCP (Prof. Dr. K. Meyer and Prof. J. Libuda) and the Professor of Catalysis within ECRC (Prof. Dr. M. Hartmann as permanent member und current speaker).

### CONTACT

Prof. Dr. Martin Hartmann  
martin.hartmann@fau.de  
www.ecrc.fau.de



## JOINT INSTITUTE OF ADVANCED MATERIALS AND PROCESSES (ZMP)

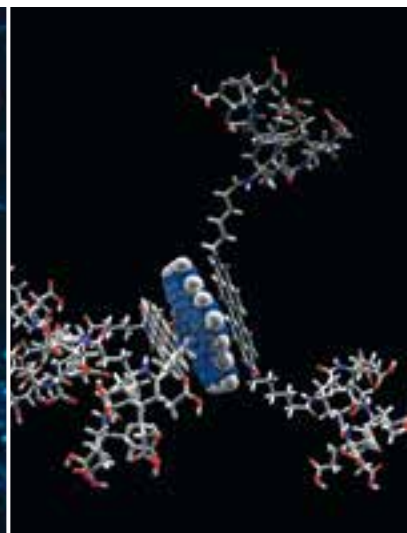
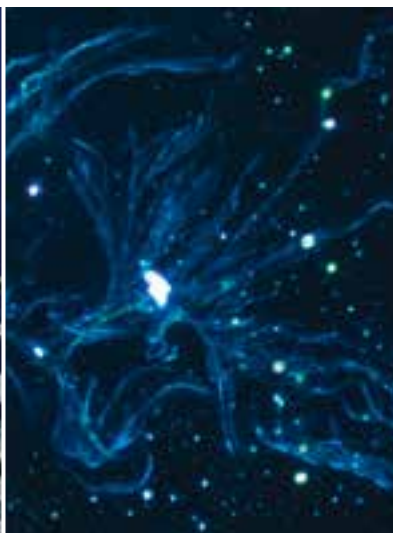
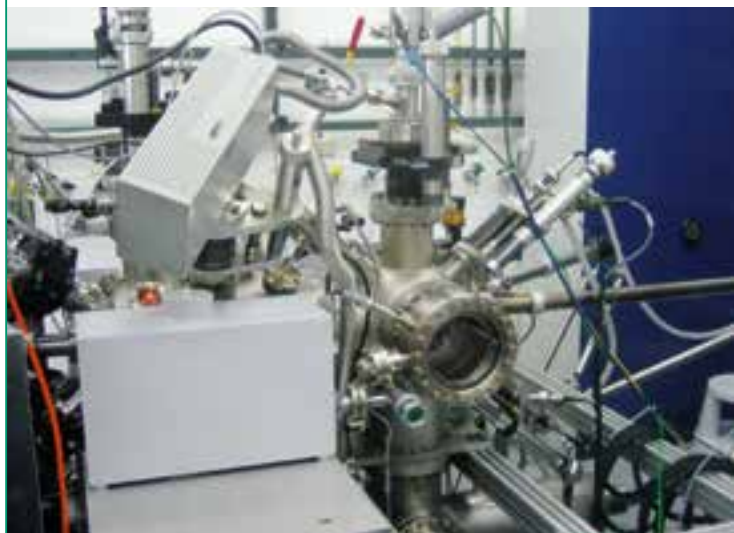
The Joint Institute of Advanced Materials and Processes (ZMP) is an interdisciplinary research center at FAU. In 2006, ZMP was established as the first institutional structure at the new high-tech campus „Uferstadt“ of the city of Fürth. ZMP research focuses on interdisciplinary topics being located in-between material sciences, mechanical engineering, chemistry, and physics. In a young and highly innovative environment, new material concepts and the corresponding production techniques concerning lightweight constructional components are developed. The advancement of ideas being formed in fundamental research to the state of prototyping forms the basic goal. The considered range of materials includes light metals, high temperature alloys, ceramics and synthetic carbon allotropes. Typical process routes include different additive manufacturing processes, rapid prototyping technologies or powder injection molding. In 2013, ZMP was expanded by the application center VerTec.

The contribution from the Department of Chemistry and Pharmacy under the supervision of Prof. A. Hirsch and Dr. F. Hauke is the development of functionalization and characterization concepts of innovative, functional carbon allotropes and novel 2D materials like black phosphorus. The interdisciplinarity aspect of ZMP is further reflected by the joint efforts of researchers also involved in other research centers of FAU such as the Cluster of Excellence Engineering of Advanced Materials (EAM), the Interdisciplinary Center for Molecular Materials (ICMM), the Graduate School Molecular Science (GSMS) and the Collaborative Research Center SFB 953 „Synthetic Carbon Allotropes“.

### CONTACT

Dr. Frank Hauke  
frank.hauke@fau.de  
www.zmp.fau.de





## INTERDISCIPLINARY CENTER FOR INTERFACE-CONTROLLED PROCESSES (ICICP)

ICICP was founded in 2004 with the idea to coordinate and strengthen cooperation between research groups in the field of surfaces, interfaces, and nanostructured materials. Today, around 20 groups from the Departments of Physics, Chemistry and Pharmacy, Chemical and Biological Engineering, and Materials Science and Engineering actively participate. The research of these groups focuses on three areas: (i) the preparation and characterization of interface-modified geometric structures, (ii) theoretical and experimental investigations of structure-property relationships in interface-modified structures and their applications, (iii) interfaces of particulate systems and interface-stabilized nanoparticles. An intrinsic strength of the center is the complementary expertise of the participating groups. Bundling this know-how, ICICP has contributed to the evolution of a lively and interdisciplinary research environment, in which numerous joint activities have been initiated. Since 2013, most ICICP groups are actively cooperating within the DFG Research Unit FOR 1878 "funCOS—Functional Molecular Structures on Complex Oxide Surfaces".

Besides research, interdisciplinary graduate and undergraduate education is the second focus of ICICP. Offering lab-courses and contributing to master programs, it aims at integrating excellent students into cutting-edge research at an early level of their studies. In terms of graduate education, ICICP is organizing a scientific seminar program and, most importantly, a 4-term interdisciplinary graduate course. These activities provide a thorough basis of interdisciplinary education in state-of-the-art research and foster direct scientific exchange between the PhD students.

### CONTACT

Prof. Dr. Jörg Libuda  
joerg.libuda@fau.de  
www.icicp.fau.de



## INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS (ICMM)

Molecular materials represent a fundamental and interdisciplinary research area at the interface between chemistry, physics and materials science. At the same time they provide the basis for a variety of future technologies. Materials based on defined molecular building blocks are characterized by tuneable performances, which is of great importance for high-end applications in nanoelectronics, medicine and energy conversion technologies. ICMM serves as a platform for interdisciplinary research projects in the field of molecular materials and nanotechnology. Currently, ICMM houses 20 research groups. Their complementary research expertise spans from the synthesis and the supramolecular organization of new molecular architectures including fullerenes, carbon nanotubes, polyynes, porphyrins and dendrimers to the development of opto-electronic devices. Next to molecules also nanoparticles, ultrathin layers and interfaces are investigated. Physical characterization is achieved, for example, by single-molecule conductivity measurements, by time resolved photophysical investigations and modern microscopy techniques including TEM, STM and AFM. The research at ICMM is supported by a variety of organizations such as DFG, BMBF, EU and the Bayerische Forschungsförderung.

In addition, close scientific collaboration with industrial laboratories serves as a major stimulus for developing new applications for molecular materials. Modern student training programs, in particular the subject Molecular Science, which was established 12 years ago at FAU as a consecutive Bachelor/Master curriculum, as well as recruitment of excellent international graduate students and post-docs guarantees a continuous supply of highly qualified researchers for ICMM.

### CONTACT

Prof. Dr. Andreas Hirsch  
icmm@fau.de  
www.chemie.fau.de/icmm





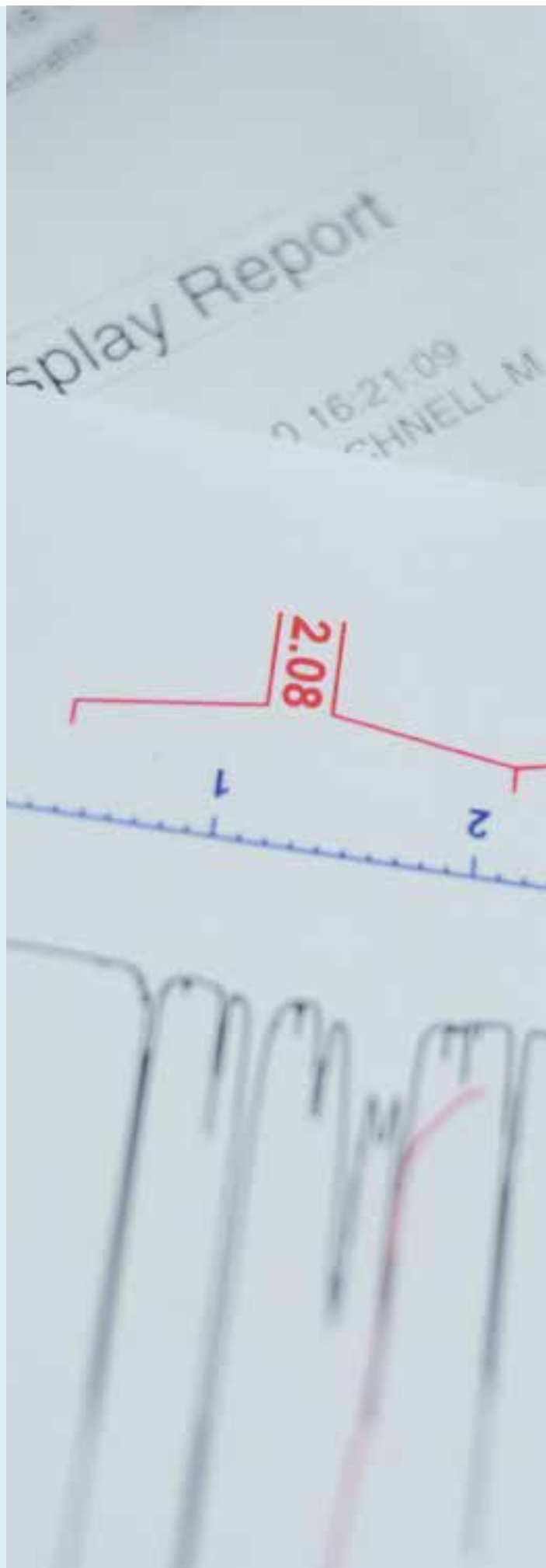
## ZENTRALINSTITUT FÜR SCIENTIFIC COMPUTING (ZISC)

The Zentralinstitut für Scientific Computing (ZISC) arose from Research Area A3 (Multiscale Modeling and Simulation) of the Excellence Cluster Engineering of Advanced Materials. ZISC is the umbrella organization for all modeling and simulation activities within FAU and currently houses more than 50 research groups from different faculties and departments. The Computer-Chemie-Centrum (CCC) is the largest single center within ZISC and the computational groups in the Department of Chemistry und Pharmacy play a major role in ZISC. Prof. Dr. B. Meyer and Prof. Dr. D. Zahn are members of ZISC, Prof. Dr. T. Clark a member of the managing board of ZISC, and Prof. Dr. A. Görling deputy speaker of the managing board.

ZISC organizes workshops on subjects such as molecular modelling and simulation techniques, parallelization and performance optimization of computer programs, coordinates cooperative research projects and international research exchange. Serving as an interface for joint projects and collaborations between Industry and University, ZISC is also the home of the Procter & Gamble Simulation Center. The ZISC management collects and coordinates short trial modeling and simulation projects within Procter & Gamble and distributes them to the relevant research groups within FAU. The aim of such projects is that, after a proof-of-principle stage, they develop into fully-fledged joint research projects between Procter & Gamble and the groups collected within ZISC.

### CONTACT

PD Dr. Harald Lanig  
harald.lanig@fau.de  
www.zisc.fau.de







## EMIL FISCHER GRADUATE PROGRAMME OF PHARMACEUTICAL SCIENCES AND MOLECULAR MEDICINE



Training future generations of scientists to discover promising new drugs and target proteins in novel ways:

The program leads to a Dr. rer. nat. degree in one of the most dynamic and expanding fields of current science. The program aims to educate students to address the major questions in pharmaceutical sciences and molecular medicine, teach students the basic sciences needed to answer these questions, and create an environment where students can develop into independent and creative scientists. The

program is multidisciplinary and has a dual focus: pharmaceutical sciences and molecular medicine.

### CONTACT

Coordinator: *Prof. Dr. Markus Heinrich*

Administrative office: *Petra Neubarth*

[petra.neubarth@fau.de](mailto:petra.neubarth@fau.de)

[www.efs.fau.de](http://www.efs.fau.de)

## GRADUATE SCHOOL ADVANCED MATERIALS AND PROCESSES



The Graduate School Advanced Materials and Processes (GS AMP) has been established within the framework of the Cluster of Excellence "Engineering of Advanced Materials" in 2009. It offers a program for graduates who are interested in research on topics related to the Cluster of Excellence.

The vision of the GS AMP is to support the evolution of young doctoral researchers into a new generation of scientists capable to pursue careers at an executive level. Successful research in natural and engineering sciences in interdisciplinary and international teams requires creative scientists who can provide cross-disciplinary and intercultural competences. The central aspect is the unique excellence of the individual doctoral project, imbedded into a training program in multidisciplinary research, international networking and soft skills development. GS AMP graduates work on innovative nanoelectronic, catalytic, optic and photonic, as well as lightweight materials focusing either on functional particle systems, nanoanalysis and micro-

scopy or multiscale modeling and simulation. Their common research approach is to develop and optimize advanced materials along the entire process chain, from the molecular level to their application in products often in close cooperation with industrial partners.

With special activities as the EAM Winter / Summer School, the EAM Young Researchers Day and lectures on EAM topics, the GS AMP successfully creates a fruitful and productive environment for an excellent education of the future generation of interdisciplinary scientists.

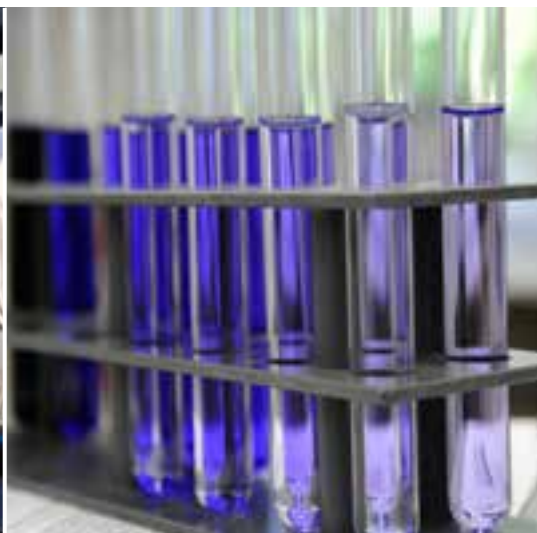
### CONTACT

Speaker: *Prof. Dr.-Ing. Hannsjörg Freund*

Program Director: *Marlene Scheuermeyer*

[eam-gsamp@fau.de](mailto:eam-gsamp@fau.de)

[www.eam.fau.de/graduate-school](http://www.eam.fau.de/graduate-school)



## GRADUATE SCHOOL MOLECULAR SCIENCE



Molecular organization and transformations form the basis for life on earth. Research on structures and properties of molecules and the ability to synthesize specific target molecules are two of the most important foundations of the progress made in medicine and technology in the last century and will gain even more importance in the future. We are living in the “age of the molecule”. The demand for adequate food, energy, pharmaceuticals, medical care and the development of new, high-performance materials can only be satisfied by cooperative, interdisciplinary research designed to develop and understand new molecular concepts.

In order to satisfy these demands, we must strengthen academic training in interdisciplinary techniques that have molecules as their common theme. The University of Erlangen-Nürnberg (FAU) has already made the first step in this direction by establishing the consecutive B.Sc. / M.Sc. degree course Molecular Science in 2001. The extraordinary success of this degree course and the large number of applications from all over Germany underline the importance of this concept. As a logical consequence and given the experience we obtained within the last years of this course, we have founded in 2008 the Graduate School Molecular Science at FAU, with support of the Bavarian initiative “Bayern excellent”. Supervised by excellent researchers, elite students from chemistry, physics, pharmacy, chemical and bioengineering, materials science, molecular science, and related fields, are trained to solve molecular problems in industrial and academic research successfully by tailored training in interdisciplinary research and techniques to enhance communication between disciplines. The basis of the GSMS, molecules, is a clearly defined and homogenous training and research area despite the broadness of the various research fields. The experimental and theoretical techniques used in the individual disciplines are complementary. Our experience so far has shown that this concept works exceptionally well and gives great stimulus to research. Newly conceived teaching concepts in frontier areas provide important impetus which already led to a

large series of seminal publications in first-class journals. Thus, we have prepared the ideal environment for the GSMS to develop into a world-leading center for academic education in Molecular Science.

In 2018, the GSMS looks back to 10 years of educational service with more than 35 academic teachers and around 185 PhD students, with an average of around 60 active students per year. More than 500 scientific contributions have been published and GSMS recognized as an outstanding institution for scientific education and support. With a lecture program hosting nationally and internationally recognized leaders in their research fields, a winter school and access to all training courses of the university for soft skill development, languages, and others, GSMS actively promotes the personal and scientific development of its graduate students.

GSMS is strongly connected and scientifically linked to three research centers at FAU. The Interdisciplinary Center for Molecular Materials (ICMM) at FAU serves as a platform for interdisciplinary research projects in the fields of Molecular Materials and Nanotechnology. The Erlangen Catalysis Resource Center (ECRC) merges scientists from chemical engineering and synthetic organic and inorganic chemistry, supplemented with expertise from physical and theoretical chemistry. The Computer Chemistry Center (CCC) offers excellent experience and capability in modeling molecules, supramolecules, and materials.

### CONTACT

Coordinator: *Prof. Dr. Andreas Hirsch*

Program manager: *Apl. Prof. Dr. Norbert Jux*

[norbert.jux@fau.de](mailto:norbert.jux@fau.de)

[www.gsms.fau.de](http://www.gsms.fau.de)



## QUALIFYING FOR THE FUTURE: OUR DEGREE PROGRAMS

The University of Erlangen-Nürnberg is part of an extended international network and maintains close ties with more than 500 partner universities all over the world. Researchers from Erlangen and Nürnberg work closely with leading universities throughout the world in more than 130 research collaborations. The University of Erlangen-Nürnberg is one of the most attractive German universities for visiting academics from abroad. Every year more and more Humboldt scholars and prize-winning researchers choose this Northern Bavarian university as their research base.

The main focus of the University of Erlangen-Nürnberg in research and teaching is to be found at the interface between Natural Sciences, Engineering and Medicine in close cooperation with the classical university disciplines Law, Theology and the Humanities. Economics, Social and Educational Sciences complete the range of subjects offered.

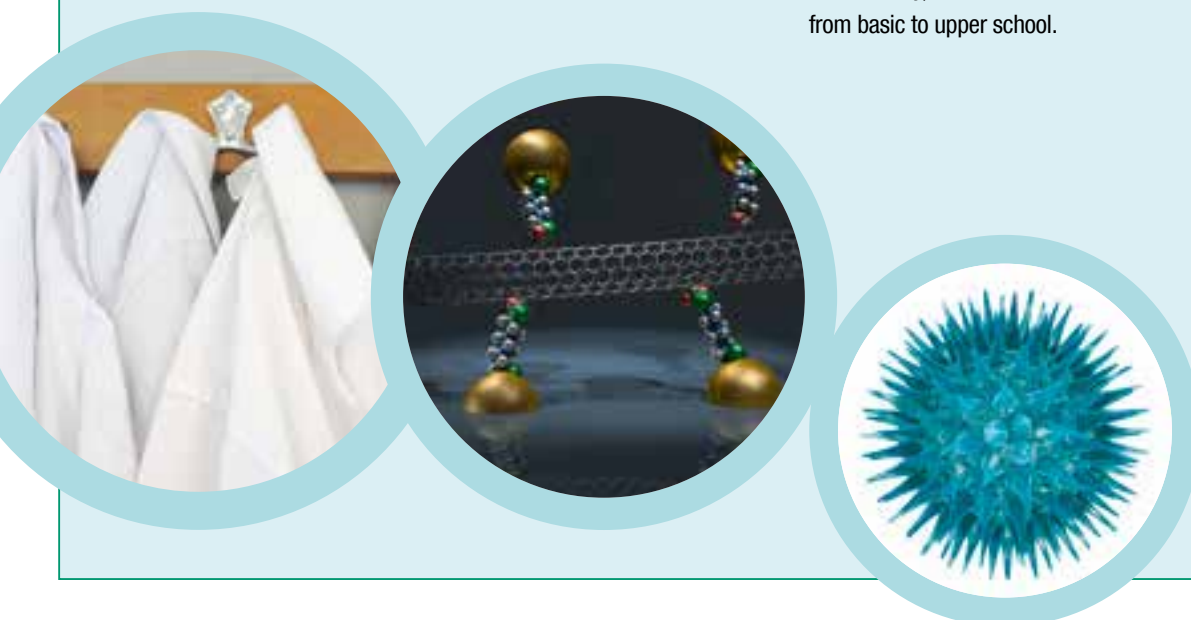
The University offers an enormous variety of subjects in more than 265 different degree courses. Even at undergraduate level students have many opportunities to experience advanced levels of research which enable them to benefit from the interdisciplinary, international and practically-oriented range of courses on offer.

The **Department of Chemistry and Pharmacy** is responsible for the following study courses

- **CHEMISTRY**  
Bachelor of Science (B.Sc.) / Master of Science (M.Sc.)
- **MOLECULAR SCIENCE**  
Bachelor of Science (B.Sc.) / Master of Science (M.Sc.)
- **CHEMISTRY TEACHER'S DEGREE**  
Gymnasium / Realschule / Hauptschule / Grundschule
- **PHARMACY**  
State Examination
- **FOOD CHEMISTRY**  
State Examination

Every year, more than 1,500 students are educated and trained in the aforementioned programs. In addition, the Department of Chemistry and Pharmacy is involved in the chemistry education of twelve other B.Sc./ M.Sc. programs ranging from medical to engineering sciences: every year more than 2,000 students from other programs attend classes and lab courses in the various fields of chemistry.

In close collaboration with the Department of Didactics (Didactics of Chemistry) we train future school teachers for different school levels, from basic to upper school.







## CHEMISTRY (B.Sc. / M.Sc.)

The established study course Chemistry is based on a wide-ranging basic and advanced education in the key subjects of chemistry. Students educated at FAU receive substantial chemical knowledge in all aspects of this natural science.

Chemistry includes the core disciplines of inorganic and general chemistry, organic chemistry, physical chemistry and theoretical/computational chemistry. The substantial education is performed by lectures and seminars and through intense experimental work. Lab courses allow direct insight into the basic and application oriented chemical research and support the lecture series.

Our consecutive Chemistry program is divided into a three-year Bachelor (B.Sc.) plus a two-year Master (M.Sc.) program. Basic principles are taught during the Bachelor program to prepare the students for graduate studies in chemical and related sciences. The Master program focuses on various subjects in chemical core disciplines. In addition, various subjects can be chosen to provide deeper insight into specific topics related to chemistry or interdisciplinary aspects. The Master program also includes a 6-month research project (master thesis) which usually concludes the course of study. The Master's degree program is taught in English.

Chemical expertise is relevant in many different fields related to energy, nutrition, health, mobility and communication. Chemical and pharmaceutical industry, research institutes, universities and the public sector are only a few employers who offer interesting job opportunities for our highly educated alumni.

The Bachelor's degree program in Chemistry is admission free.

### CONTACT

Students' Dean: *Prof. Dr. Jürgen Schatz*  
[juergen.schatz@fau.de](mailto:juergen.schatz@fau.de)  
[www.chemie.fau.de/studium](http://www.chemie.fau.de/studium)

## MOLECULAR SCIENCE (B.Sc. / M.Sc.)

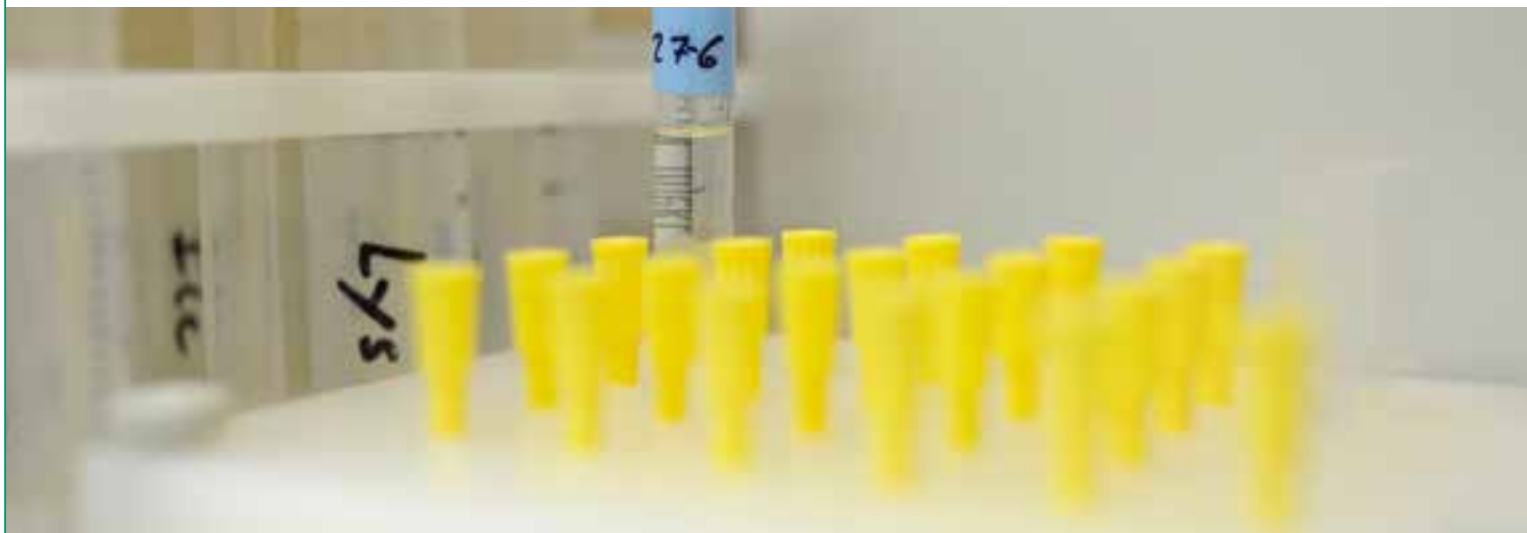
Current molecular sciences are profoundly interdisciplinary. Taking this into account, the Bachelor's and Master's degree programs Molecular Science are both science and technology oriented course programs including biochemistry, molecular biology, medicine, materials sciences, and pharmacy. The Bachelor program of six semesters consists of basic studies (which are related to the Chemistry degree program) followed by a specialization in either Molecular Nano Science or Molecular Life Science.

In both tracks, Molecular Life Science and Molecular Nano Science, the molecular aspects are the main issues differing in the relevant applications, i.e., life science or material science oriented. These aspects also serve as focus in the obligatory master modules Drug Discovery or Nano Science.

Molecular Science goes far beyond the general understanding of chemistry. The implementation of a two-year Master-level program in Molecular Science at the University of Erlangen-Nürnberg tackles new scientific and technological developments with emphasis on the smallest relevant units: the molecules. The Master's degree program is taught in English. The combination of knowledge in synthesis chemistry with a solid microbiological education is in demand in life science industry (e.g., biotechnology, bioengineering, drug discovery). In nanotechnology, various job prospects are in modern materials sciences orientated branches of technology (e.g., nanotechnology, microelectronics, energy research). With regard to the growing demand in molecular well-trained graduates in chemical and pharmaceutical companies, the job opportunities are excellent.

### CONTACT

Students' Dean: *Prof. Dr. Jürgen Schatz*  
[juergen.schatz@fau.de](mailto:juergen.schatz@fau.de)  
[www.chemie.fau.de/studium](http://www.chemie.fau.de/studium)



## PHARMACY

Pharmacy is a scientific discipline at the interface of chemistry, biology and medicine. Pharmaceutical sciences are focused on all aspects of bioactive compounds used as drugs, including the development, synthesis, quality control, preparation, and storage of pharmaceuticals, as well as their biological effects and safe of application.

Our four-year curriculum includes lectures, seminars, tutorials, as well as a range of intensive laboratory courses in which state-of-the-art scientific and instrumental methods are presented and used. Reflecting the interdisciplinary character of Pharmacy, subjects that are taught in the first two years include physics, inorganic, organic, and analytical chemistry, as well as biochemistry, physiology, and microbiology. The first section of the Pharmaceutical Examination concludes this first, basic part of the curriculum. In the third and fourth year, the curriculum focuses on specific pharmaceutical discipline, including Medicinal Chemistry, Pharmaceutical Biology, Pharmaceutical Technology / Biopharmacy, Pharmacology / Toxicology, as well as Clinical Pharmacy. Upon passing the second section of the Pharmaceutical Examination, graduates are required to perform a 12 months pharmaceutical internship before they can take the third and final section of the Pharmaceutical Examination, and subsequently, apply for the state licensure as a Pharmacist.

While the majority of Pharmacy graduates take up jobs at drug stores or hospital pharmacies, professional opportunities also include teaching and research at universities and other research institutes, the pharmaceutical industry, as well as public and private health agencies and testing laboratories.

Pharmacy graduates are also eligible to enter a PhD program at one of the graduate schools at our University.

### CONTACT

Students' Dean: *Prof. Dr. Jutta Eichler*  
[jutta.eichler@fau.de](mailto:jutta.eichler@fau.de)  
[www.chemie.fau.de/studium](http://www.chemie.fau.de/studium)

## FOOD CHEMISTRY

Food chemists are experts in the field of the chemical composition, analysis, and product design of foods and cosmetics. Moreover, they understand how food constituents affect the human organism and have a basic knowledge about the industrial processing of foodstuffs, the respective juridical evaluation, and of the role of microorganisms in food production and spoilage.

Traditionally, food chemists work in the food industry, for the food control authorities, or in commercial laboratories. However, they are also well in demand when analytic expertise is needed, for example, in forensics or in the pharmaceutical and cosmetics industry.

Especially in the second (main) study period, food chemistry courses in Erlangen are characterized by a small number of students in the respective groups and project-oriented learning. Theory lectures are mostly enlarged by practical courses. During the first four terms, students attain the scientific basics in mathematics, physics, biology, chemistry, and biochemistry. This knowledge is vital for the subsequent food chemistry courses during the following terms. During the main study period, the students concentrate on issues of food chemistry. Several extensive lab courses offer the opportunity to practice elementary analytical methods as well as to apply modern bio-analytical and instrumental techniques. The food chemistry courses are completed by lectures in nutritional physiology, food technology, microbiology, food law, toxicology, forensic analysis, quality management, and the chemistry and analytics of cosmetics.

A state examination finishes university education, usually after nine terms. Subsequently, graduates can add one year of further professional training to qualify as certified food chemists ("staatlich geprüfte Lebensmittelchemiker") and / or can do their PhD in various natural sciences or medicine.

### CONTACT

*Prof. Dr. Monika Pischetsrieder*  
[monika.pischetsrieder@fau.de](mailto:monika.pischetsrieder@fau.de)  
[www.chemie.fau.de/studium](http://www.chemie.fau.de/studium)



## STUDY COURSE INITIATIVE CHEMISTRY & MOLECULAR SCIENCE

As a collective of chemistry and molecular science students of all semesters, the Study Course Initiative Chemistry & Molecular Science (FSI) is contact for all students regarding their studies and social networking between them. As part of the University community, we are the key link between students and department executives and professors.

We dedicate our efforts to improving the situation for our students both long and short term with our services provided during the office hours in the CIP pool and our activities in committees as part of the self-administration of the university. Our services include distribution of lab coats and safety goggles, printing and advice for exam preparation and lab courses.

Besides that, we organise several events throughout the year especially for our freshmen as an introduction to a new chapter in their life like our freshmen party, campus rally and hiking. The social highlight of the department takes place at the end of the summer term with our legendary summer party where both the students and the faculty stuff come together to party.

### CONTACT

FSI Chemie & Molecular Science  
fsi-chemie@fau.de  
www.chemie.fsi.fau.de

## STUDY COURSE INITIATIVE PHARMACY & FOOD CHEMISTRY

We, the "Student Representatives" of all pharmaceutical and food chemistry students are proud to call the "Chemikum" our new home.

Located on the fifth floor (room 05.057), our office opens every Thursday from 11-12 a.m. or after making a personal appointment. We offer different services, e.g. lab coats and safety glasses, selling different kinds of booklets, journals, etc.

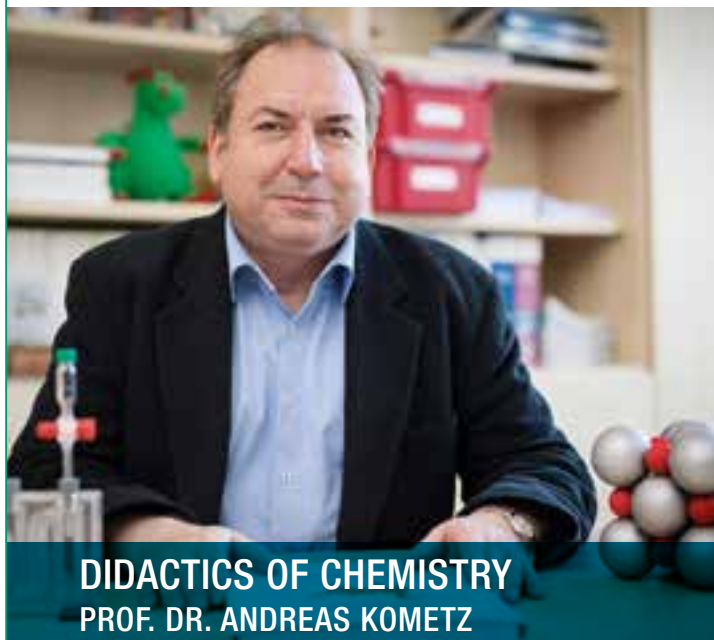
We also act as mediators between the professors and students to comfort everyone and to solve upcoming problems. Besides the above-mentioned points, we organize and promote various parties, sport events and field trips during the semesters. To support the students, we communicate with pharmacy's and the pharmaceutical industry to offer popular internships after the second state examination.

For more information about the courses you can also visit our homepage or check out our Facebook profile.

### CONTACT

FSI Pharmacy & Food Chemistry  
fsi.pharmazie@stuve.uni-erlangen.de  
www.pharmazie.fsi.fau.de





**DIDACTICS OF CHEMISTRY**  
**PROF. DR. ANDREAS KOMETZ**

[andreas.kometz@fau.de](mailto:andreas.kometz@fau.de)

[www.chemiedidaktik.fau.de](http://www.chemiedidaktik.fau.de), [www.chemie.fau.de/studium](http://www.chemie.fau.de/studium)

#### CURRICULUM VITAE

- Since 2005** University Professor of Chemistry Teaching at the University of Erlangen-Nürnberg, Germany
- 2002 – 2005** Scientific assistant for Didactics of Chemistry at Oldenburg University, Germany
- 1989 – 2002** Scientific assistant for Didactics of Chemistry at Halle University, Germany
- 1985 – 1989** Secondary school teacher and class teacher in Hoyerswerda, Germany

Chemistry education, especially chemistry didactics, is a very important part of the education and advanced training of chemistry teachers. It comprises both theory and practice of how to teach chemistry topics and how students at school learn chemistry.

Chemistry education at the Friedrich-Alexander University of Erlangen-Nürnberg (FAU) includes lectures such as the “basics of chemistry education”, seminars and laboratory practice. Laboratory practice entails “school experiments in chemistry” which students have to pass, because this lecture is a compulsory part of their training. This practical lecture consists of instructions on how to set up experiments for chemistry classes. This course is adaptable and thus able to address multiple educational levels: elementary school, secondary school, intermediate secondary school and grammar school. Experience in planning lessons can be gained through practical trainings which take place at schools. The courses offered at FAU thus range from practical exercises at the lab to lessons at schools as well as theoretical lectures at the University.

In addition to the training of students, the faculty of the Teaching Methodology of Chemistry also provides scientific training for teachers in service. The work of the Training Centre for teachers, which is supported by GDCh, is guided by three principles: “competence –



cooperation – authenticity”. Development of scientific teaching, application of didactic research to practical teaching, actual assistance in teaching classes and assistance with creating new syllabi are the program’s aims. Approximately 70 courses of various chemistry topics and their classroom implementation are offered for different levels of education annually.

Practical experience is necessary when teaching science. Therefore, the NESSI-Lab, a chemical lab for children, was founded in 2005. Once a week students between first and sixth grade can visit the University to gain experience in chemistry applications. Students of chemistry education assist the children during their experimental work on water, fire, air and earth. The lab experiments efficiently combine experiments based on real world concepts with materials that are relevant to students.

Even though these experiments could be easily arranged for the classroom, setting up the experiments in a separate location, namely the lab of the University, adds benefits of an extracurricular learning place.

Opening the NESSI-Lab for special education schools and higher school grades are current research projects at the chair of chemistry education. To adapt the experiments to special needs of children with hearing and learning disabilities, the experiments and their instructions have to be adjusted. The combination of E-Learning and practical experiments within the framework of a business game offers a context-based method for classes from 7th to 12th grades. Both projects are accompanied by studies.

Another focus of research is Microscale Chemistry and its implementation at schools. Microscale is a method of performing chemical processes in an environmentally safe and pollution preventing way. The quality and the standard of chemical applications in education are preserved, even if only small quantities of chemicals are used for the experiments. Reduced costs, shorter experiment times and less requirements are only a few examples of the benefits for its application at school. Further fields of research contents are “chemistry in context” as well as “media and experiments”.



## CLINICAL PHARMACY

### PROF. DR. FRANK DÖRJE MBA

frank.doerje@uk-erlangen.de  
www.apotheke.uk-erlangen.de

#### CURRICULUM VITAE

<b>2014</b>	Honorary Professor of Pharmacy, University of Erlangen-Nürnberg, Germany
<b>2005 – 2014</b>	Lecturer in Clinical Pharmacy at the University of Erlangen-Nürnberg, Germany
<b>2007</b>	Management degree, MBA (Health Care Management), University of Bayreuth, Germany
<b>Since 2001</b>	Head of Pharmacy Department, Erlangen University Hospital and Manager, Pharmacy and Therapeutics Committee, Erlangen University Hospital, Germany
<b>1993 – 2001</b>	Clinical Pharmacist, Pharmacy Department, Ulm University Hospital
<b>1989 – 1992</b>	PhD thesis, Institute of Pharmacology for Natural Scientists, Goethe-University Frankfurt/Main, Germany
<b>1988</b>	Licensed Pharmacist, Hannover, Germany

#### SCIENTIFIC BACKGROUND

Prof. Frank Dörje studied Pharmacy at the Technical University of Braunschweig. He received his PhD at the institute of Pharmacology for natural scientists at the Goethe-University in Frankfurt in 1992. Part of his thesis work in muscarinic receptor subtype research was carried out at the Laboratory of Molecular Biology, NINDS, NIH, USA. Prof. Dörje pursued a clinical career becoming a hospital and clinical pharmacist and working for almost eight years at the Ulm University hospital, Pharmacy Department. In 2001, he obtained the management position at the Pharmacy Department, Erlangen University Hospital. Ever since he began his clinical work, he has been a strong promoter for the evolving subject of clinical pharmacy within the German pharmacy university curriculum. Consequently, he strongly supported

the emerging field as lecturer of clinical pharmacy within the Department of Chemistry and Pharmacy at FAU. He has got comprehensive experience in the teaching and research of clinical pharmacy, also due to some foreign research stays at the University of Cincinnati (1994) and at the University of Florida, Gainesville (2013). In 2014, he was appointed Honorary Professor of Pharmacy at the University of Erlangen-Nürnberg. He and his group work in close collaboration with several groups within the Department of Chemistry and Pharmacy, particularly with the Professor of Molecular and Clinical Pharmacy as well as with clinics, research groups and units of FAU's Faculty of Medicine.

#### CURRENT RESEARCH ACTIVITIES

Prof. Dörje and colleagues are involved in advanced studies of teaching methods for clinical pharmacy (patient centred clinical pharmacy courses) as well as in comprehensive studies to substantially promote patients adherence to medication by intensified pharmaceutical care.

A large ongoing study, funded by the German Cancer Aid is currently carried out within the CCC Erlangen-EMN (Medication safety in patients treated with new oral antitumor agents: a prospective, randomized investigation on the impact of intensified clinical pharmaceutical/clinical pharmacological care on patient safety, patient knowledge and patient well-being). The clinical research work of Prof. Dörje and his group is focused on Medication Therapy Safety, intersectoral pharmaceutical care and the use of e-Health and e-Medication plan for a better medication care continuum.

Prof. Dörje as head of the Hospital Pharmacy is also responsible for a GMP-Pharmaceutical Manufacturing Unit (Core Unit) within the University Hospital. He and his coworkers are substantially involved in translational biomedical research activities of the Faculty of Medicine. The pharmacy-led task is the development, formulation and pharmaceutical production of clinical test patterns according to international GMP-regulations. The important contributing work of this GMP-Core Unit is recognized and documented by several high ranking publications.

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**1 Flavour Research**, Henkestr. 9, 91052 Erlangen

**2 Computer Chemistry Center**, Nägelsbachstr. 25, 91052 Erlangen

**3 Inorganic Chemistry**, Egerlandstr. 1, 91058 Erlangen

**4 Physical / Theoretical Chemistry**, Egerlandstr. 3, 91058 Erlangen

**5 Pharmaceuticals**, Cauerstr. 4, 91058 Erlangen

**6 Chemikum**, Nikolaus-Fiebiger-Str. 10, 91058 Erlangen

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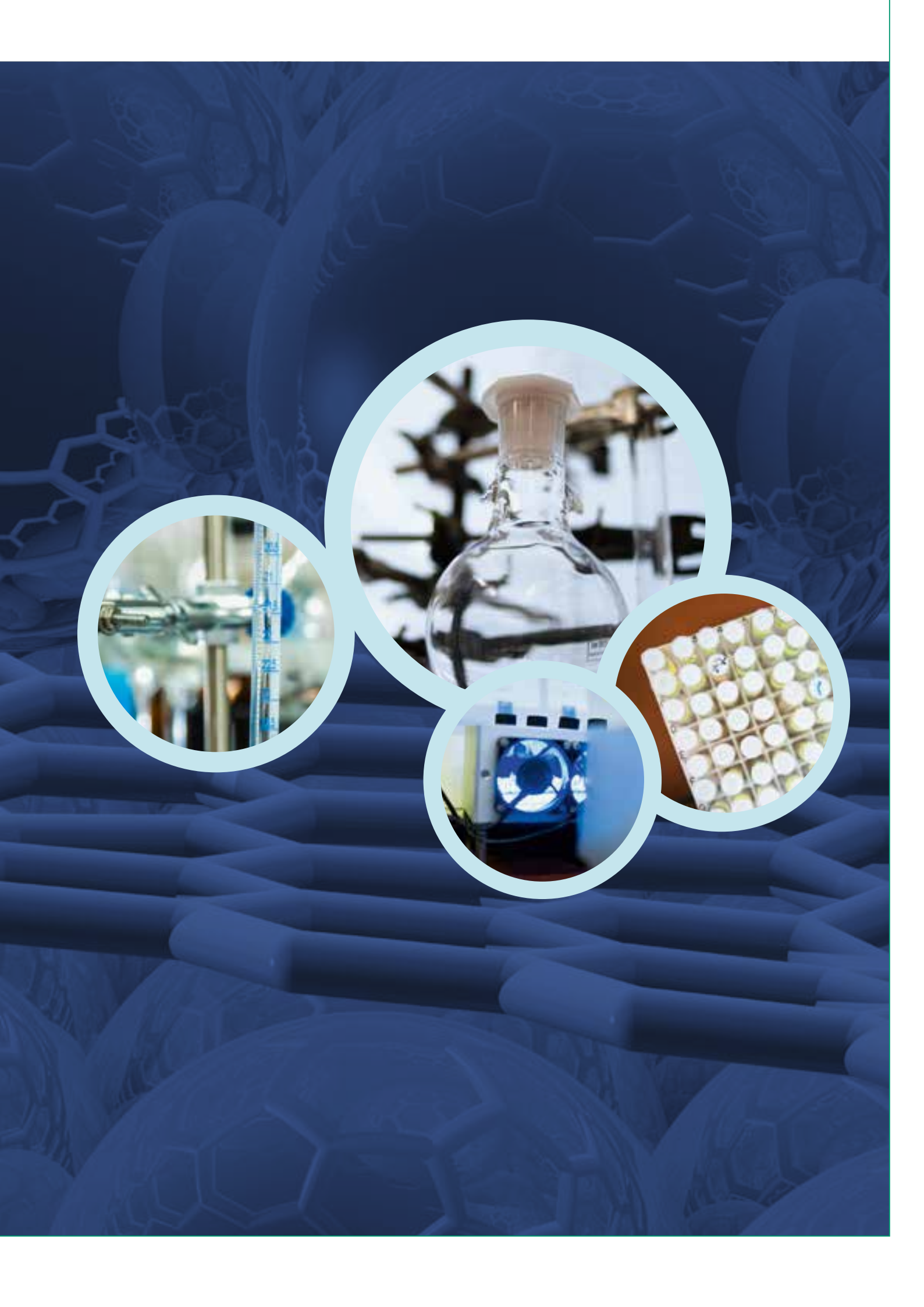
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