# TUM Catalysis Research Center

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# Catalysis – Key to the Grand Challenges of our Century

**Catalysis** is one of the key research areas to address the grand challenges of the 21st century. Catalytic processes are integral to energy storage, the generation of alternative fuels, the protection of the environment, and to the production of effective pharmaceuticals. The diversity and complexity of the associated catalytic reactions demand an interdisciplinary, cooperative approach.
Today's challenges can be successfully overcome only by providing a platform that eliminates the borders between different disciplines.

Since the groundbreaking work of the late TUM Professor Ernst Otto Fischer (1918–2007; Nobel Prize 1973), catalysis research has been strengthened not only in chemistry and physics, but also in engineering. It has become one of the key interdisciplinary research topics at the Technical University of Munich (TUM).
In light of the future potential and importance of catalytic processes for numerous scientific and industrial fields, we founded the **TUM Catalysis Research Center (CRC)** in 2008, the largest corporate research center at TUM. With the CRC, TUM thus established a unique venue to investigate collaboration among currently 19 prominent researchers and their teams; these research groups represent different, yet complementary scientific fields, tackling various aspects of catalysis research, including theory, catalyst development and technology applications. The CRC is further strengthened by the involvement of Munich Catalysis, an Alliance of Clariant and TUM (MuniCat).

TUM was awarded a 57 Million Euro grant from the Federal and Bavarian governments for the construction of a new research building, which is situated next to the chemistry department on the Garching TUM Campus and will be inaugurated on May 9th, 2016. The CRC will enhance the working environment of the researchers by providing state-of-the-art laboratory facilities, and support the scientific cooperation among the members and partners of the CRC.

Beyond the CRC and associated with it, research at the **TUM Research Center on Industrial Biotechnology** and the **TUM Research Center on Synthetic Biotechnology**, open yet another horizon.
Our university is thus prepared to set the new standards in the fields of energy, sustainability, environmental protection, and avantgardistic production processes in the chemical industry of tomorrow.

*„In daily life we often hear that something is catalyzed or that someone must act as a catalyst. Even persistent catalysis is mentioned when a complex process must be kept in motion. It is always people, individuals with special talents, who bring others together and ensure that progress is made."*

*- Wolfgang A. Herrmann*

Prof. Wolfgang A. Herrmann
TUM President and
Inorganic Chemistry Chair Emeritus

# CRC Mission

Life on earth could not have emerged without catalytic processes that have been optimized over the course of evolution. Since industrialization, humanity has been strongly affected by man-made catalysis in a myriad of ways. To face the many challenges of today, catalysis will be one, if not the most important technologies, e.g. in energy science or environmental protection.

Catalysts are chemical engines on a nanoscale level that power the transformation of chemical structures by breaking and making chemical bonds. They thereby alter the energy landscape of a reaction and accelerate the rates of specific reaction pathways that are thermodynamically accessible. Catalysts ideally function over millions and millions of reaction cycles without being consumed. Thus, very small quantities of catalytic materials can transform large quantities of a feedstock into valuable chemicals.

Over the last decades, catalysis research led to the discovery of key approaches for facilitating novel chemical reactions and to transition our society to renewable energy and resource sustainability.

While the emphasis on catalytic processes has led to impressive successes in understanding and realizing the pathways of individual reactions qualitatively and quantitatively, our knowledge is far too limited at present to practically develop *de novo* catalysts.

These would allow us to successfully master the challenges of the future, i.e., decentralized production and conversion of energy carriers, organic synthesis with high carbon efficiency, and reactions accelerated by catalysts, which combine the activity and specificity of enzymes with the robustness of solid catalysts. All chemical transformations associated with these challenges are characterized by a need for catalysts that are highly active and selective at low temperatures.

In order to develop such catalysts and catalytic routes, several approaches are possible. The most prominent, widely used strategy is to rely on the knowledge and insight accumulated over the last decades and to develop the leads further. Another would be to parallelize synthesis efforts, while deliberately minimizing the input outside of the results achieved in massive parallel screening.

*"Chemistry without catalysis would be like a sword without a handel, a light without brilliance, a bell without sound."*

*- Alwin Mittasch*

## CRC Mission

The third option is to understand on a molecular level the elementary steps of reactions and to use the resultant insight for the design of efficient and selective catalytic materials on an atomic level. This borders on the ultimate goal to selectively catalyze a desired reaction pathway on the complex energy landscape with the highest efficiency, the minimal use of energy, and the least consumption of the catalytic material.

While it is difficult to weight the benefits and drawbacks, the third approach is certainly best suited for an academic environment, such as the TUM Catalysis Research Center (CRC).

The knowledge-based route requires a highly intra- and interdisciplinary approach, whereby barriers between classical disciplines of research, e.g. chemistry and physics, nanoscience and catalysis, engineering and fundamental research, or experiment and theory, must be broken.

In this respect, the newly inaugurated CRC plays a key role in bringing together the expertise of almost 20 research groups at TUM – five among them ERC grant holders – across a wide range of disciplines: molecular science, surface science, nanoscience, materials science, bioscience, photophysics, spectroscopy, and computational science.

Encouraging the discovery and innovation in catalysis research by bringing together these diverse scientists is indeed one of the aims.

The CRC bundles the excellent scientific potential in the area of catalysis. It strives to become a globally competitive scholarly environment, where problems in basic and industrial catalysis are explored, and new routes for the sustainable production of energy carriers, value-added intermediates, and tailored materials are created. The research teams will address challenging problems by applying a comprehensive and interdisciplinary knowledge-based approach.

Synergistic effects will be created and benchmarks set together with the international network that has been created by the founding director, Prof. Rösch. The CRC will leverage its scientific findings from academic research through close interaction with industry, thus amplifying the benefits to society.

In the short term two immediate actions have been identified.
With this diverse team of scientists in the CRC, the first goal is to disentangle and elucidate the impact of the chemical environment on a specific catalytic center. While we hypothesize that fundamental analogies exist between reactive interactions at catalytic sites of solids, enzymes, and molecular complexes, rigorous information is lacking. This understanding, in combination with the kinetics of catalyzed processes, is required to develop more active and selective catalysts. Thus, we seek to draw a rigorous comparison between elementary reactions at the solid gas interface and the analogous reactions in liquid phase using molecular, enzymatic, and solid catalysts. This topic will form the basis of a graduate school, educating young researchers in a truly interdisciplinary fashion.

In a second goal, we focus on establishing a common research program to elucidate concepts and develop materials, which efficiently transform abundant carbon based molecules (e.g. $CO_2$, $CH_4$, …) into fuels or fine chemicals by the absorption of photons and via reactions, such as C-C coupling or C-H activation.
At present, two different approaches exist, which either use metal-(bio)-organic complexes (homogeneous approach) or metal-loaded semiconductor materials (heterogeneous approach). In both cases, the underlying fundamental principles are the same: the two systems share the common mechanistic pathways of light harvesting, separation and transport of the charge carriers, as well as the actual catalytic reaction. One of the challenges of this research project lies in its interdisciplinary nature, hereby the CRC defines a common umbrella that will stimulate a conceptual exchange between the associated research groups.
The unifying concepts and fundamental mechanistic insights in the homo- and heterogeneous approaches will result in building blocks, such as the light-harvesting center, that may be exchanged in order to design novel hybrid materials. Furthermore, we envision the development of optimized light sources with an emission spectrum matched to the characteristics of the absorbers and/or operated in a pulsed mode to match the photochemical reaction kinetics. This allows for additional optimization of the photo-catalytic conversion efficiency and is in contrast to the broad and continuous spectrum of solar irradiation.

With the newly inaugurated CRC, the members have unique and outstanding facilities at their disposal that not only allow for common and individual research goals to be achieved, but also to benefit society through their acquired knowledge.

Prof. Ueli Heiz
Director
TUM Catalysis Research Center

CRC Building, Infrastructure and Organization

# CRC Building and Infrastructure

## CRC Building

The CRC building is solely dedicated to laboratory research work and offers state-of-the-art infrastructure for chemical and physical research ranging from fundamental to applied research.
Seven large laboratory areas with in total 75 separate laboratories are located on the north and south of the building on three levels. In between these facilities, the area of the CRC analytical core labs are located. In addition the building accommodates two seminar rooms, three offices for administration and a spacious entrance area with a cafeteria.

## Key facts

Construction time: 2009 – 2015

Useful area: 6.500 m$^2$
Brutto area: 16.000 m$^2$
Brutto volume: 66.300 m$^3$

Project lead/Client:
Staatliches Bauamt München 2, Freistaat Bayern

Architect:
Klein und Sänger Architekten, Munich

## CRC Analytical Core Labs

The analytical core labs, open to all CRC members provide a wide range of analytical techniques applicable to solve a large amount of analytical problems in catalysis research.
Characterization and analysis techniques are performed and provided under the supervision of trained technicians.

# CRC Organization

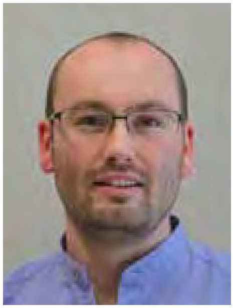
**Academic Director**

**Prof. Dr. Ueli Heiz**

**Technical Business Manager**

**Dr. Dimitrios Mihalios**

**Scientific Coordinator**



**Dr. Florian Schweinberger**

**Administration**

**Irmgard Grötsch**

**Stefanie Wölfl**

CRC Members

## CRC Members

The TUM Catalysis Research Center realizes a structural paradigm shift in university based, fundamental research exemplary for one key technology of the future.

Overcoming the traditional university structures, i.e. faculties and small institutes, an interdisciplinary main research hub at the interface of engineering and natural sciences is created.

Members with different scientific background and originating from various faculties are key for the successful interdisciplinary research performed at the TUM CRC.
The principal investigators and their teams are focused on a wide range of problems, covering all significant aspects of catalysis from theoretical basics to technology applications – from spectroscopy and surface catalysis to heterogeneous, homogeneous and biocatalysis.

**Assistant Professorship of Molecular Engineering at Functional Interfaces**

**Prof. Dr. Wilhelm Auwärter**

The research focus of Prof. Auwärter lies on the creation of nanoscale model systems on atomically tailored surfaces, enabling the study and control of single-molecule processes as well as the self-assembly of supramolecular structures.
This approach includes the use of ultra-thin textured layers of boron nitride as a substrate. The studies are inspired by the chemistry of life – which shows how functionally versatile a single set of molecular building blocks can be – and oriented toward innovation in nanotechnology.

**e20.ph.tum.de**

**Chair of Organic Chemistry I**

**Prof. Dr. Thorsten Bach**

The research of Prof. Bach is focused on organic synthesis chemistry, in particular stereoselective transformations.
He has developed new methods using, among others, photochemical processes, the research into and use of new catalytic reactions (C-H activation, oxidation catalysis, Lewis acid catalysis) and the total synthesis of complex natural products (including GE 2270 A, meloscine, podophyllotoxin, punctaporonin C).

**oc1.ch.tum.de**

### Chair of Molecular Nanoscience and Chemical Physics of Interfaces

**Prof. Dr. Johannes Barth**

The research activities of Prof. Barth center on the fundamental understanding of phenomena at interfaces and the design of functional molecular nanosystems.
His work notably focuses on the characterization and control of surface chemical reactions, complex molecules and highly-organized supramolecular architectures at the atomic scale.

**e20.ph.tum.de**

### Chair of Inorganic and Organometallic Chemistry

**Prof. Dr. Roland Fischer**

Prof. Fischer's research team is interested in metal-organic frameworks (MOFs), metal clusters and nanostructures which fulfill advanced tasks in a complex chemical-physical system.
Catalysts are such functional material systems, nanoelectronic architectures for chips as well. As inorganic chemists we are playing for this purpose on the keyboard of the whole periodic table pushing the limits of synthesis and chemical bonding.

**amc.ch.tum.de**

### Chair of Technical Electrochemistry

**Prof. Dr. Hubert Gasteiger**

Prof. Gasteiger is working in the areas of electrocatalysis, polymer electrolyte fuel cells and electrolyzers, as well as lithium ion and lithium sulfur batteries. Activities include synthesis of novel catalysts and incorporation into high-performance fuel cell, electrolyzer and battery electrodes. Analytic and spectroscopic methods are applied to study catalytic processes and to elucidate material degradation mechanisms. The research is performed in close collaboration with the engineering faculty, where the fundamental learnings will aid to design battery and fuel cell systems which can be incorporated into, e.g. electrified vehicles.

**tec.ch.tum.de**

## CRC Members

### Associate Professorship of Physical Chemistry with Focus on Catalysis

**Prof. Dr. Sebastian Günther**

Prof. Günther conducts research into surface science and heterogeneous catalysis. He uses models to image catalytic reactions and processes at interfaces. Microscopy and spectroscopic techniques are combined, with particular use made of scanning tunnelling microscopy, photoelectron spectro-/ microscopy and low energy electron microscopy (LEEM).
With respect to heterogeneous catalysis, the aim is to enable elevated pressure conditions for the models used in the ultra-high vacuum.

**pc5.ch.tum.de**

### Chair of Physical Chemistry

**Prof. Dr. Ueli Heiz**

Prof. Heiz explores the physical and chemical properties of the smallest matter particles in the non-scalable size regime.
In this regime, the properties of the clusters are determined by the exact number of atoms. His research findings create a better understanding of nanocatalysis, asymmetric catalysis and photo-catalysis. He also works on characterizing and developing new optic materials based on size-selected clusters.

**pc.ch.tum.de**

### Assistant Professorship of Bioinorganic Chemistry

**Prof. Dr. Corinna Hess**

The research of Prof. Hess spans the areas of inorganic and bioinorganic chemistry. Central themes include the coordination chemistry of synthetic and biological systems, catalysis, and spectroscopic studies for structure elucidation.
A key research area centers on the development of bio-inspired inorganic catalysts for multi-electron reactions, including $H_2$ production and $O_2$ activation. These small molecule transformations are central to life and at the heart of renewable energy and sustainable chemistry processes.

**bioinorganic.ch.tum.de**

### Chair of Chemical Technology I

**Prof. Dr.-Ing. Kai-Olaf Hinrichsen**

Prof. Hinrichsen researches in the field of industrial catalysis at the interface between natural science and engineering science. His research work is oriented along the process chain, starting from particle design through reactor design to process design. Particular focus is placed on particle technology and catalyst forming as well as multi-scale modeling. In the latter discipline, research is centered on describing chemical reactions at the elementary level, the numerical simulation and modeling of chemical reactors with respect to their apparatus design, dimensioning and operating characteristics.

**tc1.ch.tum.de**

### Associate Professorship of Organic Chemistry

**Prof. Dr. Lukas Hintermann**

The research of Prof. Hintermann focuses on the development of highly active and selective catalysts for organic synthesis, with potential applications both in basic molecular research and in industrial production.
The group is active in the field of homogeneous catalysis with metal complexes or small organic molecules. A key goal is to realize general, efficient and sustainable methodology for the chemical synthesis of any organic target molecule.

**oca.ch.tum.de**

### Assistant Professorship of Silicon Chemistry

**Prof. Dr. Shigeyoshi Inoue**

The research interests of Prof. Inoue focus on the synthesis, characterization and reactivity investigation of compounds containing low-valent main group elements (groups 13, 14 and 15) with unusual structures and unique electronic properties, with the goal of finding novel applications. A particular emphasis is laid on low-coordinate silicon compounds.

**si.ch.tum.de**

## CRC Members

### Associate Professorship of Inorganic Chemistry

**Prof. Dr. Klaus Köhler**

The work of Prof. Köhler focuses on the preparation, structural characterization and catalytic properties of transition metal compounds on surfaces of solids (interfacial coordination chemistry, surface organometallic chemistry).
The synthesis of solids and the modification of their surfaces centres on the development of materials with tailored surface properties and new heterogeneous catalysts for the abatement of nitrogen oxides, for oxidation and hydrogenation reactions and for fine chemical syntheses.

**ch.tum.de/akkoehler**

### Associate Professorship of Nonequilibrium Chemical Physics

**Prof. Dr. Katharina Krischer**

Research activities of Prof. Krischer cover self-organization in physical and physicochemical systems as well as electrocatalysis.
She focuses in particular on efficient photoelectrochemical and electrocatalytic energy conversion and universal mechanisms of structure formation processes in nonequilibrium systems.

**chemphys.ph.tum.de**

### Associate Professorship of Molecular Catalysis

**Prof. Dr. Fritz Kühn**

Prof. Kühn’s areas of research are organometallic chemistry, medicinal chemistry and molecular catalysis. In the field of catalysis, mechanistic behavior, practical and industrial uses of efficient catalysts are of prime interest.
Prof. Kühn cooperates with several industrial companies on applied catalysis projects.

**ch.tum.de/molcat**

### Chair of
### Chemical Technology II

**Prof. Dr. Johannes Lercher**

Prof. Lercher aims to gain elemental understanding of the chemical reactions on surfaces and in the pores of nanostructured catalysts and use this knowledge to develop new catalysts and reaction channels. Processes like the sustainable generation of clean energy sources through selective conversion of biogenous or fossil raw materials are examined. This is done by combining physical-chemical characterization of catalysts and determining their kinetics. Based on the findings new catalysts and reaction paths are developed, combining different functions that allow several reaction steps to be run in one process.

**tc2.ch.tum.de**

### Chair of
### Theoretical Chemistry

**Prof. Dr. Karsten Reuter**

Prof. Reuter's research activities are mainly focused on quantitative modeling of material properties and functionalities. Heterogeneous catalysis and energy research are particular areas of interest.
He makes widespread use of modern multi-scale modeling, which unites methods and concepts from the disciplines of physics and chemistry as well as materials science and engineering.

**th4.ch.tum.de**

### Chair of
### Macromolecular Chemistry

**Prof. Dr. Bernhard Rieger**

The research activities of Prof. Rieger are focused on polymerization catalysis. His work provides on the one hand the opportunity to selectively control the microstructure of polymers and on the other hand leads to completely new functional polymer materials. He also explores the use of $CO_2$ as a resource for the synthesis of polymers. This process produces biodegradable polycarbonate.
Other research areas include low-valent organo-functionalized silicon compounds and the development of new catalysts as well as materials on the basis of main group elements compounds.

**makro.ch.tum.de**

## CRC Members

**Chair of**
**Chemistry of Biogenic Resources**

**Prof. Dr. Volker Sieber**

The research activities of Prof. Sieber focus on biocatalysis and its combination with heterogeneous catalysis and electrochemistry in single processes. By learning from mechanisms of biochemical reactions and evolving enzymes for new activities he is developing new routes for the sustainable production of chemicals and fuels from biomass (biobased chemicals and materials) as well as from carbon dioxide ("Power to Chemicals").

**rohstoffwandel.de**

**Chair of**
**Experimental**
**Semiconductor Physics**

**Prof. Dr. Martin Stutzmann**

The research of Prof. Stutzmann explores fundamental and application-oriented aspects of semiconductor physics. His main areas of interest are the production, nanostructuring and biofunctionalizing of semiconductors with a large band gap like gallium nitride, zinc oxide and diamond, as well as thin layers and silicon nanoparticles.
Possible applications include biosensors, model systems for quantum information processing and semiconductor-based photovoltaic and thermoelectric energy conversion, as well as sophisticated photo-catalyst materials.

**wsi.tum.de**

# Directions, Imprint and Contact

# Orientation on Garching TUM Campus

## Travelling by public transport

### City Center/Munich Central Station
- S-Bahn direction ‚Ostbahnhof', exit station Marienplatz, change to
- U-Bahn U6 with direction to ‚Garching Forschungszentrum'

### Munich Airport
- S-Bahn S8 to ‚Ismaning'
- take bus 230 until stop ‚Garching Forschungszentrum'

**or**
- S-Bahn S1 to ‚Neufahrn'
- take bus 690 (weekdays only) to ‚Garching Forschungszentrum'

## Travelling by car

### Arriving from north
- Highway A9, ‚München-Nürnberg'
- Exit ‚Garching-Nord',
- Follow signs: ‚Forschungszentrum'

### Munich International Airport
- Highway A92 towards direction ‚München'
- Exit ‚Freising-Süd'
- follow B11 towards direction ‚München' via ‚Dietersheim'
- left turn after ca. 2 km
- Follow signs: ‚Forschungszentrum'

## Imprint

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Academic Director
TUM Catalysis Research Center

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