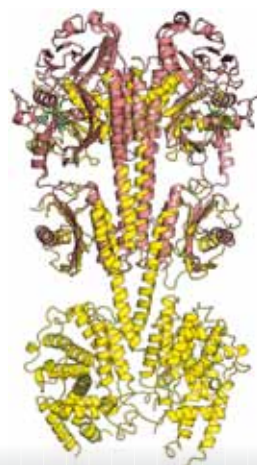


## Biocatalysis in Cellular Systems

- Elucidation and manipulation of complex biocatalytic processes in cellular systems by skillful combination of synthetic chemistry and genetic code engineering
- Synthesizing non-canonical amino acids (ncAAs) with unique side chain chemistries for incorporation into the target proteins by expanding the genetic code
- Transferring the chemical synthetic laboratory into the biochemistry of living cells
- Large-scale biological production of tailored peptide antibiotics
- Expanding our synthetic and biosynthetic approaches to combinatorial biosynthesis with nonribosomal peptide synthetases to further overcome the limits of ribosomal peptide synthesis
- Elucidating and steering light-gated enzymes in physiological reaction cascades



## BIG-NSE: UniCat's Graduate School

UniCat promotes young scientist and students. The Berlin International Graduate School of Natural Sciences and Engineering is an important part of UniCat. Excellent students are encouraged to apply for a fellowship.

[www.big-nse.tu-berlin.de](http://www.big-nse.tu-berlin.de)

## BasCat: UniCat-BASF Joint Lab

In 2011 UniCat and the chemical company BASF founded the new UniCat-BASF Joint Lab, or BasCat for short. BasCat is dedicated to the development of new catalytic processes for raw material change.

[www.bascat.tu-berlin.de](http://www.bascat.tu-berlin.de)

“Unifying Concepts in Catalysis” (UniCat) is supported by the German Research Foundation (DFG) within the framework of the German Initiative for Excellence. Six institutions are involved in UniCat hosted by the Technische Universität Berlin.



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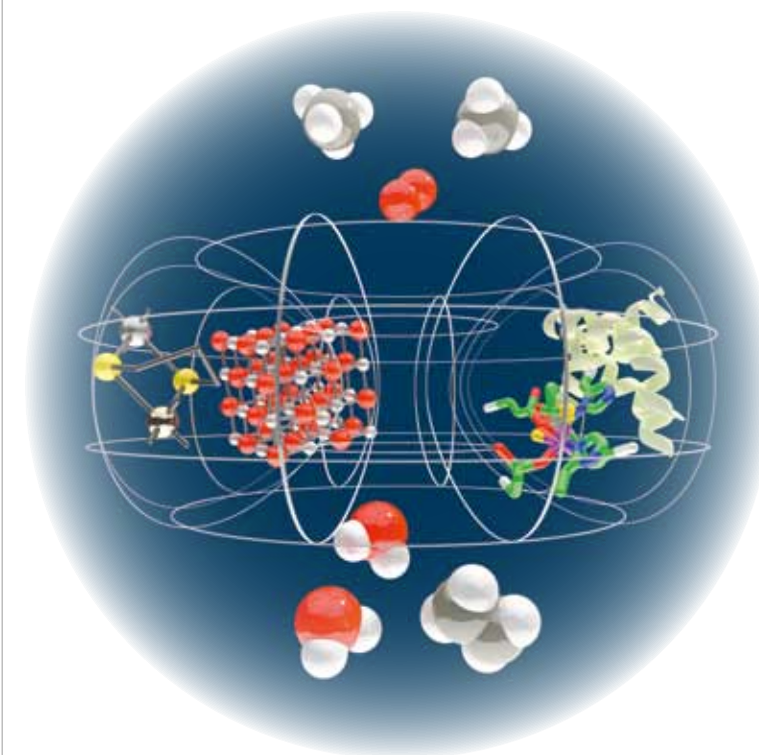
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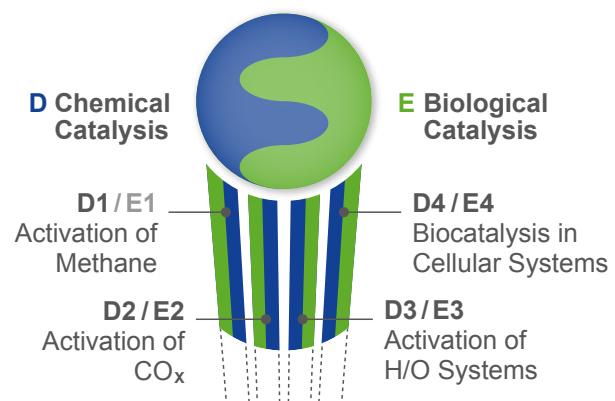
[www.unicat-berlin.de](http://www.unicat-berlin.de)



## Cluster of Excellence Unifying Concepts in Catalysis



## Catalysis is a Key Technology



### UniCat aims at

- Determination of similarities and differences in the concepts of chemical (heterogeneous, homogeneous) and biological catalysis
- Identification of a platform where chemical and biological catalysis can be unified
- Identifying key parameters that control mechanism and dynamics of specific catalytic processes at different levels of complexity
- Promoting a more general understanding of catalysis to enable a knowledge-based prediction of catalyst performance and potential new applications.

### Challenges

- Efficient use of resources by activation of small molecules e.g. methane, oxygen, hydrogen, carbon oxides
- Tailoring enzymes for biotechnological use
- Catalyst-assisted drug synthesis
- Upscaling

## RESEARCH BAND D1/E1

### Activation of Methane

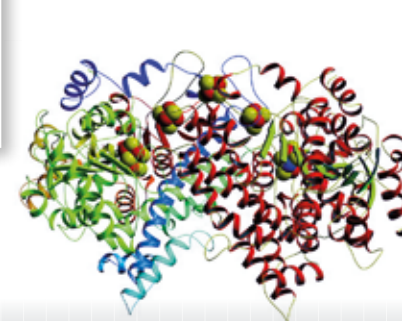
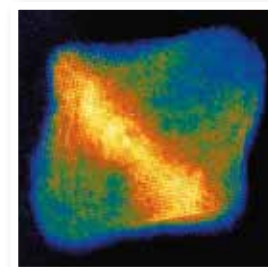
- Elucidation of the molecular mechanism of oxidative coupling of methane (OCM), including identification of reactive intermediates and active sites
- Understanding of the interaction of surface-confined and gas phase elementary reactions
- Comprehensive kinetic and mechanistic description of OCM at all relevant time and length scales from model systems to the mini-plant level
- Synthesis and structural and dynamic characterization of model and performance catalysts
- Synthesis and structural characterization of bio-inspired methane monooxygenase (MMO) models based on Cu metal sites



## RESEARCH BAND D2/E2

### Activation of Carbon Oxides

- Elucidation of the molecular mechanism of dry reforming of methane (DRM), including identification of reactive intermediates
- Comprehensive kinetic and mechanistic description of dry reforming at all relevant time and length scales from model systems to the mini-plant level
- Synthesis of molecular model systems for comparative mechanistic analysis of enzymes and chemical catalysts converting carbon oxides: CO, CO<sub>2</sub>, HCOOH, CH<sub>3</sub>COOH
- Mechanistic analysis of enzymes converting the above mentioned carbon oxides, including identification, characterization and modification of active sites for specific functions
- Engineering of enzymes and enzyme complexes towards novel functions in the activation of small molecules
- Stabilization of enzymes for biofuel cell applications: engineering of oxygen tolerant enzymes, reverse the reaction of enzymes by modulation and generation of mini-enzymes



## RESEARCH BAND D3/E3

### Activation of H/O Systems

- Fundamental coordination chemistry studies by combining essential features of [NiFe]-Hydrogenases
- Development of bioinspired hydrogenation catalysts and understanding of their mechanism
- Investigation of the molecular details of aerobic H<sub>2</sub> cycling in a multidisciplinary effort
- Application of novel innovative silicon- and germanium-based frustrated Lewis pairs (FLP) capable of activating H<sub>2</sub> and catalytic hydrogenation
- “High load” biofuel cells based on nanoporous electrode materials (capacity and long-term stability)
- Light-driven hydrogen production from water in aerobic cellular systems
- Mechanistic “in-operando” spectro-electrochemical studies
- New approaches in X-ray spectroscopy combined with advanced EPR studies and DFT calculations
- Insights into the light-driven self-assembly of the catalytic Mn complex
- Developing functional systems capable of activating oxygen for the oxidation of hydrocarbons

