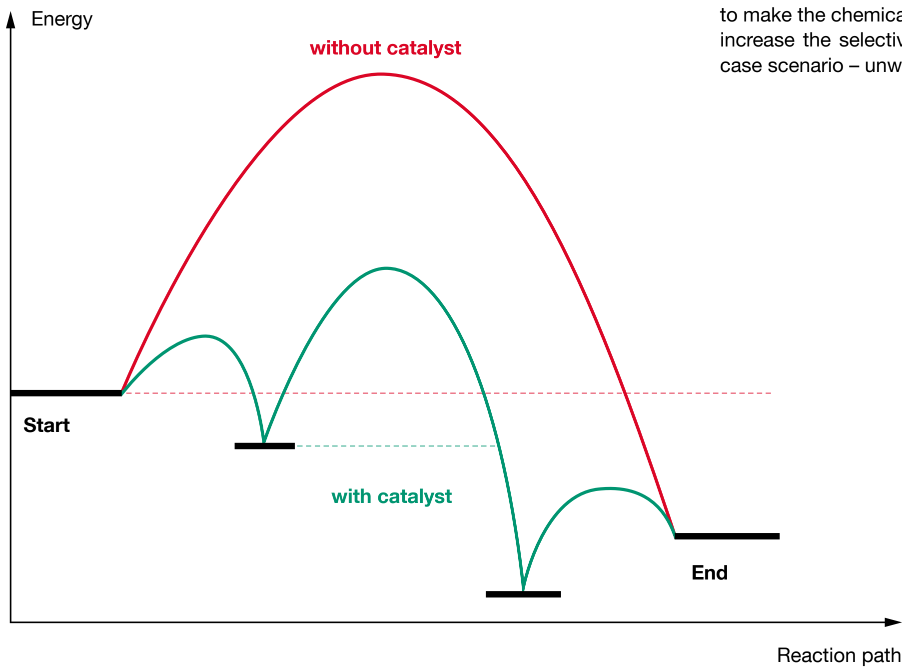
Picture credit: Hoeglmeier

Catalysis – the Frontier Technology

By TUM President Prof. Wolfgang A. Herrmann

The development of new catalysts and catalytic processes will play a crucial role in the future success of Germany as a key location in the chemical industry. With its high-tech infrastructure and dense competence network of national and international reach, TUM's new Catalysis Research Center provides an ideal scientific platform for the country that invented industrial catalysis to shine.

Picture credit: Hoeglmeier



Catalysts lower the energy barriers which chemical reactions normally have to overcome in order to create a target product, and therefore help to make the chemical industry more energy efficient. At the same time they increase the selectivity of chemical reactions and eliminate – in the best case scenario – unwanted by-products.

Of all technology principles, catalysis is unique in its ability to add value by closely aligning both economic and ecological interests. In future, the wide variety of chemical products required by high-tech societies will only be technically and economically feasible if we can harness specific catalysts to create valuable materials, reduce waste and avoid hazardous substances. Examples include the manufacture of stereochemically pure pharmaceuticals, the development of polymer substances with specific properties from simple precursors, the breakdown of end-of-life plastics, as well as the elimination of harmful emissions from manufacturing plants and combustion engines such as cars or power plants. The production, storage and conversion of energy – one of the biggest challenges of our time – also depends on advances in catalysis research – exemplified by electrochemistry and fuel cells.

Catalysis is a way to manipulate chemical reactions and achieve a specific outcome with a minimal energy and resource bill. Considering the massive volume of potential substance conversions – which is what chemistry is essentially all about – and the raw material, energy and waste problems which these generate, catalysis is at the top of today's scientific, economic, environmental and policy-making agenda. Growing resource scarcity is shining the spotlight even more on this key technology. Seriously neglected during the oil age, the future use of biogenic raw materials will heavily depend on advances in catalysis research, as will the chemical

"The catalytic force is reflected in the capacity that some substances have, by their mere presence and not by their own reactivity, to awaken activities that are slumbering in molecules at a given temperature."

Jöns Jakob Berzelius (1779–1848), who discovered the principle of catalysis

In the chemical industry, over 80 percent of value is added through catalytic processes even today. The international catalyst market is already worth more than USD 18 billion, and the trend is upward. Ultimately, catalysts are the key to an efficient and environmentally friendly chemical industry.

use of natural gas – methane in particular. Previously combusted without a second thought, this gas belongs in catalyst-filled chemical reactors – and not in industrial turbines! The omnipresent gas carbon dioxide should also prove to be a valuable chemical raw material as soon as catalysts to activate this inert gas can be found.

This applies in particular to the Federal Republic of Germany which, with few natural resources, will only remain at the vanguard of the world economy if it keeps on developing technological innovations to renew, expand and improve industrial production. In the chemical industry, catalysis is dominating the scientific discussion around technology leadership. Given the sheer product diversity and production volumes of the chemical, pharmaceutical and biofuel industries, it is obvious that for the foreseeable future, no other field of research has the potential to secure the success of the German chemical industry on the international stage.

The main purpose of applied catalysis is to activate largely inert components and cause a specific reaction. Industrial-scale examples include ammonia (NH_3) synthesis from N_2 and H_2, the conversion of CO and H_2 into fuel using the Fischer-Tropsch process and the conversion of ethylene derived from refining into polyethylene. Several Nobel Prizes have been awarded for breakthroughs in catalytic science since the achievements of Fritz Haber (1918) and Carl Bosch (1931).

To be effective, a catalyst has to be tailored to its specific purpose. This adaptation process ensures that it demonstrates the key characteristics required of a catalyst:

- Selectivity: Only selective products, i.e. the desired ones, are formed.
- Activity: The catalyst function repeats itself as often as possible in the exact same way, i.e. the effect is reproducible.

A catalyst is said to be highly selective if it achieves the target product at a rate of ≥99%. It is regarded as highly active – depending on the situation – at turnover frequencies of up to 10^6/h. This means that a catalyst unit activates one million molecular substance conversions per hour up until its deactivation. This level of performance is achieved not only by many enzymes, which are natural biological catalysts, but also by lab-created catalysts (like metallocene) in the technical synthesis of polyolefins from ethylene and propylene.

The search for new catalysts and catalytic processes is driven by three overarching goals: higher activity (smaller reactors, less energy), higher selectivity (smaller separation units, less waste) and greater sustainability (variable and, if possible, renewable raw materials; industrial biotechnology).

Catalysis research at TUM

Between 1964 and 1984, Ernst Otto Fischer achieved international acclaim at our university for his ground-breaking work in organometallic synthesis enabling a host of new substance classes. In 1973, he received the Nobel Prize in Chemistry for his research. Fischer laid the foundations for the application of these families as catalysts in chemical reactions. An early example of the work produced by his students (Hafner and Jira) was the Wacker-Hoechst process for the simple and clean production of the base chemical acetaldehyde (1958). The Munich laboratory where he worked has since become a top-flight center for organometallic catalysis research. Over the years, TUM's Department of Chemistry has prioritized catalysis research, with practically all disciplines now involved following a number of new appointments. Particular mention should go to the systematically expanded field of Biological Chemistry within the Department, which the Shanghai Ranking places among the top ten in the world for the quality of its research. Today, catalysis research at TUM is renowned for the depth and breadth of its coverage, its interdisciplinary approach and close ties with industry.

Now TUM is taking catalysis research to the next level with the *TUM Catalysis Research Center* (CRC). The initial application submitted to the German Council of Science and Humanities (WR) on August 1, 2007 was promptly approved. Representing an investment of over EUR 70 million, the new building, located at Ernst-Otto-Fischer Strasse 1 in Garching, has now been completed. The scientific aims, according to the strategy paper "are specifically focused in the medium-term on the investigation of multifunctional, nanostructured catalysts based on an interdisciplinary approach incor- ▷

Graphics: ediundsepp (source: TUM)

porating fields of engineering." Even back then, the paper pointed out that "in the chemical industry alone, today over 80 percent of value is already added through catalytic processes." The international catalyst market is already worth more than USD 18 billion, and the trend is upward. Ultimately, catalysts are the key to an efficient and environmentally friendly chemical industry.

The TUM Catalysis Research Center

The CRC steps up to the interdisciplinary challenges of modern catalysis research. It is home to a host of highly varied yet synergized methodological approaches that interact to identify the molecular chemisms of catalytic reactions, for instance, or gain an understanding of fundamental processes with solid state catalysts. This type of research breaks down the boundaries between traditional scientific disciplines. The investigation of new, structurally tailored catalysts will hinge on instrumental analysis of molecule to surface spectroscopy, as well as on reaction kinetics, theoretical models and simulation calculations, as well as technical developments in the area of process control. Parallel screening in miniature reactors in combination with numerical modeling on ▷

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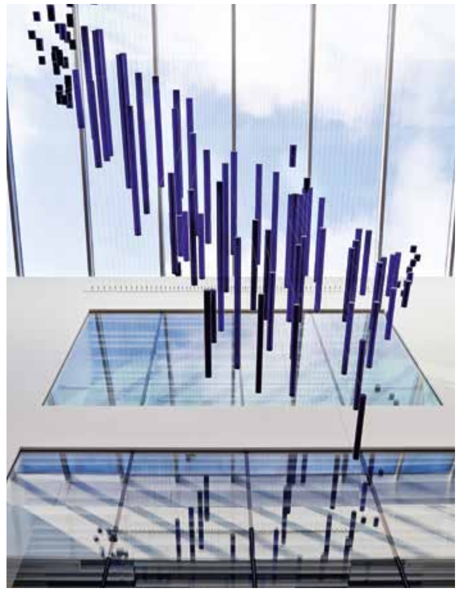

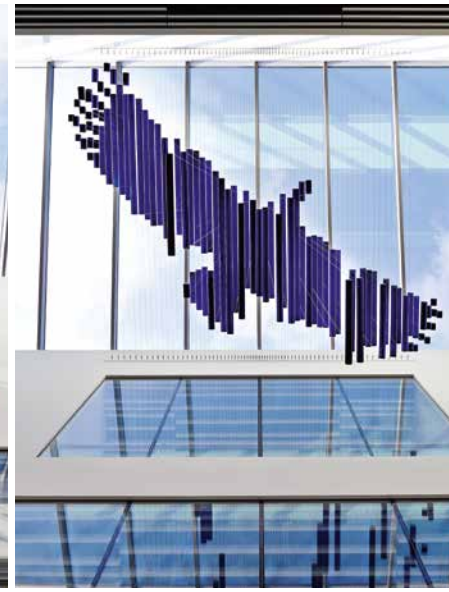

The Catalysis Research Center

The CRC is an interdisciplinary research hub at the interface of engineering and natural sciences. The building with a net area of 6,500 m^2 is solely dedicated to laboratory research work. It offers state-of-the-art infrastructure for chemical and physical research including lab-scale pilot plant facilities. Seven large laboratory areas with a total of 75 separate laboratories are complemented by well-equipped analytical core labs and two seminar rooms. □

supercomputers is set to significantly speed up progress in catalyst optimization. The Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities in Garching has the facilities to support this work. On the Garching research campus, scientists have access to a unique combination of methods to determine catalyst structures with great precision. As well as X-ray structure analysis, there is the Bavarian Nuclear Magnetic Resonance Center and the Heinz Maier-Leibnitz neutron source research reactor (FRM II).

The CRC planning and building phase was used to expand the research portfolio and adapt it to the latest scientific and technical challenges. The following institutes have been established at TUM in the meantime:

- The Research Center for Industrial or White Biotechnology – a center of excellence in engineering sciences equipped with a Pilot Plant for White Biotechnology;
- The teaching and research domain Synthetic Biotechnology funded by the Werner Siemens Foundation (EUR 11.5 m);
- New catalysis-relevant Chairs for bioinorganic chemistry, computer-aided biocatalysis, industrial biocatalysis, technical electrochemistry, physical chemistry/catalysis, silicium chemistry, solid-state NMR spectroscopy, biomolecular NMR spectroscopy, selective separation technology, systems biotechnology;
- The Bavarian NMR Center (BNMRZ) with its 1.2 gigahertz spectrometer;
- The TUM International Graduate School of Science & Engineering (IGSSE; under the 2006 Excellence Initiative), which is the scene of numerous catalysis research projects;
- The Institute of Silicon Chemistry in cooperation with Wacker Chemie AG;
- Munich Catalysis Alliance of Clariant and TUM (MuniCat).

The research activities of the Center of Excellence for Renewable Resources in Straubing are associated with the CRC. The development of biochemistry and biophysics research at TUM, likewise supported by the creation of several new professorships, lays the foundation for an expansion of catalysis research into the biopharmaceutical sphere. Our coherent overall concept puts us in a strong position to compete on the international stage in the future.

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