# The Max-Planck-Institut für Kohlenforschung: basic chemical research with a focus on catalysis

The Max-Planck-Institut für Kohlenforschung has been conducting basic chemical research for over 100 years. Following its foundation in 1914, numerous chemical discoveries of historical significance have been made at the institute. The major achievement of the early years of coal research was the invention of the Fischer-Tropsch process by Franz Fischer and his co-workers, which allows mineral coal to be transformed into transportable fuels, such as gasoline or diesel oil.

After the appointment of Karl Ziegler as director of the institute in 1943, research efforts were primarily directed towards organometallic chemistry. Among the numerous important developments, the polymerization of ethylene or propylene via "Ziegler-Natta catalysis" stands out and was rewarded with the Nobel prize to Karl Ziegler in 1963. Another milestone was the cyclooligomerization of 1,3-butadiene to carbocycles by Günther Wilke (Ziegler's successor) and his co-workers.

Today, the institute consists of five scientific departments, each headed by a director. About 370 students and employees from all over the world are dedicated to basic chemical research with a focus on catalysis. They are supported by service groups that provide state-ofthe-art analytics, IT and technology.





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Our researchers develop methods for resource-conserving sustainable chemical processes.







Basic chemical research with a focus on catalysis in all of its aspects

# Bilder: Frank Vinken für MPI für Kohlenforschun

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### Department of Organometallic Chemistry: Prof. Dr. Alois Fürstner

Carbon is able to engage in bonding with any metal of the periodic table of the elements. Our research tries to make targeted use of the reactivity of metal-carbon single, double, triple or  $\pi$ -bonds in catalytic transformations. Specifically, we are interested in the metathesis of alkenes and alkynes using complexes of ruthenium, molybdenum and tungsten, the development of ironcatalyzed cross-couplings, the emerging field of gold and platinum catalysis, and metal carbene chemistry in general. The development of new synthetic methods is complemented by mechanistic investigations and applications to the synthesis of structurally complex and biologically relevant natural products.

# **Department of Homogeneous Catalysis: Prof. Dr. Benjamin List**

For a long time, chemists thought that there were only two types of well-functioning catalysts: On the one hand there are enzymes, which are used by all living organisms to catalyze essentially all biological processes, and on the other hand there are synthetic metal-containing compounds and materials. The List group discovered a third class of general catalysts, metal-free small molecules such as amino acids.



This discovery has given chemists new tools, known as "organocatalysts", which they can use to produce scents, materials and medicines, for example, in a more environmentally friendly and energy-saving way.

# Department of Molecular Theory and Spectroscopy: Prof. Dr. Frank Neese

Using modern computers, it is possible to calculate molecular structures, energies and properties with high accuracy and to realistically simulate chemical processes. The activities of the department range from theoretical method development in guantum chemistry (within the framework of the worldwide wide extensively used ORCA program) to computational chemistry applications in transition metal chemistry, magnetism and catalysis to the experimental application of modern spectroscopic methods (EPR, ENDOR, MCD, resonance Raman, Mößbauer ...). The emphasis of our approach to science is a close interaction between theory with particular attention to advanced spectroscopy. A second general aim of our studies is to not only compute accurate numbers, but to also interpret and understand the results in chemical terms.



# Department of Organic Synthesis: Prof. Dr. Tobias Ritter

The focus of research is on the development of new chemical reactions. The aim is to discover new molecular structures and reactivities that can contribute to interdisciplinary scientific challenges. The laboratory works in the field of synthetic organic chemistry, organometallic chemistry and the synthesis of complex molecules. Scientists are also engaged in mechanistic studies to gain easier access to molecules of interest in catalysis, medicine and materials science.



# Department of Heterogeneous Catalysis: Prof. Dr. Ferdi Schüth

Most of the catalysts used in industry today are solids. Therefore they are in the center of the department's activities. The properties of the solids on the nanometer scale are manipulated using a number of different methods in order to tailor the catalysts to the desired application.

The aim is to develop better catalysts for chemical processes and for reactions that are important for our energy supply, such as the use of biomass. Other interesting solid state properties, such as optical and magnetic effects, are also being investigated on these nanomaterials.