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# Green Methanol for the Circular Economy - New Catalyst Developed at LIKAT

This is the vision: to produce the raw material methanol at the edge of the field or on the farm using renewable energies. In addition to wind or sun, water and  $CO_2$  would be needed to produce the raw materials for the green methanol process: Carbon monoxide (CO) and hydrogen ( $H_2$ ), which react catalytically to form methanol. This is made possible by a new catalyst developed in Rostock. A process based on this completely dispenses with fossil raw materials. And it is highly selective, i.e. it produces virtually no by-products.

The catalyst is based on manganese, as Gordon Neitzel from the Leibniz Institute for Catalysis (LIKAT) explains: "The metal atom forms the catalytic center. It is fixed and protected by a kind of scaffold, the so-called ligand." As part of his doctorate, Gordon Neitzel optimized the molecular structure of this ligand and put the finishing touches to the catalyst complex, so to speak. The results were published in the journal CHEMCATCHEM.

## Climate-neutral Management with E<sup>4</sup>MeWi

The work is part of the E<sup>4</sup>MeWi research network. The abbreviation stands for "Energie-Effiziente Erneuerbare Energien basierte Methanol-Wirtschaft" (Energy-Efficient Renewable Energy-based Methanol Economy). The joint project was funded by the Federal Ministry for Economic Affairs and Energy for three years with two million euros. The project partners are also CreativeQuantum GmbH in Berlin, Ineratec GmbH in Karlsruhe, Ruhr University Bochum and the Bitterfeld-Wolfen Chemical Park.

"A climate-neutral economy, as the Federal Republic of Germany is aiming for by 2045, also needs basic chemicals," Gordon Neitzel continues. Methanol is needed for plastics and resins, for example, which are used everywhere from the furniture to the automotive industry. Methanol production, currently 110 million tons per year worldwide, traditionally runs on natural gas - at high pressures of around 50 to 100 bar and temperatures between 200 and 300°C, depending on the process. With every tonne of methanol, the huge plants emit one and a half tons of carbon dioxide. This has no future.

#### Reduced Pressure and Temperature Requirements

The  $E^4$ MeWi project aims to provide an alternative to the conventional process. Its core element is the catalyst, which allows  $H_2$  and CO to react in a dissolved state to produce methanol. The carbon monoxide is first extracted from  $CO_2$ .

The manganese catalyst used for this was originally developed at LIKAT in the research group led by Dr. Kathrin Junge and Prof. Dr. Matthias Beller. It enables a completely new process that halves the pressure and temperature required for methanol production.





Fig. 1: Supply of the starting materials for the production of methanol: carbon monoxide (CO) and hydrogen (H<sub>2</sub>). In the E<sup>4</sup>MeWi project, these substances come from sustainable sources. (picture: LIKAT, nordlicht)

In addition, the process does not require fossil raw materials, which makes the catalyst a key element of a future  $CO_2$ - and climate-neutral circular economy. Especially as methanol, produced in a green way, is also well suited as a chemical storage medium for hydrogen, one of the hopes of the energy transition.

#### Methanol Plants in Container Size

The  $E^4$ MeWi project participants envision a container-sized plant that uses local resources for sustainable value creation virtually at the edge of the field, on the farm or on the farmyard: Wind and solar energy,  $CO_2$  emissions from point sources and from biogas, plastic waste or wood waste.  $CO_2$  and water are initially combined to produce synthesis gas, a mixture of hydrogen and carbon monoxide, which is converted into methanol using the new catalyst.

Gordon Neitzel has significantly optimized the well-known manganese catalyst by developing new structures for the ligand that protectively surrounds the catalytically active center. "Without this shell, carbon monoxide would attack the manganese atom in the center of the catalyst and destroy the complex compound." This work has now doubled the reaction speed in methanol production.



Simplified scheme of the reaction: Carbon monoxide (CO, obtained from CO<sub>2</sub>) reacts with hydrogen to form methanol (CH<sub>3</sub>OH).

Above the arrow: This is what a model of the catalyst might look like. A manganese atom (Mn) is the reactive center, which is protected by a shell, the ligand. Phosphorus and nitrogen atoms (P and N) play a special role in this ligand. They clasp the Mn atom like pincers. Scheme: LIKAT/Neitzel

This brings the project partners a good deal closer to an economically viable plant. After all, this is also part of the aim of such decentralized production: to establish a completely new market for the methanol trade and thus promote economic transformation processes.

#### Publication:

"An Improved Manganese Pincer Catalyst for low Temperature Hydrogenation of Carbon Monoxide to Methanol"

G. Neitzel, R. Razzaq, A. Spannenberg, K. Stier, M. P. Checinski, R. Jackstell, M. Beller, ChemCatChem 2024, e202301053.

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### Contact:

Gordon Neitzel
PhD in the "Applied
Carbonylations" Group
Gordon.neitzel@catalysis.de



Dr. Ralf Jackstell
Group Leader of the "Applied Carbonylations" Group ralf.jackstell@catalysis.de