Catalyst cleans up CO2 better with different preparation

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CO_2 molecules land on the surface of the catalyst during CO_2 hydrogenation. At a high pretreatment temperature, titanium atoms (brown) remain on the nickel (gold). Credit: Utrecht University

An international research team led by Bert Weckhuysen (Utrecht University) and Sara Bals (University of Antwerp) has shown that a promising catalyst for clearing CO_2 becomes significantly more active and selective if its pretreatment is modified. The scientists have visualized the mechanism underlying this concept with unparalleled precision. The results of the study are published in *Science* on May 11. Matteo Monai, Kellie Jenkinson and Angela Melcherts are the first authors.

Cleaning up carbon dioxide or converting it into something useful is becoming increasingly common, for example in the energy and transportation sectors, where huge amounts of the greenhouse gas are emitted. Catalysts are necessary for such a cleanup process to proceed properly and quickly. In the case of CO_2 hydrogenation, which is a widely used chemical reaction to clean up CO_2, a nickel-supported titanium dioxide catalyst is used.

In this study, the scientists show that the catalyst's performance is highly dependent on the temperature at which it is prepared. The selectivity and activity of the catalyst were much better during CO_2 hydrogenation at a pretreatment temperature of 600°C than at 400°C. Better selectivity is desirable because the catalyst provides fewer unwanted by-products. Improved activity results in a faster progression of the catalytic reaction. The researchers expect the same principle to apply to catalysts with metal oxides other than titanium oxide.

The team of scientists made the principle visible using advanced electron microscopy. And they did so with unparalleled precision: at the atomic level. They inserted a special nanoreactor, in which the catalytic process took place, into the microscope and were able to see exactly what happened to the catalyst.

"During the process, you see the titanium atoms crawling onto the nickel like layers and coming off again," Bert Weckhuysen says. "At a high pretreatment temperature, some titanium atoms remained on the nickel. At a low temperature, the layers of titanium atoms disappeared completely."

Two chemical elements, such as nickel and titanium, interacting and forming a catalyst, is an old concept known as strong metal support interaction (SMSI). This study reveals for the first time what happens at the atomic level during this interaction. The sliding layers of titanium have never been seen before. "The new technique has made it possible for us to observe this with our own eyes," says Weckhuysen. "With, moreover, a very high resolution. We can count the titanium atoms on the nickel."

The international research team that worked on the study is extremely interdisciplinary. According to Sara Bals, this was critical to achieving the results obtained. "We used electron microscopy techniques that are generally difficult to combine with experiments in a nanoreactor," she says. "Researchers with different backgrounds and access to a variety of advanced techniques each laid out small pieces of a larger puzzle. Ultimately, these pieces combined led to the complete picture."

More information: Matteo Monai et al, Restructuring of titanium oxide overlayers over nickel nanoparticles during catalysis, *Science* (2023). DOI: 10.1126/science.adf6984.
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