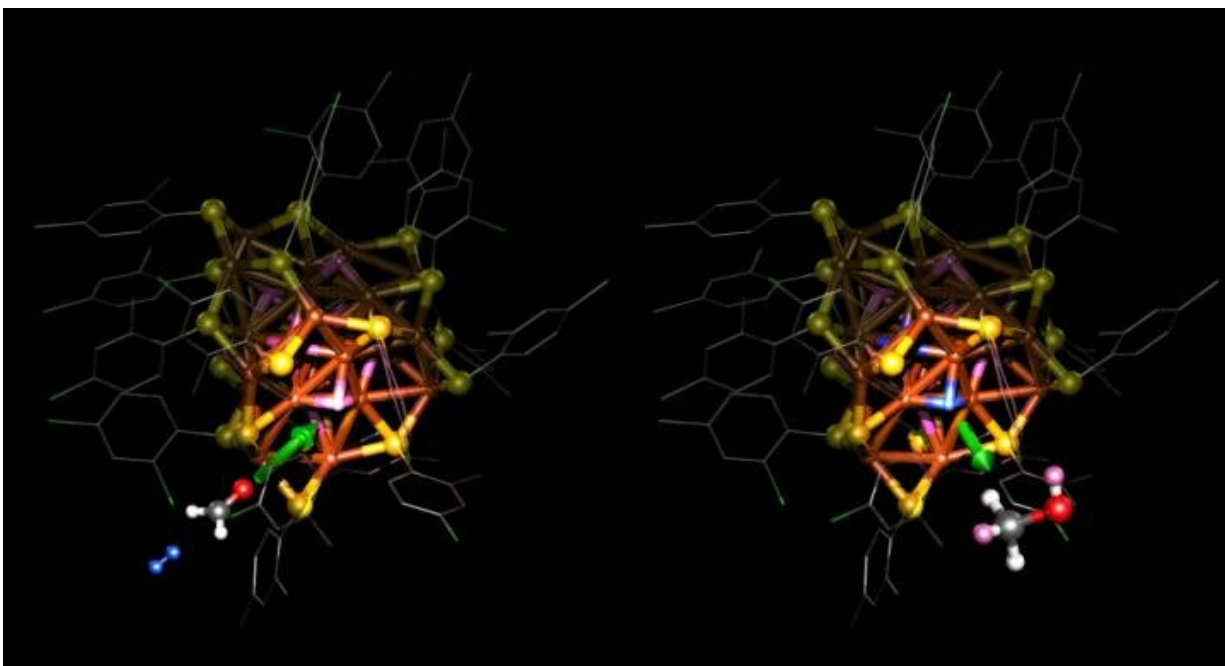


Researchers discover how a nanocatalyst works at the atomic level

May 29 2019



Atomic structure of the copper catalyst used in the hydrogenation reaction of a carbon-oxygen bond. Formaldehyde H_2CO (on the left), used as the model molecule in the simulations, takes two hydrogens from the copper; they move to the carbon-oxygen bond so that the molecule changes into a simple alcohol (methanol CH_3OH on the right). After the reaction, a hydrogen molecule (blue, on the left) in the vicinity splits into two hydrogen atoms inside the copper. Credit: Sami Malola, University of Jyväskylä

Researchers of the Nanoscience Center (NSC) at the University of

Jyväskylä, Finland, and Xiamen University, China, have discovered how copper particles at the nanometer scale operate in modifying a carbon-oxygen bond when ketone molecules turn into alcohol molecules. Modification of the carbon-oxygen and carbon-carbon bonds found in organic molecules is an important intermediate stage in catalytic reactions in which the source material is changed into valuable end products.

Understanding the operation of catalysts at the level of the atomic structure of a single particle makes it possible to develop catalysts with desired features, such as making them efficient and selective for a specific end product. The study was published in *ACS Nano*. In Finland, the study was led by Academy Professor Hannu Häkkinen.

The catalytic [copper particles](#) used in the study were made and structurally characterized at Xiamen University, and their operation in changing a strong carbon-oxygen bond in a hydrogenation reaction was studied by the researchers of the Nanoscience Center (NSC) at the University of Jyväskylä in [computer simulations](#). The precise atomic structure of the copper particles was determined through X-ray diffraction and nuclear magnetic resonance (NMR) spectroscopy. The particles were found to contain 25 copper atoms and ten hydrogens, and there were 18 thiols protecting the surface of the particle. While the experimental work in Xiamen revealed its excellent performance in catalytic hydrogenation of ketones, the simulations predicted that the hydrogens bound to the copper core of the particle act as a [hydrogen storage](#), which releases two [hydrogen atoms](#) to the carbon-oxygen bond during a reaction. The hydrogen storage is refilled after the reaction, when a hydrogen molecule attached to the particle from its surroundings splits into two hydrogen atoms, which are bound again to the copper core (see image). The NMR measurements carried out in Xiamen revealed an intermediate product of the reaction, which confirmed the predictions of the computational model.

"This is one of the first times that it has been possible to discover how a catalytic particle works when its structure is known this accurately, thanks to a cooperation involving both experiments and simulations," says Academy Professor Hannu Häkkinen from the University of Jyväskylä, who led the computational part of the study.

Häkkinen's collaborator, Karoliina Honkala, professor of computational catalysis, says, "Traditionally, expensive platinum-based catalysts are used in hydrogenation reactions. This study proves that nanoscale copper hydride particles also act as hydrogenation catalysts. The results give hope that in the future, it will be possible to develop effective and inexpensive copper-based catalysts to transform functionalized organic molecules into products with a higher added value."

More information: Cunfa Sun et al, Atomically Precise, Thiolated Copper-Hydride Nanoclusters as Single-Site Hydrogenation Catalysts for Ketones in Mild Conditions, *ACS Nano* (2019). [DOI: 10.1021/acsnano.9b02052](https://doi.org/10.1021/acsnano.9b02052)

Provided by Academy of Finland

Citation: Researchers discover how a nanocatalyst works at the atomic level (2019, May 29) retrieved 28 April 2024 from <https://phys.org/news/2019-05-nanocatalyst-atomic.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.