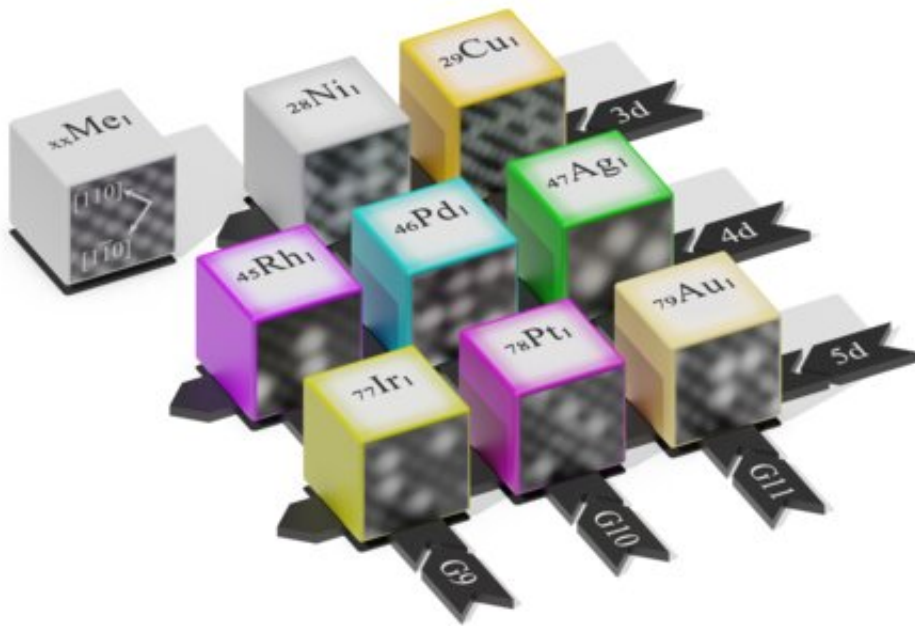


Single atoms as a catalyst

January 22 2021



Using single atoms lowers the cost of catalysts. Credit: Vienna University of Technology

For years, the metal nanoparticles used in catalysts have been getting smaller and smaller. Now, a research team at TU Wien in Vienna, Austria have shown that everything is suddenly different when you arrive at the smallest possible size: a single atom.

Metals such as gold or platinum are often used as catalysts. In the catalytic converters of vehicles, for example, platinum nanoparticles

convert poisonous carbon monoxide into non-toxic CO₂. Because platinum and other catalytically active metals are expensive and rare, the nanoparticles involved have been made smaller and smaller over time.

Single-atom catalysts are the logical end point of this downsizing: The [metal](#) is no longer present as particles, but as individual atoms that are anchored on the surface of a cheaper support material. Individual atoms can no longer be described using the rules developed from larger pieces of metal, so the rules used to predict which metals will be good catalysts must be revamped—this has now been achieved at TU Wien. As it turns out, [single atom](#) catalysts based on much cheaper materials might be even more effective. These results have now been published in the journal *Science*.

Smaller is sometimes better

Only the outer atoms of the piece of metal can play a role in chemical processes—after all, the atoms inside never come into contact with the environment. In order to save material, it is therefore best to use tiny metal particles instead of large lumps, so that a greater proportion of the atoms reside at the surface. If we go to the ultimate limit and use individual atoms, every single atom is chemically active. Over the last decade the field of "single atom" catalysis has grown dramatically, achieving great success.

Wrong model, right solution

"The reasons why some [precious metals](#) are good catalysts was already researched in the 1970s," says Prof. Gareth Parkinson from the Institute for Applied Physics at TU Wien. "For example, Gerhard Ertl was awarded the Chemistry Nobel Prize in 2007 for providing atomic-scale insights into catalysis."

In a piece of metal, an electron can no longer be assigned to a specific atom; the electronic states result from the interaction of many atoms. "For individual atoms, the old models are no longer applicable" says Gareth Parkinson. "Individual atoms do not share electrons like a metal, so the electron bands, whose energy was key to explaining catalysis, simply do not exist in this case."

Gareth Parkinson and his team have therefore been intensively investigating the atomic mechanisms behind this single-atom catalysis in recent years. "In many cases the metals that we think of as good catalysts remain good catalysts in the form of [individual atoms](#)" says Gareth Parkinson. "In both cases it is the same electrons, the so-called d electrons, that are responsible for this."

Customized properties through tailored surfaces

Entirely new possibilities arise in single-atom catalysis that are not available when using ordinary metal particles: "Depending on the surface on which we place the metal atoms and which atomic bonds they form, we can change the reactivity of the atoms," explains Parkinson.

In some cases, particularly expensive metals like platinum are no longer necessarily the best choice. "Individual nickel atoms show great promise for carbon monoxide oxidation. If we understand the atomic mechanisms of single atom catalysis, we have a lot more leeway to influence the [chemical processes](#)," says Parkinson.

Eight different metals were precisely analyzed in this way at TU Wien—the results fit perfectly with the theoretical models that have now been developed in a collaboration with Prof. Cesare Franchini at the University of Vienna.

"Catalysts are very important in many areas, especially when it comes to

chemical reactions that play a major role in attempts to develop a renewable energy economy," emphasizes Gareth Parkinson. "Our new approach shows that it doesn't always have to be platinum." The decisive factor is the local environment of the [atoms](#)—and if you choose it correctly, you can develop better catalysts and at the same time save resources and costs.

More information: Jan Hulva et al. Unraveling CO adsorption on model single-atom catalysts, *Science* (2021). [DOI: 10.1126/science.abe5757](#)

Provided by Vienna University of Technology

Citation: Single atoms as a catalyst (2021, January 22) retrieved 26 April 2024 from <https://phys.org/news/2021-01-atoms-catalyst.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.