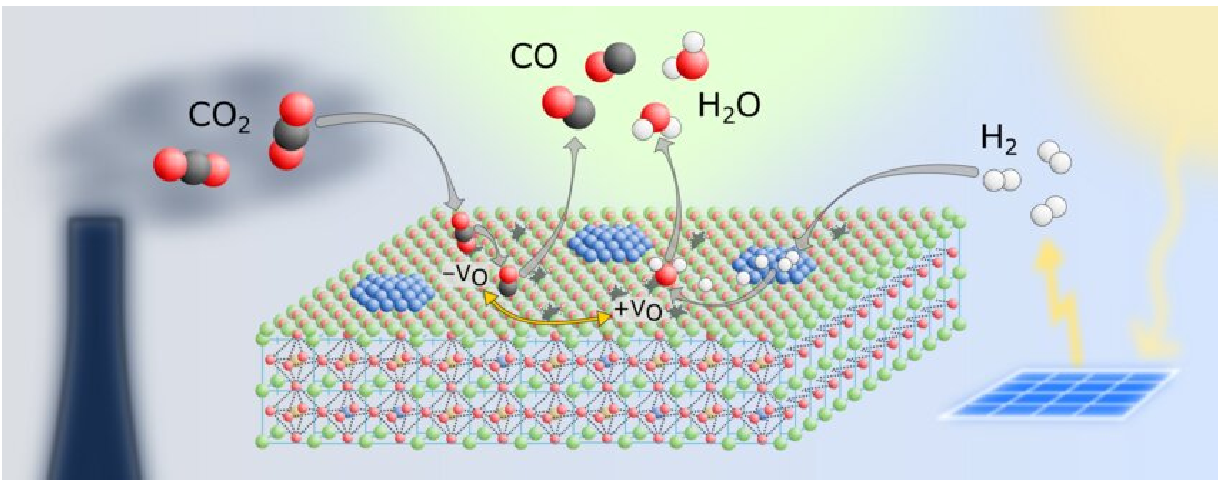
New catalyst for lower carbon dioxide emissions

April 20 2021



Credit: Vienna University of Technology

If the CO_2 content of the atmosphere is not to increase any further, carbon dioxide must be converted into something else. However, as CO_2 is a very stable molecule, this can only be done with the help of special catalysts. The main problem with such catalysts has so far been their lack of stability: after a certain time, many materials lose their catalytic properties.

At TU Wien, research is being conducted on a special class of minerals—the perovskites, which have so far been used for solar cells, as anode materials or electronic components rather than for their catalytic properties. Now scientists at TU Wien have succeeded in producing a special perovskite that is excellently suited as a catalyst for converting CO_2 into other useful substances, such as synthetic fuels. The new perovskite catalyst is very stable and also relatively cheap, so it would be suitable for industrial use.

How to close the carbon cycle

"We are interested in the so-called reverse water-gas shift reaction," says Prof. Christoph Rameshan from the Institute of Materials Chemistry at TU Wien. "In this process, carbon dioxide and hydrogen are converted into water and carbon monoxide. You can then process the carbon monoxide further, for example into methanol, other chemical base materials or even into fuel."

This reaction is not new, but it has not really been implemented on an industrial scale for CO_2 utilization. It takes place at high temperatures, which contributes to the fact that catalysts quickly break down. This is a particular problem when it comes to expensive materials, such as those containing rare metals.

Christoph Rameshan and his team investigated how to tailor a material from the class of perovskites specifically for this reaction, and he was successful: "We tried out a few things and finally came up with a perovskite made of cobalt, iron, calcium and neodymium that has excellent properties," says Rameshan.

Atoms migrating through the crystal

Because of its crystal structure, the perovskite allows certain atoms to migrate through it. For example, during catalysis, cobalt atoms from the inside of the material travel towars the surface and form tiny nanoparticles there, which are then particularly chemically active. At the same time, so-called oxygen vacancies form—positions in the crystal where an oxygen atom should actually sit. It is precisely at these vacant positions that CO_2 molecules can dock particularly well, in order to then be dissociated into oxygen and carbon monoxide.

"We were able to show that our perovskite is significantly more stable than other catalysts," says Christoph Rameshan. "It also has the advantage that it can be regenerated: If its catalytic activity does wane after a certain time, you can simply restore it to its original state with the help of oxygen and continue to use it."

Initial assessments show that the catalyst is also economically promising. "It is more expensive than other catalysts, but only by about a factor of three, and it is much more durable," says Rameshan. "We would now like to try to replace the neodymium with something else, which could reduce the cost even further."

The industrial plant with built-in fuel production

Theoretically, you could use such technologies to get CO_2 out of the atmosphere—but to do that you would first have to concentrate the carbon dioxide, and that requires a considerable amount of energy. It is therefore more efficient to first convert CO_2 where it is produced in large quantities, such as in industrial plants. "You could simply add an additional reactor to existing plants that currently emit a lot of CO_2, in which the CO_2 is first converted into CO and then processed further," says Christoph Rameshan. Instead of harming the climate, such an industrial plant would then generate additional benefits.

More information: L. Lindenthal et al. Novel perovskite catalysts for CO2 utilization - Exsolution enhanced reverse water-gas shift activity, *Applied Catalysis B: Environmental* (2021). DOI:

10.1016/j.apcatb.2021.120183

Provided by Vienna University of Technology