Nanoparticle catalysts convert carbon dioxide to carbon monoxide to make useful compounds

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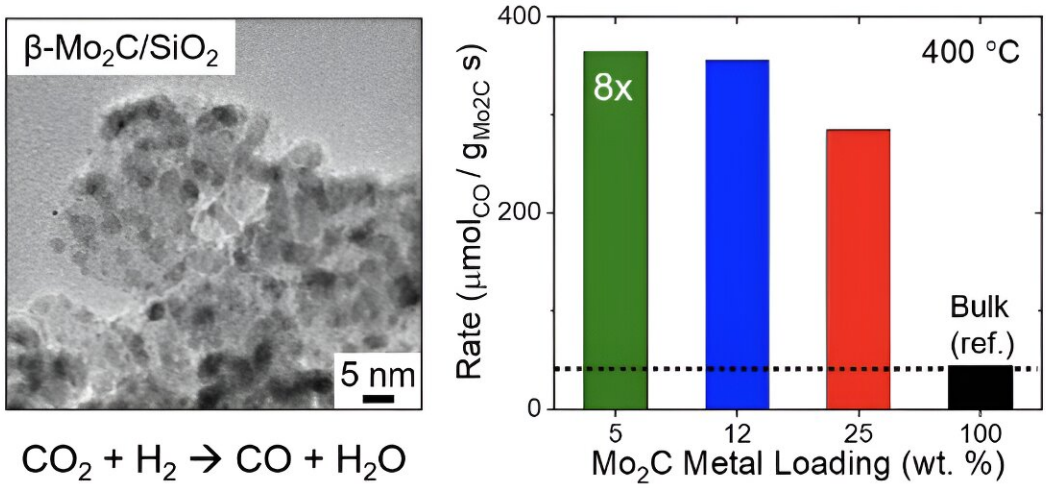

The image to the left depicts β-Mo_2C nanoparticles supported on SiO_2 (β-Mo_2C/SiO_2). The graph on the right represents the increased catalytic activity of β-Mo_2C/SiO_2 in CO production rate in the RWGS reaction compared to bulk β-Mo_2C, represented by the black bar. Each bar represents a different percentage of Mo_2C loading weight based on the mass of the SiO_2 support. Catalytic activity for this data was measured at 400°C. Credit: Carbon Future, Tsinghua University Press

As a greenhouse gas, carbon dioxide (CO_2) contributes to climate change as it accumulates in the atmosphere. One way to reduce the amount of unwanted CO_2 in the atmosphere is to convert the gas into a useful carbon product that can be used to generate valuable compounds.

A recent study attached nanoparticles of beta phase molybdenum carbide (β-Mo_2C) catalysts on a silicon dioxide (SiO_2) support to speed the conversion of CO_2 into more useful carbon monoxide (CO) gas.

CO_2 is a very stable molecule, which makes conversion of the greenhouse gas into other molecules challenging. Catalysts can be used in chemical reactions to lower the amount of energy required to form or break chemical bonds and are used in the reverse water gas shift (RWGS) reaction to convert CO_2 and hydrogen gas (H_2) into CO and water (H_2O).

Importantly, the CO gas produced by the reaction is called syngas, or synthesis gas, when combined with H_2 and can be used as a carbon source to create other important compounds.

Traditional catalysts in the RWGS reaction are made from precious metals, including platinum (Pt), palladium (Pd) and gold (Au), limiting the cost efficiency of the reaction. Because of this, new catalyst materials and formation methods are developed to increase the practicality of the RWGS reaction as a means of lowering atmospheric CO_2 and generating syngas.

In order to address the cost issues of traditional RWGS catalysts, a team of researchers from the University of Illinois in Urbana-Champaign studied the formation and catalytic activity of cheaper nanoparticle β-Mo_2C catalysts on a SiO_2 support to determine if the lower-cost catalyst could enhance activity levels of β-Mo_2C with a silica oxide support in the RWGS reaction.

The team published their study in *Carbon Future* on April 30.

"Society is moving towards a carbon-neutral economy. Carbon dioxide is a greenhouse gas, thus any technology that can break down the carbon-oxide bond in this molecule and turn carbon into a value-added chemical could be of great interest.

"One important C1 chemical is carbon monoxide, which is an essential feedstock to produce a range of products, such as synthetic fuels and vitamin A," said Hong Yang, Alkire chair professor in the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign and senior author of the paper.

Specifically, the researchers synthesized β-Mo_2C nanoparticle catalysts absorbed onto a SiO_2 support (β-Mo_2C/SiO_2). The amorphous structure of the SiO_2 support was critical for nanoparticle formation, activity and stability of the β-Mo_2C/SiO_2 catalyst.

The team additionally tested cesium (Ce), magnesium (Mg), titanium (Ti) and aluminum (Al) oxides as potential supports, but catalyst on SiO_2 produced the best catalyst formation at the temperature of 650°C.

"It appears the disordered nature of amorphous silica, which behaves like glue to catalyst nanoparticles, is a key factor of our success in achieving high metal loading and the corresponding high activity," said Siying Yu, graduate student in the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign and co-author of the paper.

Importantly, the SiO_2 catalyst support structure improves the catalytic activity of β-Mo_2C 8-fold compared to bulk β-Mo_2C. Even with improved catalytic activity, the β-Mo_2C/SiO_2 catalyst demonstrated high CO conversion and increased stability compared to bulk β-Mo_2C in

RWGS reactions.

"A major discovery of our work is a new process for producing high metal-loading catalysts made of molybdenum carbide nanoparticles. Such metal carbide catalysts are developed for converting carbon dioxide into carbon oxide at high production rate and selectivity," said Andrew Kuhn, former graduate student in the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign and first author of the paper.

The researchers performed their study under reaction conditions that favored conversion to CO gas, with a H_2:CO_2 ratio equal to 1:1. This ratio differs from the more commonly tested ratio of less than 3:1.

Reactions were also performed at temperatures between 300 to 600°C. Under these conditions, the team produced more concentrated CO, which is more efficient for downstream compound synthesis.

The team sees this research as a launching point for other catalysts that leverage support structures to increase activity. "Our ability to synthesize phase-pure metal carbide nanomaterials at high loading opens the door for the development of new catalysts for the process of CO_2 utilization," said Yang.

"I hope through in-depth study of the synthesis-structure-property relationship of this catalyst we will soon be able to uncover new important applications for value-added conversion of CO_2 and the sustainable development of our economy."

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More information: Andrew N. Kuhn et al, Valorization of carbon dioxide into C1 product via reverse water gas shift reaction using oxide-supported molybdenum carbides, *Carbon Future* (2024). DOI: 10.26599/CF.2024.9200011

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