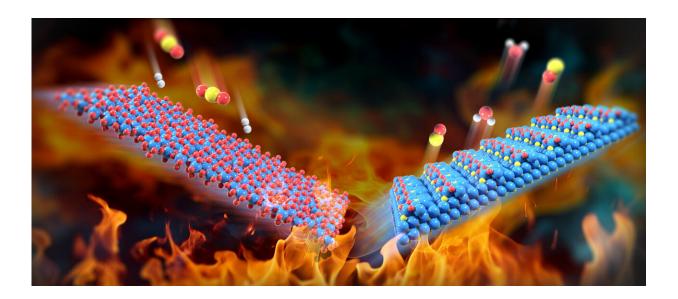


## New Mo carbide catalysts show high stability and activity in CO<sub>2</sub> conversion

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Abstract image. Credit: DICP

Molybdenum (Mo) carbides, known for their unique electronic and structural properties, are considered promising alternatives to noble metal catalysts in heterogeneous catalysis. However, traditional methods for preparing Mo carbides suffer from complex processes, stringent synthesis conditions, challenging crystal regulation, and high energy consumption. Additionally, Mo carbides are susceptible to oxidation and deactivation, which poses a significant barrier to their widespread application.



In a study <u>published</u> in *Nature Chemistry*, a research group led by Prof. Sun Jian from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) has developed a facile strategy to establish Mo carbide catalysts for efficient  $CO_2$  conversion, bypassing the complicated carburization process of traditional methods.

The researchers fabricated an Ir-modified MoO<sub>3</sub> <u>catalyst</u> using a onestep flame spray pyrolysis (FSP) method, resulting in metastable Mo oxide species due to the rapid quenching from high temperatures. This unique structure facilitated reaction-induced carburization during the RWGS reaction, thus creating oxidation-resistant Mo oxycarbide (MoO<sub>x</sub>C<sub>y</sub>) active sites.

The catalyst exhibited excellent activity and stability, highlighting the superiority of reaction-induced Mo carbide catalysts. At 600°C, it achieved a CO production rate of 17.5 mol gcat<sup>-1</sup> h<sup>-1</sup> with 100% CO selectivity. No significant deactivation was observed over a 2,000-hour stability test, showing its great potential for industrial applications.

Further investigation revealed that the crucial <u>active sites</u> in the RWGS reaction were the unsaturated  $MoO_xC_y$  species on the surface of Mo carbides. These species could maintain a dynamic equilibrium in the combined reduction, carburization, and oxidation atmosphere, preventing severe deactivation.

Additionally, the researchers proposed a new carbon cycle pathway in the RWGS reaction that was more thermodynamically favorable than the traditional redox pathway by promoting the  $H_2$  dissociation through \*COH species. This pathway could act as a supplement to the redox mechanism, enhancing CO<sub>2</sub> conversion on Mo carbides and leading to superior catalytic performance.

"Our study provides a low energy-consuming strategy for developing Mo



carbides as efficient catalysts and paves the way for the application of a low-cost Mo-based catalyst system for  $CO_2$  utilization," said Prof. Sun.

**More information:** Reaction-induced unsaturated Mo oxycarbides afford highly active CO<sub>2</sub> conversion catalysts, *Nature Chemistry* (2024). DOI: 10.1038/s41557-024-01628-4

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