Basic Research

Novel Catalyst Boosts Hydrogenation of CO_2 to Methanol: Higher Activity, Selectivity and Stability

The hydrogenation of carbon dioxide (CO_2) to methanol using a renewable energy-based "green hydrogen" source is one of the promising methods to alleviate energy crisis and achieve the goal of carbon neutrality.

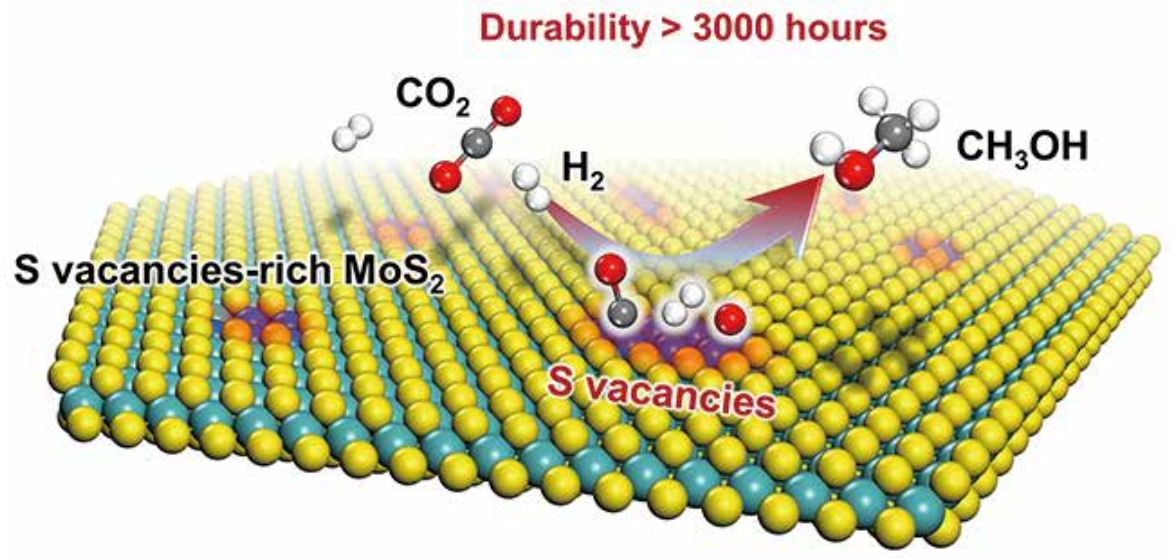
Recently, a group led by Prof. DENG Dehui from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS), in collaboration with Prof. WANG Ye from the College of Chemistry and Chemical Engineering, Xiamen University, for the first time, achieved hydrogenation of CO_2 to methanol at low temperature and with high efficiency.

The study was published in *Nature Catalysis* on March 22, 2021.

Traditional metal oxide catalysts for CO_2 to methanol reaction typically require a high temperature of above 300°C, which causes undesired reverse water-gas shift (RWGS) side reactions, and thus produces a large amount of CO as the by-product.

Introduction of transition metal components onto metal oxides can promote the activation of H_2, thereby reducing the reaction temperature, but this also facilitates excessive hydrogenation of CO_2 to CH_4, leading to lower methanol selectivity.

In this study, the sulfur vacancy-rich few-layered MoS_2, as the catalyst, could simultaneously activate and dissociate CO_2 and H_2 at low temperatures and even at room temperature, thereby facilitating the hydrogenation of CO_2 to methanol with high activity and selectivity.



Sulphur vacancies-rich MoS_2 as catalyst for the hydrogenation of CO_2 to methanol. (Image by HU Jingting and YU Liang)

In situ characterizations combined with theoretical calculations demonstrated that the in-plane sulfur vacancies on MoS_2 were the active centers for catalyzing the highly selective hydrogenation of CO_2 to methanol.

In addition, the researchers found that the RWGS reaction and excessive hydrogenation of methanol to CH_4 were effectively suppressed. At 180°C, the methanol selectivity could reach 94.3% at a CO_2 conversion of 12.5%; this result was better than that obtained with the commercial $Cu/ZnO/Al_2O_3$ catalyst and previously reported catalysts.

The activity and selectivity were steadily maintained for over 3,000 hours over the MoS_2 catalyst, making it a promising candidate for industrial applications.

"This work reveals the potential of in-plane vacancies in two-dimensional materials for catalysis and provides a novel strategy for the development of new catalysts to be used in CO_2 hydrogenation," said Prof. DENG.

This work was highlighted in a *News & Views* article in Nature Catalysis. Prof. Felix Studt from Karlsruhe Institute of Technology appraised it as an amazing and interesting work, which may bring large efficiency gains in CO_2 conversion to methanol.

(DICP)

Reference

Jingting Hu, Liang Yu, Jiao Deng, Yong Wang, Kang Cheng, Chao Ma, . . . Dehui Deng, (2021) Sulfur vacancy-rich MoS_2 as a catalyst for the hydrogenation of CO_2 to methanol. *Nature Catalysis* 4, 242. doi: 10.1038/s41929-021-00584-3.