Researchers realize direct conversion of methane with oxygen at room temperature

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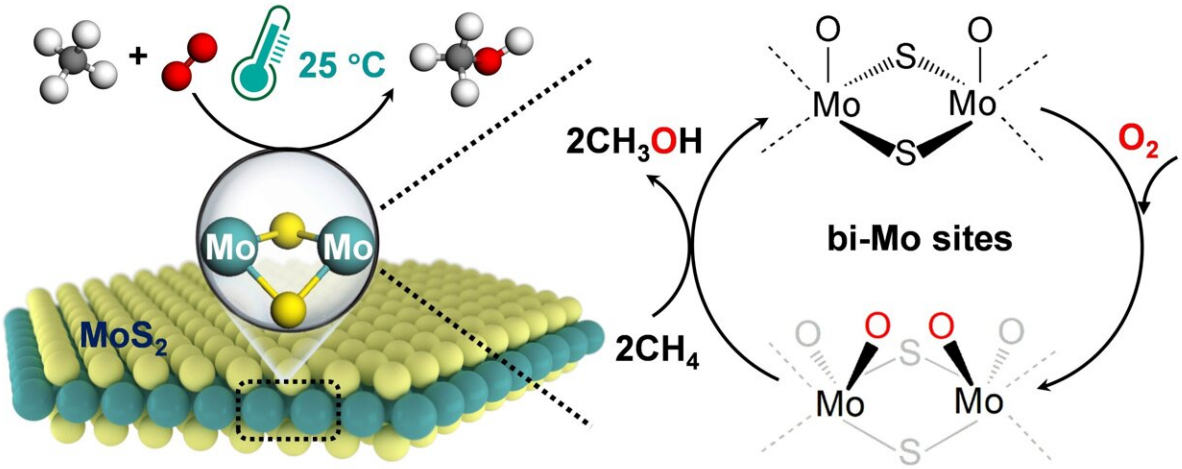

Room-temperature CH_4 conversion by O_2 over bi-Mo sites confined in MoS_2 edge. Credit: Mao Jun and Liu Huan, *Nature Catalysis* (2023). DOI: 10.1038/s41929-023-01030-2

Direct conversion of methane (CH_4) to high-value-added chemicals at room temperature, by directly using abundant and low-cost molecular oxygen (O_2) as an oxidant, is an ideal route for CH_4 utilization. But it remains a challenge due to the chemical inertness of methane and low activity of O_2.

Recently, a research group led by Prof. Deng Dehui and Assoc. Prof. Yu

Liang from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) realized direct CH_4 conversion to C1 oxygenates (CH_3OH, $HOCH_2OH$ and HCOOH) with O_2 at room temperature (25°C) over an edge-rich MoS_2 catalyst. The study was published in *Nature Catalysis* on Sept. 21.

Catalytic conversion of methane to high-value-added chemicals is a tough problem due to the low polarization rate and high C-H bond energy (439 kJ mol^{-1}) of methane.

Typical catalytic conversion of CH_4 usually operates at high temperatures (over 600°C), or in the aid of strong oxidants (such as fuming sulfuric acid) or external fields (such as plasma). Nevertheless, such harsh reaction easily leads to excessive conversion of the target product, such as overoxidation to CO_2.

Direct conversion of CH_4 and O_2 at low temperatures or even at room temperature is an appealing strategy for CH_4 conversion. However, it is challenging due to the difficulty in continuous formation of active oxygen species under mild conditions for C-H activation.

In-situ characterizations and theoretical calculations demonstrated that the unique binuclear molybdenum (bi-Mo) site of sulfur vacancies at the MoS_2 edge was able to directly dissociate O_2 to form O=Mo=O* active species at 25°C, which could activate the C-H bond of CH_4 and thereby driving the catalytic conversion of CH_4 to C1 oxygenates via CH_3O* intermediates at room temperature.

In this study, the researchers achieved CH_4 conversion of up to 4.2% with a high selectivity of over 99% for the C1 oxygenates for CH_4 conversion with O_2 at room temperature.

More information: Jun Mao et al, Direct conversion of methane with

O2 at room temperature over edge-rich MoS2, *Nature Catalysis* (2023). DOI: 10.1038/s41929-023-01030-2