Researchers reveal oxygenate-based routes in syngas conversion over oxide-zeolite bifunctional catalysts

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Solid-state NMR studies reveal that the oxygenate-based routes regulate syngas conversion over OXZEO bifunctional catalysts. Credit: DICP

A research team led by Prof. Hou Guangjin and Prof. Bao Xinhe from

the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) has revealed the oxygenate-based routes in syngas conversion over oxide–zeolite (OXZEO) bifunctional catalysts by solid-state Nuclear Magnetic Resonance (NMR).

This study was published in *Nature Catalysis* on June 23.

OXZEO catalysis was proposed in 2016 by Prof. Bao Xinhe and Prof. Pan Xiulian from DICP. It provides a platform for the efficient utilization of coal and other carbon resources. However, the reaction mechanism in OXZEO catalysis still remains unclear.

In this study, the researchers chose the syngas conversion over the $ZnAlO_x$/H-ZSM-5 bifunctional catalyst as a model system to highlight the mechanistic difference in the OXZEO-based syngas direct conversion. $ZnAlO_x$ is a typical metal oxide for syngas to methanol process while H-ZSM-5 is a typical zeolite for methanol to hydrocarbons (MTH) reaction.

They used the quasi-in situ solid-state NMR (ssNMR)-Gas Chromatography (GC) analysis strategy to reveal the dynamic evolution of abundant critical and/or transient intermediates, including multi-carbon carboxylates, alkoxyls, acid-bounded methyl-cyclopentenones, and methyl-cyclopentenyl carbocations, from the very early induction period to the steady-state conversion under high-pressure flow-reaction conditions.

Oxygenate-based routes were proved to be contributed to the outlet olefins and aromatics, where the feed, i.e., CO and H_2, was also a vigorous participant in these secondary reactions. In addition to the $ZnAlO_x$/H-ZSM-5 catalyst, the researchers also discovered that the key intermediates exist in multiple OXZEO catalysts, proving the universality of oxygenate-based routes in OXZEO-based syngas

conversion.

"Our findings provide new insights into the reaction mechanism of syngas conversion on bifunctional catalysts, and may also help to better understand the mechanism of CO_2 and biomass conversion," said Prof. Hou.

More information: Guangjin Hou, Oxygenate-based routes regulate syngas conversion over oxide–zeolite bifunctional catalysts, *Nature Catalysis* (2022). DOI: 10.1038/s41929-022-00806-2. www.nature.com/articles/s41929-022-00806-2

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