Dynamic confinement of SAPO-17 cages on selectivity control of syngas conversion

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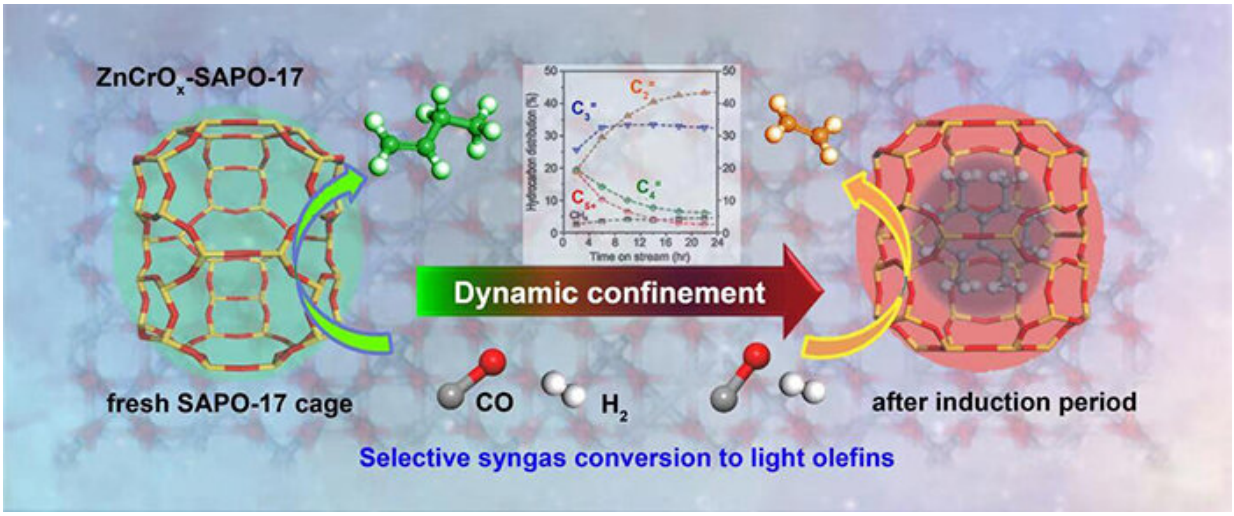

Dynamic confinement of SAPO-17 cages on the selectivity control of syngas conversion. Credit: Wang Haodi and Jiao Feng

A research team led by Prof. Pan Xiulian and Prof. Bao Xinhe from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) discovered dynamic confinement of SAPO-17 cages on the selectivity control of syngas conversion.

This study was published in *National Science Review* on July 26.

In 2016, the team proposed a new catalyst concept based on metal oxide-

zeolite bifunctional catalysts (OXZEO), which enabled the direct conversion of syngas to light olefins with high selectivity.

In this study, the researchers reported the dynamic confinement effect of zeotype cages, which controlled the product selectivity during the induction period of syngas conversion. They increased the ethylene selectivity from 19% gradually to 44% whereas decreased C_{4+} hydrocarbon selectivity from 39% to 9% within the first 22 hours on stream. After the induction period, the catalytic performance leveled off.

"This was induced by the gradual accumulation of carbonaceous species inside the SAPO-17 cages as the reaction proceeds. It led to a gradually decreased free space inside the cage," said Prof. Bao.

They found that the diffusion coefficient ratio of C_2 to C_4 was correlated negatively with an Effective Space Coefficient (ESC), a descriptor that was defined to describe the effective space inside the SAPO-17 cage. It indicated more hindered diffusion for C_4 than for C_2 with the reduced free space of the cage. Furthermore, a restricted free space would also hinder the secondary reaction of ethylene and therefore benefited C_2 selectivity.

"This study reveals a significant effect of the dynamic confinement of SAPO-17 cage on the product selectivity," said Prof. Pan. Although the most of micropores was occupied (93%) when the induction period was completed, the catalyst was not deactivated and it was running rather stably in syngas conversion.

This dynamic confinement is expected to be general for a number of reactions involving hydrocarbons over zeolites. The understanding is essential for further design of high-performance zeolites-based catalysts for C_1 chemistry as well as other reactions involving hydrocarbons.

More information: Haodi Wang et al, Dynamic confinement of SAPO-17 cage on the selectivity control of syngas conversion, *National Science Review* (2022). DOI: 10.1093/nsr/nwac146

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