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Designing the right protection

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Designing the right protection

A new iron-based catalyst helps avoid common pitfalls for making olefins

By Jingxiu Xie

Olefins are used to manufacture our everyday essentials, including plastics, detergents, and hand sanitizers. Olefins are conventionally produced from crude oil cracking, but environmental concerns drive the urgent search for alternative, more sustainable carbon feedstocks. Carbon-containing waste streams ranging from biomass to industrial carbon dioxide (CO₂) to municipal waste are increasingly explored for the synthesis of chemicals and fuels (1, 2). These waste streams may first be converted to carbon monoxide (CO) and hydrogen (H₂) called synthesis gas or syngas. The gas is further converted to olefins. Because the waste streams may be contaminated with impurities, catalysts with higher resistance to poisons would be advantageous for these processes. On page 610 of this issue, Xu *et al.* (3) report iron catalysts that are particularly suitable for this task owing to their robustness and the low selectivity toward CO₂ and methane (CH₄).

The current industrial process to produce lower olefins (ethylene, propylene, and butenes) from syngas is indirect and requires two steps, the first to synthesize methanol and the second to convert methanol to olefins (4, 5). The process is mainly commercialized in China, by using syngas derived from coal gasification or by the import of methanol produced from natural gas. Direct processes, namely Fischer-Tropsch to olefins (FTO) (6) and oxide-zeolite (via oxygenate intermediates) (7, 8), are more attractive owing to cost and material savings along with being able to avoid the thermodynamic constraints for methanol synthesis.

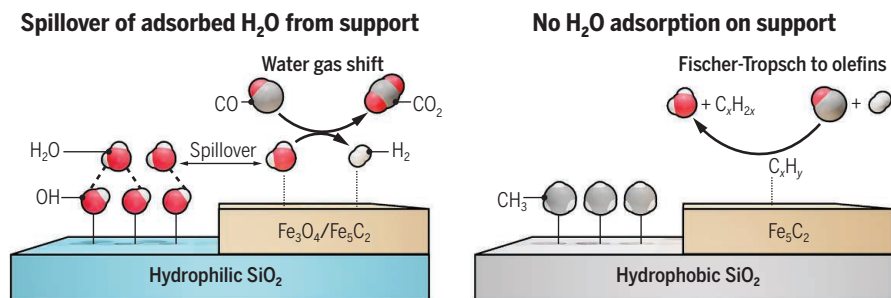
Several strategies suppress the formation of CO₂ and CH₄ in the FTO process. One approach is to use promoted metallic cobalt catalysts, which are not active for the water gas shift (WGS) reaction (CO + H₂O → CO₂ + H₂), that gives rise to formation of CO₂ (9). The other approach is to use pure iron carbide catalysts and prevent the phase transitions to iron oxides, which are presumed to be more active for WGS (10, 11). For these types of catalysts, high steam partial pres-

ures are often detrimental to the catalytic performance because of oxidation or sintering of the active phase.

Xu *et al.* present a catalyst composed of iron carbide nanocrystals encapsulated in hydrophobic amorphous silica shells. This may be a viable solution to overcome the limitations brought about by high steam partial pressure. A high steam partial pressure in the reactor is inevitable at high conversion levels because H₂O is a by-product of FTO, but the hydrophobic silica shell is effective

Getting water out of the way

Olefins are used for making polymers and plastics. A catalyst on a support that adsorbs water may produce CO₂ from the water gas shift reaction (left), which reduces the efficiency for making olefins. Replacing the support with one that is hydrophobic (right) allows for a more effective Fischer-Tropsch reaction and olefin production.



at suppressing the WGS reaction. Hence, the authors achieved a relatively high CO conversion of 56% and a low CO₂ selectivity of 13%.

Xu *et al.* used water-droplet contact angle and water vapor adsorption and desorption tests to support the claim on the catalyst hydrophobicity, which has two functions. It stabilizes the iron carbide phase and suppresses its phase transition to iron oxide. This decreases the primary CO₂ formation from FTO. Additionally, the authors suggest that the hydrophobicity may facilitate the timely desorption of H₂O and prevent its readsorption. This decreases the secondary CO₂ formation by the WGS reaction. A possible scenario to higher WGS activity is spillover of H₂O species from the hydrophilic silica shell to the active sites, which is absent with the hydrophobic silica shell (see the figure).

To reduce CH₄ production, Xu *et al.* added manganese to the iron carbide catalyst because it can promote carbon-carbon coupling to longer hydrocarbon products. Therefore, at the industrially relevant conditions of

320°C, 20 bar, and H₂/CO = 2, with a 56% CO conversion and 13% CO₂ selectivity, the selectivity of methane was less than 10% and the olefin selectivity reached more than 60%.

Conceptually, the use of a hydrophobic shell to reduce the coverage of the catalytic surface with H₂O is interesting and could very well be applicable to other reactions that are kinetically inhibited by H₂O adsorption. A common strategy to overcome this issue has been the addition of adsorbents in the reactor, but this requires a temperature and/or pressure swing to release the adsorbed steam, which drives up production costs. As such, the approach of Xu *et al.* could improve process efficiency, although the hypothetical mechanism still needs to be verified. The hydrophobicity tests were carried out with liquid H₂O, which means the surface species and coverages of the active sites with H₂O still need to be established.

Xu *et al.* demonstrate the feasibility of this catalyst in the coal-based FTO process with a techno-economic analysis. Despite the focus on a coal-based FTO process, the technological advancement should be transferable to other FTO processes that use more sustainable and renewable raw materials. Nonetheless, it remains to be shown if the unit product cost would be competitive when this catalyst and technology are used with more sustainable feedstocks from, for example, municipal waste and CO₂ with H₂ from water electrolysis. ■

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