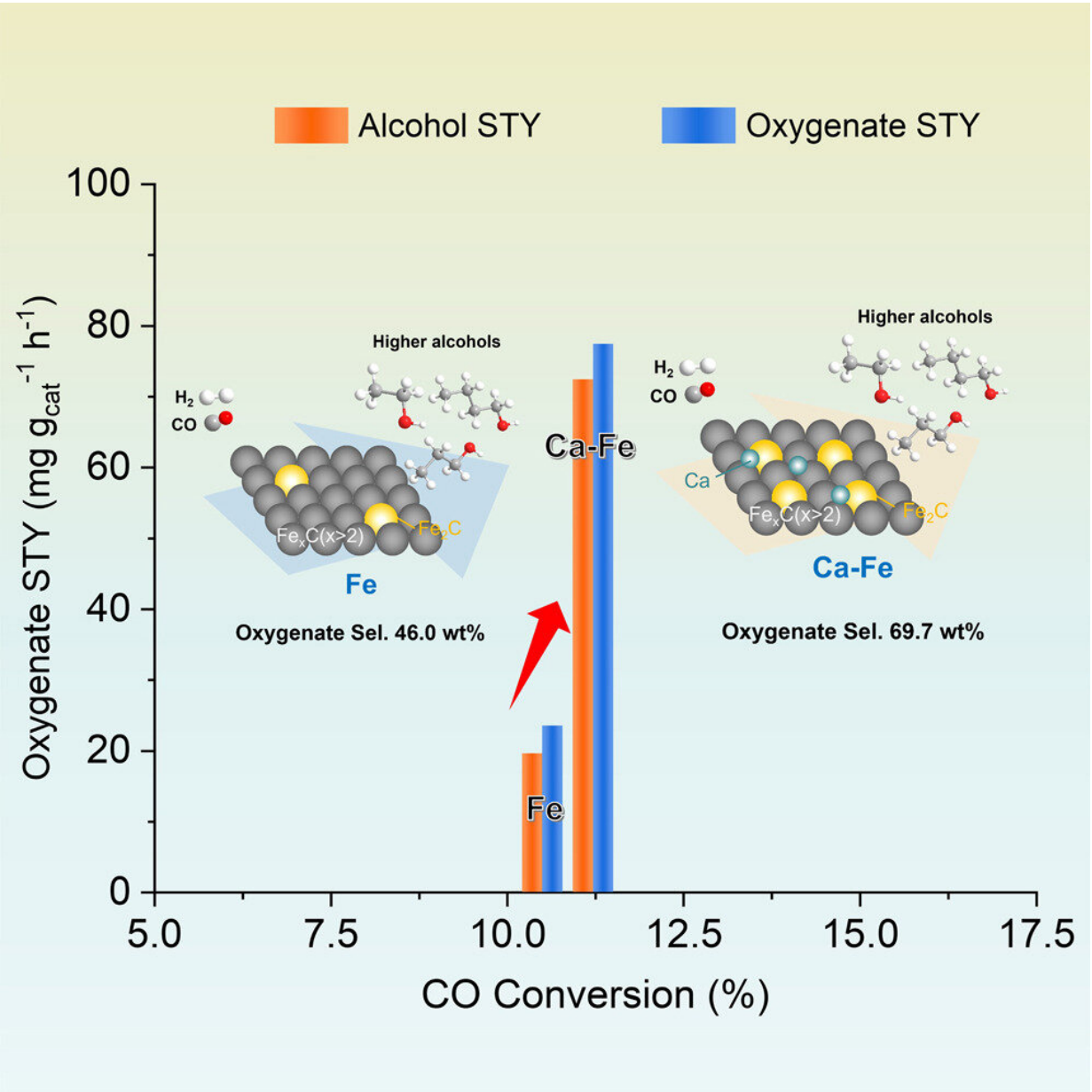
Synergistic iron carbide catalysts enable direct conversion of syngas into higher alcohols

March 24 2023



Graphical abstract. Credit: *Chem Catalysis* (2023). DOI: 10.1016/j.checat.2023.100584

Higher alcohols (C_{2+} alcohols), which are important raw materials, have been used as the intermediates of valued products. They are also widely applied in various fields of fuel, food, fine chemicals, pharmaceuticals and energy.

With the gradual depletion of petroleum resources, the direct synthesis of higher alcohols from syngas has become a sustainable and potential process because of its wide source of raw materials and high atomic utilization. However, the low yield of higher alcohols restricted industrial application.

Recently, a research team led by Prof. Sun Jian and Prof. Ge Qingjie from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) has realized the direct synthesis of higher alcohols from syngas and achieved the highly selective production of higher alcohols from CO hydrogenation over synergistic iron carbides catalysts.

This study was published in *Chem Catalysis*.

"The proposed synergistic Ca-Fe series catalysts could realize a oxygenate selectivity of 69.7 wt% under mild conditions, alongside the alcohols fraction of 86.4 % in oxygenates," said Prof. Sun. "The total oxygenates and alcohols selectivity outperformed the results of previously reported catalysts."

With multiple characterizations, the researchers found that the Ca loading enabled the Ca-Fe catalyst to have high surface iron carbides with a proper $Fe_2C/(Fe_5C_2+Fe_3C)$ ratio. The Fe_5C_2 and Fe_3C as CO dissociative sites could be assisted by a synergistic effect with Fe_2C (CO non-dissociative sites) to produce higher alcohols.

Therefore, the proper $Fe_2C/(Fe_5C_2+Fe_3C)$ ratio facilitated the balance of the CO dissociative and non-dissociative abilities, and boosted the better cooperation of *CO and $*CH_x$ to form the $*CH_x$-*CO species, further promoting the higher alcohols formation.

"This study extends the understanding of the important role of Ca and provides a new strategy for the design of catalysts in CO hydrogenation to higher alcohols," said Prof. Sun.

More information: Qingjie Ge, Precisely synergistic synthesis of higher alcohols from syngas over iron carbides, *Chem Catalysis* (2023). DOI: 10.1016/j.checat.2023.100584. www.cell.com/chem-catalysis/fu … 2667-1093(23)00091-X

Provided by Chinese Academy of Sciences