Inorganic Materials & catalysis

Research Project – Emiel Hensen/Shiyue Li

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Towards high-performance iron-carbide catalysts for CO hydrogenation: understand the role of promoters

Background

Fischer-Tropsch synthesis (FTS), which converts coal, natural gas, and biomass to chemicals and liquid fuels, has attracted increasing attention in recent years as a way to diversify both the feedstock base for obtaining liquid transportation fuels and the monetization of natural gas and coal resources. In heterogeneous catalysis, Typical transition metals for catalyzing the FTS reaction are ruthenium (Ru), cobalt (Co), and iron (Fe). All of these present high activity and selectivity toward liquid hydrocarbons in the low-temperature FTS reaction [1]. Ru is usually deemed to be too expensive for this purpose despite its high activity, so Fe and Co are the only viable transition metals for the active phase in commercial FTS catalysts. Despite the higher activity, higher paraffin selectivity and higher stability of Co-based FTS catalysts, Fe-based FTS catalysts are better choice for coal-derived syngas conversion, because Fe catalysts (i) can be operated in wider range of temperatures and H_2/CO ratios; (ii) are more tolerant to sulfur compounds in the synthesis gas; (iii) display higher selectivity to olefins and C_{5+} hydrocarbons at lower CH_4 selectivity; and (iv) can be used to produce short-chain (unsaturated) hydrocarbons and short-chain oxygenates at elevated temperature.

In the industry there usually adds promoters into Fe-based catalyst to enhance the catalytic performance. A challenge in Fe-based FT catalyst is the complexity of the catalyst composition under reaction conditions, and it is difficult to clearly understand the function of promoters over FTS. To exclude the influence of iron-carbides, preparing phase-pure carbides are necessary, and Wang et al. [2] synthesized phase-pure ε (')-Fe_2C catalysts via controlling the pretreatment and carburization conditions. According to this theory, a series of metal modified catalysts based on pure phase iron-carbides will be studied.

Main research goals:

- Synthesis and development of alkali metal (Li, Na, K, Rb, Cs) modified pure phase Fe-based catalyst in Fischer-Tropsch synthesis reaction, and compare the catalytic performance on FTS.
- Analyze and investigate the reaction mechanism of modified catalysts in complex FTS system by means of advanced in situ characterization.
- Explore the different function of alkali promotors on iron-carbides over FTS and attempt to find the chemical principals.

Techniques used:

- Catalyst evaluation will be performed in fixed-bed reactor equipped with GC.
- Catalyst characterization like XRD, TEM, XPS, ICP, TPH, SSITKA and Mössbauer spectroscopy will be carried out.

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[2] Wang, P.; Chen, W.; Hensen, E. J. M., Synthesis of stable and low-CO_2 selective epsilon-iron carbide Fischer-Tropsch catalysts. *Sci. Adv. 2018*, 4 (10), 6.