

Supporting Information

**Silicalite Zeolite Supported Iron Catalysts for Enhancing
Isoparaffin Selectivity from CO Hydrogenation**

Wuqiang Si,^a Xuangan Liu,^a Zhiren Xu,^a Chunyang Zeng,^d Mingquan Li,^a Chuang Xing,^a Bin Huang,^{*c} Peng Wang,^b Yan Xu,^b Shuai Wei^{*b}

- a. School of Biological and Chemical Engineering, Zhejiang University of Science and Technology, Hangzhou 310023, China.
- b. School of Materials and Chemical Engineering, Xuzhou University of Technology, Xuzhou 221018, China.
- c. Zhejiang Benli Technology Co.,Ltd. Taizhou 317016, ChinaChina Petroleum and Chemical Industry Federation, Beijing 100723, China

Corresponding authors:

huangbinbin74@163.com (B. Huang);

Weishuai@xzit.edu.cn (S. Wei)

1. ICP results of catalyst

Table S1. ICP results of catalyst

Catalyst	Mass fraction of Fe
Fe@S1	16.73%
Fe/S1	18.13%
Fe@S2	17.86%
Fe/S2	18.54%

Compared to the anticipated 20% iron content at the time of preparation, an actual loss is observed.

2. Acid alkalinity of iron carbide

Due to the presence of iron carbides after the catalyst reaction, the acidity and basicity of iron carbide were also characterized. We synthesized a small quantity of iron carbide for ammonia temperature-programmed desorption (NH₃-TPD) by treating activated carbon with ferric nitrate at high temperature, aiming to investigate its acidic and basic properties. As shown in the XRD results in Figure S1 (a), we successfully prepared iron carbide.

NH₃-TPD experiments were conducted on activated iron carbide and iron oxide, yielding the results depicted in the accompanying Figure S1 (b). Between 100 and 200 °C, a weak NH₃ desorption peak was observed, suggesting that both iron oxide and iron carbide possess some degree of acidity, with iron carbide exhibiting stronger acidity than iron oxide. Owing to the poor stability of iron carbide and the potential presence of activated carbon residue in the sample, a significant decomposition peak emerges beyond 500 °C, which holds no referential value.

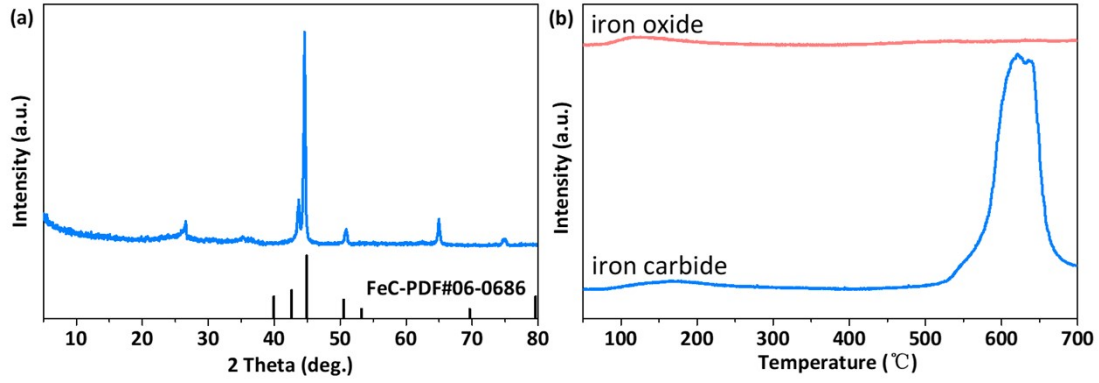


Figure S1 (a) The XRD of the prepared iron carbide;(b) NH₃-TPD of iron carbide and iron oxide

3. Calculation of experimental results

Syngas consists of Ar, CO and H₂. The CO conversion rate is calculated using the peak area of the chromatography, where in and out represent the inlet and outlet gases:

$$CO\% Conv = \frac{\left(\frac{A_{CO}}{A_{Ar}}\right)_{in} - \left(\frac{A_{CO}}{A_{Ar}}\right)_{out}}{\left(\frac{A_{CO}}{A_{Ar}}\right)_{in}}$$

The molar quantity of the outlet gas is calculated by using the exit flow rate of the reaction and the ideal gas state equation:

$$n_{out} = \frac{PV}{RT}$$

The amount of methane produced is calculated using a standard gas of known concentration:

$$n_{CH_4} = n_{out} \times \text{The amount of } CH_4 \text{ in a standard gas} \times \frac{A_{produced CH_4}}{A_{CH_4 \text{ in standard gas}}}$$

The CO₂ conversion rate can be calculated by comparing the amount of CO₂ before and after the reaction. The methane peak area detected by the FID and the calculated methane content are used as the internal standard to calculate the amount of other hydrocarbons, where n is the molar amount, S is the selectivity, and i represents various hydrocarbon products.

$$n_i = \frac{A_{i}}{A_{CH_4}} \times n_{CH_4}$$

$$S_i = \frac{n_i}{n_{CO \text{ conversion}}} \times 100\%$$

The liquid phase products were collected for off-line analysis in FID, and n-dodecane was added as internal standard to calculate various hydrocarbon contents:

$$n_i = \frac{A_{era_i}}{A_{era_{C12}}} \times n_{C12}$$