

Design of novel porous Fe₂O₃ cage catalyst for production of gasoline fuels via coupling Fischer-Tropsch with zeolite cracking

Yulan Zhang,^{a*} Xizhu Lin^a

^aGuizhou Institute of Technology, Key Laboratory of Light Metal Materials Processing of Guizhou Province, No. 1 Caiguan Road, Guiyang 550003, P.R. China

*Corresponding author E-mail: zyl_6688@163.com

Table S1 Catalytic performances of the cage catalysts.

Time (h)	Mass balance (%)	^a CO conv.	CO ₂ (%)	^b Product selectivity (wt%)					Products in C ₅₊ (%)	
				CH ₄	C ₂ -C ₄ ⁰	C ₂ -C ₄ ⁼	C ₅ -C ₁₁	C ₁₂₊	aromatic	i-C ₅₊
24	96.5	86.2	35.3	21.1	17.3	24.2	28.0	9.40	8.39	26.5
48	97.3	82.4	33.5	20.5	16.5	21.7	30.1	11.2	5.80	27.6
72	98.7	83.5	37.2	22.4	18.2	21.9	27.1	10.4	4.95	27.2

^aCO conversion: $(\text{CO}_{\text{syngas}} - \text{CO}_{\text{tailgas}}) / \text{CO}_{\text{syngas}} \times 100\%$, CO_{syngas} and CO_{tailgas} represent the moles of CO at the syngas and tailgas, respectively.

^bProduct selectivity: $W_n / \sum W_n \times 100\%$, W_n represents the weight of hydrocarbons at the carbon number of n, including gaseous and liquid hydrocarbons.

Table S2 FTS performances of the prepared catalysts after FTS for 24 h.

Sample	Mass balance	^a CO conv. (%)	^b CO ₂ (%)	^c Product selectivity (wt%)					Products in C ₅₊ (%)	
				CH ₄	C ₂ -C ₄ ⁰	C ₂ -C ₄ ⁼	C ₅ -C ₁₁	C ₁₂ +	arom atic	i-C ₅ +
Fe+ZSM5 (16)	96.6	69.9	32.6	14.7	10.2	22.3	49.4	3.40	7.34	63.3
Fe+ZSM5 (24)	96.4	75.3	40.0	16.4	12.3	4.41	64.8	2.09	24.6	42.8
1Fe+ZSM5 (27)	97.2	69.9	26.6	20.8	11.6	3.86	58.6	5.04	34.8	34.1
Fe+ZSM5 (27)	97.4	93.6	43.6	18.6	13.7	3.09	62.7	1.91	22.1	48.8
2Fe+ZSM5 (27)	97.1	74.1	32.1	21.4	13.0	3.30	60.0	2.30	36.9	35.7
Fe+ZSM5 (33)	96.6	84.6	38.7	15.3	11.1	5.52	65.1	2.98	15.7	57.0
Fe+ZSM5 (40)	96.4	91.6	41.4	21.1	15.0	3.80	55.8	4.30	21.3	51.5

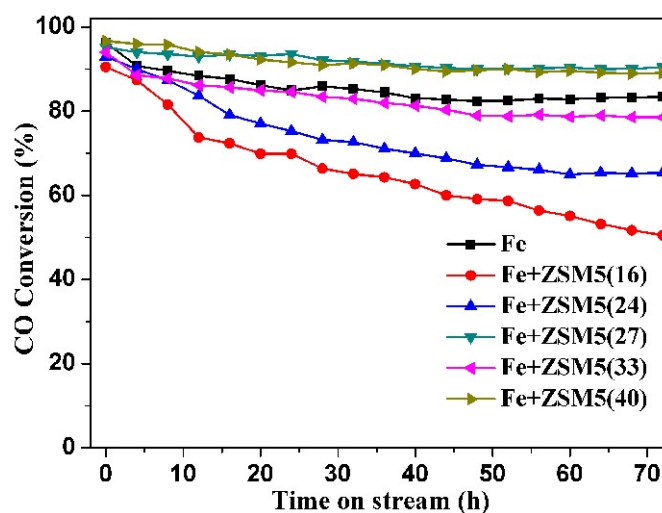
^aCO conversion: $(\text{CO}_{\text{syngas}} - \text{CO}_{\text{tailgas}}) / \text{CO}_{\text{syngas}} \times 100\%$, CO_{syngas} and CO_{tailgas} represent the moles of CO at the syngas and tailgas, respectively.

^bCO₂ selectivity: $(n_{\text{tailgas}} \text{ mol} \times \text{CO}_{2\text{tailgas}} \text{ mol}\%) / (n_{\text{syngas}} \text{ mol} \times \text{CO}_{\text{syngas}} \text{ mol}\% - n_{\text{tailgas}} \text{ mol} \times \text{CO}_{\text{tailgas}} \text{ mol}\%) \times 100\%$

^cProduct selectivity: $W_n / \sum W_n \times 100\%$, W_n represents the weight of hydrocarbons at the carbon number of n, including gaseous and liquid hydrocarbons.

Table S3 Catalytic performance of the prepared catalysts.

Catalysts	C ₂₊ paraffins (wt%)	C ₂₊ olefins (wt%)	Naphthene in C ₅₊ (%)	Aromatics in C ₅₊ (%)	Olefins/ Paraffins	Si (10 ⁻³ mol)	Al (10 ⁻³ mol)	Si/Al
Fe	31.4	41.1	3.20	8.39	1.31	0	0	0
Fe+ ZSM5(16)	20.6	56.9	16.9	7.34	2.77	9.79	0.60	16
Fe+ ZSM5(24)	32.3	22.0	21.8	24.6	0.68	9.21	0.38	24
Fe+ ZSM5(27)	32.2	25.4	17.1	22.1	0.79	8.06	0.30	27
Fe+ ZSM5(33)	33.3	30.5	17.9	15.7	0.92	9.89	0.30	33
Fe+ ZSM5(40)	31.5	23.9	20.0	21.3	0.76	8.34	0.21	40

**Fig. S1** CO conversion with time on stream over the as-prepared catalysts.