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A series of Fe-based catalysts for CO2 hydrogenation into light olefins

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PURPOSE OF THE ABSTRACT

In recent decades, global attention has increasingly focused on the challenges posed by human-induced climate change. One of the most prominent concerns is the rising concentration of CO2 in both the Earth's atmosphere and oceans, which contributes to the greenhouse effect (1) and water acidification (2). Although CO2 levels remained nearly unchanged for thousands of years during the pre-industrial period, they are now surging dramatically (3). In response to these challenges, CO2 utilization technologies are being developed. These strategies offer a fresh perspective on CO2, treating it not only as a greenhouse gas but also as an inexpensive renewable source of carbon (4-6).

Light olefins, including ethylene, propylene, and butylenes, have attracted considerable interest among the diverse range of products that can be synthesized from CO2. As essential industrial feedstocks for plastics, synthetic rubbers, solvents, surfactants, paints, and various other chemicals, their demand continues to grow year after year (7). Fe-based heterogeneous catalysts have shown great promise for converting CO2 into hydrocarbons. Their widespread availability, affordability, high catalytic performance, and stability have spurred significant research aimed at optimizing their use in CO2 hydrogenation. Additionally, their highly tunable surface properties offer extensive opportunities to adjust product selectivity. Nevertheless, modern scientific literature contains relatively few studies that systematically compare the effects of various additives, especially transition metals.

In this study, a series of K-Fe-M materials, where M is Zn, Co, Mn, or Cu, as well as a reference K-Fe sample, were prepared and investigated as catalysts for CO2 hydrogenation into light olefins. In a typical synthesis procedure, Fe and M metal nitrates were mixed and dissolved in deionized water. Then, sodium bicarbonate was added dropwise as a precipitating agent under intensive stirring. After the precipitation was completed, the sediment was maintained under vigorous stirring at 40°C for 8 h. The aged precipitate was then washed 3 times with deionized water and dried at 110°C for 8 h. The resulting material was promoted with potassium by impregnation with a KNO3 solution. Finally, the samples were dried and calcined at 400°C for 6 h.

For catalytic investigations, 0.5 g of the prepared K-Fe-M or K-Fe material was loaded into a packed-bed tubular flow reactor. Then, the sample was partially reduced in a H2 flow at 400°C for 4 h. Finally, the CO2 hydrogenation reaction was carried out at 320 °C, 20 bar and a stoichiometric H2/CO2 ratio of 3. A suite of detailed

characterization techniques, including N2 physisorption, X-ray diffraction, scanning electron microscopy, and energy-dispersive X-ray analysis, were employed to correlate the structural properties as well as the elemental and phase composition of the Fe-based materials with their catalytic performance. Among the series, the 3K-Fe-5Co catalyst sample with a molar ratio K/Fe/Co = 0.03/1/0.5 demonstrated the best CO2 conversion of 32% and light olefins fraction of 54% in the gaseous product mixture. This performance was attributed to the highest dispersion of the sample, the close proximity of Fe and Co species, and the increased surface basicity, as evidenced by the highest surface concentration of potassium among the materials studied.

The study provides clear insights into how catalyst composition can significantly influence CO2 conversion and selectivity toward light olefins. These findings not only contribute to a deeper understanding of iron catalyst behavior under realistic conditions but also suggest promising directions for improving the efficiency and sustainability of CO2 utilization processes.

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FIGURES

FIGURE 1

FIGURE 2

KEYWORDS
CO2 utilization | Heterogeneous catalysis | Iron-based catalysts | Light olefins

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