Catalytic materials for the hydrogenation of carbon dioxide to liquid fuels

Climate change and the related global warming created by the carbon dioxide emissions are among the most critical global issues. The linear relationship between cumulative CO$_2$ emissions and global temperature rise according to various scenarios has been recently re-emphasized, stressing that global net emissions need to reach zero at some point in time. Carbon dioxide hydrogenation is a viable catalytic process that converts the greenhouse gas and hydrogen, potentially produced from water, into renewable chemicals and fuels. CO$_2$ hydrogenation conducted on Fe-based catalysts consists of a wide range of reactions with CO$_2$ and H$_2$ reacting in the reverse water–gas shift (RWGS) to produce CO and CO and H$_2$ reacting in the Fischer–Tropsch (FT) type reactions leading to hydrocarbons. The catalytic system is very complex, posing challenging issues that require fundamental understanding of the dynamics of changes in the catalytic phases, mechanism of key reactions, and effects of catalyst composition including key promoters. It was established that the ratio of Fe$_{\text{carbide}}$/Fe$_{\text{oxide}}$ atoms at the surface of an activated catalyst responsible for its selectivity is determined by the environment of iron ions in oxide precursors changed by insertion of ions of other metals. The effects of chemical composition, texture, and promotion with potassium of BaFe-hexaaluminates catalysts on their performance in RWGS reaction were studied. It was established that the rate of RWGS is strongly affected by catalysts iron content gradually increasing up to 45% Fe. Decreasing the catalyst nanocrystals platelets size in 3.5 times by implementing the carbon templating increased the surface area and the rates of reaction. Modelling of the redox cycle of RWGS by CO$_2$-TPD, TP reaction, TP reduction indicated that H$_2$ reduction is needed for regeneration of active sites Fe$^{2+}$ ions associated with oxygen vacancies. Potassium displayed a strong promotion effect on the activity of Ba-Fe-hexaaluminates. At optimal K content of 6 wt%, the RWGS rates increased by a factor of 12-15 without changing the TOF number.
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