Preparation of model catalyst systems to optimize sustainable aviation fuel production via Fischer-Tropsch synthesis

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Abstract

In the era of energy transition with the goal to lower greenhouse gas emissions and to overcome the impact on climate changes, the Power-to-Liquids (PtL) technology poses as a key potential solution, especially in the hard to abate aviation sector. Sustainable aviation fuel (SAF) may be produced through Fischer-Tropsch (FT) synthesis, the conversion of synthetis gas into long-chained hydrocarbons using iron or cobalt-based FT catalysts. The CARE-O-SENE consortium[1] that connects German and South African partners is driven to accelerate the development of cobalt-based FT catalysts for green and efficient production of SAF. The cobalt FT catalyst with oxidic supports have a nano-scale active phase with large mass specific surface area. However, nano-structuring and strong metal-support interaction would lead to deactivation with sintering and/or forming metal-support compounds (MSCs).[2] Manganese promotion of cobalt was demonstrated to efficiently increase the production yield of SAF and the presence of Mn^{2+} on the edge of manganese oxide structure has been hypothesized to interact with adsorbed carbon monoxide species.[3] Nevertheless, the role of Mn and the level of participation in the FT process is still under discussion.
The role of Mn promotion and support interaction on selectivity, activity, and stability in cobalt-based FT catalyst are the focus of CARE-O-SENE. At KIT, the synthesis of well-defined model catalysts[4] is accompanied by theoretical chemistry and *operando* characterization of the catalysts. In our contribution, we will provide an overview on our recent progress in catalyst preparation, *ex situ* and *in situ* characterization, and DFT modelling. For example, $Co_{3-x}Mn_xO_4$ nanoparticles in the spinel structure were synthesized and used in model catalysts to understand the role of Mn on the reduction behavior of the catalyst materials using X-ray absorption spectroscopy (XAS) at the CAT-ACT beamline of the KIT Light Source.[5] Together with suitable reference materials and DFT modelling, these analyses allow for identification of size and coordination of MnO_x clusters in the catalysts. Such insight can be transferred into deeper understanding with respect to Mn promotion, metal-support interaction, long-term stability and deactivation phenomena to improve the commercially-relevant catalysts in the overall FT process to efficiently produce SAF. This work was supported by the German Federal Ministry of Education and Research (BMBF) within the CARE-O-SENE project (03SF0673B).

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