***In situ* Studies of Model High-Temperature Shift Catalysts**

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High-temperature shift (HTS) catalysts are used to catalyze the water-gas shift reaction in which CO with steam is converted to CO_2 and H_2. This reaction is an intermediate process in the industrial production of hydrogen used for e.g. the synthesis of ammonia. The product gas from a steam reformer is cooled in two processes: a high-temperature (320-500°C) step over a Cr containing magnetite catalyst and a low-temperature step (~220°C) over a Cu-Al_2O_3-ZnO based catalyst that reduces the CO concentration to about 0.1%.

In this combination of in situ studies, model HTS catalysts were prepared in order to determine the structure of pure and Cr containing iron oxides under industrially relevant conditions. From XRD it was observed that the addition of Cr resulted in lower crystallite sizes of the activated magnetite catalysts. Quantitative phase analysis using Rietveld refinement, the Avrami- and Arrhenius expressions, resulted in activation energies for the reduction process. XAFS, at the Cr- and Fe K-edges, showed the short-range order and oxidation states. TEM images illustrated that elongated particles become more dominant with increasing Cr concentration for the chloride-based synthesis. The sizes are generally in good agreement with XRD results. STEM studies combined with EDS suggested that the Cr concentration at the surface of the reduced particles was enhanced. Finally, electron diffraction showed transformations of crystallographic axes from Cr containing hematite particles to Cr containing magnetite particles.

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