hp spectroscopy

Optimizing catalysts for synthesis gas conversion with lab-based XANES

Catalysis

Today's chemical products, such as plastics or cosmetics, are synthesized in processing steps involving several chemical reactions. Many of these reactions are enabled or optimized by catalyst materials. Catalysts can improve conversion rates, lower energy consumption, or tune the selectivity of chemical reactions, thus saving costs and reducing environmental impact. Consequently, catalysis is of utmost importance for the chemical industry.

Current research efforts strive to improve the understanding of the relationship between structure and chemical state of a catalyst and its performance. Tracking the chemical state during preparation, activation, and cycling is the crucial key to a profound understanding of this relation. X-ray Absorption Near Edge Structure Spectroscopy (XANES) is one of the powerful tools for monitoring the oxidation state of a catalyst.

Synthesis gas conversion is one of the primary applications of catalysts. Synthesis gas is one of the nodes in a complex network of reactions for the mass production of primary hydrocarbons in chemical industry. Hydrocarbons form the basis for plastics such as polyester, polypropylene or paraffin wax.

Silica supported Rh catalysts are used to produce methane, but also a broad range of other products. The addition of Mn and Fe tunes the selectivity of the reaction, hence the promoter effects of Mn and Fe are of considerable interest for investigations. However, with only 1.4 wt.% Mn content, the measurement poses a major challenge to the instrument sensitivity.

Novel lab-based XANES

The HPS hiXAS is a lab-based XAS solution for both high-resolution XANES and wide-band EXAFS measurements in an energy range extending from 5-12keV. hiXAS uses a highly efficient HAPG crystal in von Hamos configuration. Its improved sensitivity permits rapid measurements even with analyte concentrations around one weight-percent. Applications in several research areas have already benefitted from this novel tool [1-8].

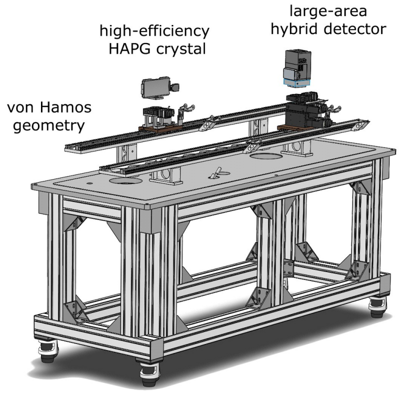

Fig. 1. hiXAS configuration for wide-band recording of spectra with extremely high efficiency

In this study, hiXAS is used to determine the oxidation state of the Mn in the Rh catalyst. Figure 2 shows the XANES spectrum of Mn after calcination of the catalyst in comparison with reference spectra. The oxidation state is clearly indicated by the edge position and the shape of the spectrum, suggesting the predominance of Mn^{3+}.

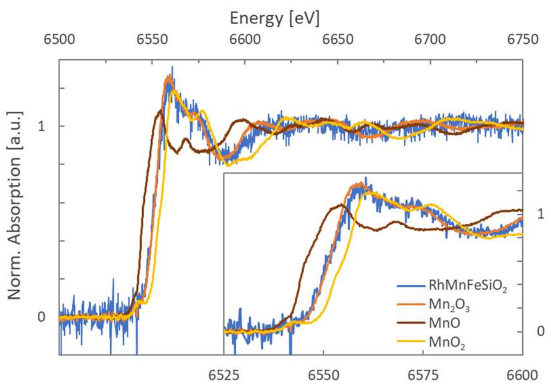

Fig. 2. XANES spectrum at the Mn K-edge of Rh-Mn-Fe/SiO2 recorded in air under ambient pressure [3]. Spectra of binary manganese oxides with Mn in different oxidation states shown for reference. Data acquisition time 50min.

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With XANES as a non-destructive and rapid measurement method, tracking the evolution of a catalyst in-situ or operando becomes a reality. With this method, HPS hiXAS offers researchers continuous and valuable insight into the catalyst oxidation state.

References

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