XANES and EXAFS characterization of FeBEA catalysts for the use in NH₃-SCR

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FeBEA samples can be applied as highly active catalysts in the selective catalytic reduction of NOₓ with NH₃ (NH₃-SCR) [1].

\[ 4 \text{NH}_3 + 4 \text{NO} + \text{O}_2 \rightarrow 4 \text{N}_2 + 6 \text{H}_2\text{O} \]

FeBEA catalysts synthesized by wet-ion exchange of zeolite BEA were steam treated under NH₃-SCR conditions, consisting of 1000 ppm NO, 1000 ppm NH₃, 5% O₂ and 5% H₂O at temperatures between 450°C and 600°C and characterized by XANES and EXAFS analysis. Although the Fe content of the samples was only 1 wt% Fe, a sufficient quality of the spectra was reached by measuring in transmission geometry.

![EXAFS spectra](image1)

Figure 1: EXAFS of untreated (left) and at 450°C steam treated (right) FeBEA catalysts.

The analysis of the EXAFS region showed that an unsteamed reference sample is coordinated by 6 oxygen atoms with a Fe-O distance of 2.05 Å. This refers to an isolated extraframework Fe ion saturated with water. The analysis of the EXAFS for the steam treated samples reveals a coordination number of four with a shorter Fe-O distance of 1.86 Å. The shorter distance and lower coordination number gives evidence that during the steaming treatment under NH₃-conditions extraframework Fe species can be incorporated into framework positions of zeolite BEA.

The XANES of the respective samples also support these observations as the steamed samples all show an intense pre-edge peak. This peak is due to the 1s to 3d transition which is spin-forbidden in octahedral coordination and can be only observed if the metal is tetrahedrally coordinated [2]. The unsteamed sample does not show this transition and hence, the Fe in this sample is octahedrally coordinated.

References