



	<b>Experiment title:</b> Valence-to-core XES studies on Cu-SSZ-13 for NO <sub>x</sub> removal by selective catalytic reduction with NH <sub>3</sub> in the presence of HCHO	<b>Experiment number:</b> CH-6331
<b>Beamline:</b> ID26	<b>Date of experiment:</b> from: 24/05/2022 to: 30/05/2022	<b>Date of report:</b> 07/10/2022
<b>Shifts:</b> 18	<b>Local contact(s):</b> Sami Juhani Vasala	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists): Prof. Dr. Jan-Dierk Grunwaldt <sup>1,2</sup> , Dr. Maria Casapu <sup>1</sup> , Dr. Dmitry Doronkin <sup>2*</sup> , Simon Barth <sup>2</sup> <sup>1</sup> Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany <sup>2</sup> Institute for Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany		

### Report:

Reducing greenhouse gas and pollutant emissions is one of the most stringent priorities of our society, with emission control playing an important role. Zeolite-based catalysts are widely used for the removal of toxic nitrogen oxides resulting from mobile or stationary sources, via the selective catalytic reduction (SCR) process with NH<sub>3</sub> as reductant. Due to the present shift to renewable fuels like methane and ethers, such catalysts are also used for the emission control of natural gas engines. However, under these conditions the SCR catalyst can be additionally exposed to methane and partial oxidation by-products. Our recent results indicate that the presence of formaldehyde leads to a major drop in the low temperature activity for a Cu-SSZ-13 catalyst and toxic HCN emissions [2]. Hence, our study aimed to elucidate the catalyst deactivation mechanism by systematic investigations of the Cu local structure at different temperatures and along the catalyst bed during SCR of NO<sub>x</sub> with NH<sub>3</sub> in the presence of HCHO. The tests were conducted in a capillary microreactor heated by a hot gas blower (Oxford). Reactive gases were dosed with mass flow-controllers provided by the users. The reacted gas mixture was monitored at the outlet using a mass spectrometer (Pfeiffer Vacuum) and a FTIR (MKS, Multigas 2030).

The catalysts were analysed under model conditions relevant for NH<sub>3</sub>-SCR, varying from simple single gas conditions (NO, NH<sub>3</sub>, O<sub>2</sub>, HCHO) to complex mixtures of those gases. Additionally, spatially resolved measurements were conducted under SCR reaction conditions in absence and presence of HCHO.

Preliminary evaluation of the obtained *in situ / operando* HERFD-XANES data indicate a strong influence of formaldehyde presence on Cu local structure. This trend is supported by the complementary V2C-XES measurements. The obtained data is currently analysed in detail at KIT and will be included in future publications.

### References:

1. Zengel, D.; Koch, P.; Torkashvand, B.; Grunwaldt, J.-D.; Casapu, M.; Deutschmann, O., *Angew. Chem. Int. Ed.* **2020**, *59* (34), 14423-14428.