

Multi-scale holistic approach at the BESSY II synchrotron light source for investigating Fischer-Tropsch catalysts

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The CARE-O-SENE project focuses on the optimization and development of knowledge driven Fischer-Tropsch (FT) catalysts to enable highly efficient production of sustainable aviation fuels. Within CARE-O-SENE, a unique, multi-scale combination of complementary imaging and spectroscopic tools for *ex-situ*, *in-system*, *in-situ*, and *operando* analysis of FT catalysts at the BESSY II Synchrotron Light Source is developed and used to guide the project's catalyst optimization. This holistic approach is demonstrated by exemplary results from cobalt-based catalysts characterized *in-system* with soft- and hard- X-ray photoelectron and absorption spectroscopies yielding chemical profile information and how they are affected by redox cycles without exposure to air. Extending this *in-system* approach, a dedicated FT reactor designed for achieving industrial FT conditions (20 bar at up to 500 °C), compatible with the vacuum conditions of the attached thin-film synthesis and spectroscopic soft and hard X-ray analysis is currently being set up. Near-ambient pressure X-ray photoelectron and absorption spectroscopy is further exploited to *in-situ* investigate the catalyst activation and catalyst-promoter interaction for thin-film model FT catalysts. Ultimately, thin-film model catalysts are also studied at reduced pressure conditions in H₂:CO:H₂O gas mixtures at 1 mbar. This multi-scale concept is also applied to imaging techniques, using a commercially relevant FT catalyst characterised by synchrotron tomography and scanning electron microscopy enabling 3D data analysis strategies using machine learning approaches to identify regions of interest for detailed focus ion beam (FIB) tomography. The selected examples showcase how electrons, soft- and hard X-rays probes combined provide insights on all relevant information depth and size scales, ultimately aiming at a complete (locally resolved) picture of the chemical, electronic, and geometric properties of FT catalysts to lay the foundation for deliberate catalyst optimization beyond the current state-of-the-art in terms of activity, selectivity, and stability.