

***In situ* and *operando* spectroscopy of Fischer-Tropsch catalysts: Opportunities and challenges for advanced characterization and development of next-generation cobalt catalysts**

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The development of next-generation cobalt catalysts for Fischer-Tropsch synthesis (FTS) is crucial for advancing this key process in sustainable fuel production. To improve catalyst performance (activity, selectivity) and durability, it is essential to understand the active sites and deactivation mechanisms that govern catalytic behavior. However, the identification is challenging due to the dynamic nature of the catalysts and traditional characterization methods are insufficient for capturing real-time changes under industrially relevant conditions. This is where advanced *in situ* and *operando* spectroscopy plays a pivotal role.

In the CARE-O-SENE project [1], we address these challenges by combining complementary *in situ* characterization tools like X-ray diffraction, magnetometry, hard and soft X-ray spectroscopy with catalytic studies, defined model catalysts and modelling [2]. This integrated approach enables us to set a basis for in-depth characterization of Co and Mn-doped FT catalysts. Especially *in situ* and *operando* X-ray absorption spectroscopy (XAS) studies under industrially relevant conditions are crucial. For this purpose, we have developed and continue to design *operando* spectroscopic cells [3,4] that allow XAS studies at 30 – 50 bar and 250 °C for more than 300 h. These cells allow for the direct observation of structural changes and their correlation with catalytic performance. One of the challenges is the insufficient (only differential) conversion of the reactants, which is less representative for an industrial process. Recently, an alternative reactor/*operando* concept for conversions close to equilibrium has been developed that will be presented [5].

[1] Partners in South Africa and Germany in CARE-O-SENE, see <https://care-o-sene.com/en/> (accessed 08.01.2025.)

[2] R. Elbuga-Ilica et al., publication to be submitted (2025)

[3] M. Loewert, M.-A. Serrer, T. Carambia, M. Stehle, A. Zimina, K.F. Kalz, H. Lichtenberg, J.-D. Grunwaldt et al., *React. Chem. Eng.* 5 (2020) 1071–1082.

[4] L. Pandit, M.-A. Serrer, E. Saraçi, A. Boubnov, J.-D. Grunwaldt, *Chem. Methods* 2 (2022).

[5] M. Schulte, et al. *Angew. Chem.*, in revision (2025).