Operando investigation of Fischer-Tropsch catalysts via soft and hard X-ray spectroscopic techniques in a dedicated reactor cell

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Fischer-Tropsch Synthesis (FTS) is a promising route for sustainable fuels production via the conversion of renewably derived H₂ and CO. Supported cobalt-based catalysts can exhibit high conversions towards the formation of long-chain hydrocarbons at relatively low temperatures (~220 °C) ^[1]. The catalyst's performance depends on various parameters, such as the nature of the support and the existence of promoters. Condensation of products in the pores leading to mass transport limitations can also have important influence ^[2,3]. In-situ/operando characterization techniques are powerful tools for investigating catalytic materials under working conditions. Understanding the nature of the active sites can further guide the rational design of more efficient catalysts. However, the high pressure conditions during FTS make any operando study especially challenging. In our contribution, we will present a first design of a dedicated FTS reactor cell that is compatible with X-ray Absorption and Emission Spectroscopy (XAS, XES) measurements in the soft and hard X-ray regime. In this design, a thin X-ray transparent membrane made of SiN_x separates the high-pressure reaction volume from UHV conditions (Figure 1).

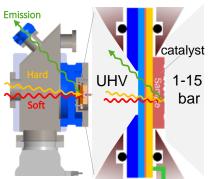


Figure 1:Figure 1. Scheme of operando cell for soft and hard X-ray XAS and XES
measurements of catalyst materials under FTS relevant conditions.

Both powder samples and thin film model catalysts can be studied. The deliberated combination of soft and hard X-ray spectroscopies will be exploited to reveal depth-

dependent information. Additionally, transmission-metal elements of the active phase and lighter elements (like O and C) can be probed in the same setup, paving the way for sound conclusions regarding the chemical structure of the catalyst under working conditions. These unique experimental capabilities are currently set up at the Operando Absorption and Emission Spectroscopy (OÆSE) endstation in the Energy Materials In-situ Laboratory Berlin (EMIL) at the BESSY II synchrotron facility. Preliminary tests of the reactor cell are presented as proof of concept regarding the possibility of conducting the aforementioned measurements under FTS relevant conditions. The present work aims at further closing the pressure gap between surface science and high-pressure, industrially relevant conditions, opening a route to investigate catalyst candidate materials under realistic FTS conditions.

References

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