



Contribution ID: 27

Type: **Oral contribution**

Optimizing cobalt catalyst for CO Preferential Oxidation with the aid of X-ray photoelectron and absorption spectroscopies

Wednesday, 7 December 2022 15:00 (20 minutes)

Catalysis plays a central role in the design of efficient processes for energy production and environmental remediation. One of the main obstacles for finding sustainable catalysts is related to the relatively poor understanding of the material properties, especially under working conditions. This presentation illustrates a characteristic example where ambient pressure soft X-ray photoelectron (APXPS) and absorption (XAS) spectroscopies were applied to identify critical parameters governing the reactivity of cobalt for CO Preferential Oxidation in H₂-rich mixtures (COPrOx), an important catalytic reaction involved in the purification of H₂. At first, CoO was identified as the surface oxidation state with the highest activity for COPrOx, by combining in situ spectroscopy and first-principles calculations [1]. Nevertheless, it appears that CoO is unstable under reaction conditions and is readily oxidized to the less active Co₃O₄. In an attempt to stabilize Co²⁺ oxidation state, cobalt was impregnated with V [2] and Mn [3] promoters. The nature of the catalytic active sites of the promoted catalysts during COPrOx was established by operando APXPS, while the stability of the CoO surface under reaction-relevant conditions was verified by in situ XAS at 1 bar. The promotion effect of the two metals on cobalt will be discussed in terms of enhanced redox stability of CoO surface based on by spectroscopic evidence. In addition, the influence of the spatial distribution of the promoter on the stability of CoO will be discussed. Furthermore, deeper insights regarding the surface composition and electronic structure of the promoted catalysts were deduced from theoretical simulation of XPS peak intensities and L₃-absorption edges using SESSA [4] and CTM4XAS [5] software, respectively. Overall, our results correlate surface state and catalytic performance of cobalt-based COPrOx catalysts and validate the application of in situ and operando spectroscopies to provide the concept for designing better performing catalysts.

[1]L. Zhong, et al., Correlation between Reactivity and Oxidation State of Cobalt Oxide Catalysts for CO Preferential Oxidation, *ACS Catal.* 9 (2019) 8325–8336.

[2]L. Zhong, et al. Improving the Catalytic Performance of Cobalt for CO Preferential Oxidation by Stabilizing the Active Phase through Vanadium Promotion, *ACS Catal.* 11 (2021) 5369–5385.

[3]L. Zhong, et al., Effect of manganese promotion on the activity and selectivity of cobalt catalysts for CO preferential oxidation, *Appl. Catal. B Environ.* 297 (2021) 120397.

[4]W. Smekal, et al, Simulation of electron spectra for surface analysis (SESSA): A novel software tool for quantitative Auger-electron spectroscopy and X-ray photoelectron spectroscopy, *Surf. Interface Anal.* 37 (2005) 1059–1067.

[5]E. Stavitski, et al, The CTM4XAS program for EELS and XAS spectral shape analysis of transition metal L edges, *Micron.* 41 (2010) 687–694.

if "Other", please specify:

I apply for a travel grant

No

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Track Classification: Catalysis