

Impact of Mn on the Surface Chemistry of Co(0001) Fischer-Tropsch Model Catalysts

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Fischer-Tropsch Synthesis (FTS) converts syngas (H_2+CO) into valuable hydrocarbons including diesel and jet-fuel. Cobalt (Co) is mainly used as active metal due to its high activity and selectivity for C_{5+} hydrocarbons^[1]. Tucker et al. reported Manganese (Mn) as an efficient FT promoter for Co, provided the catalyst has an optimal Mn:Co ratio, with Co in the metallic (Co^0) and Mn in the divalent (Mn^{+2}) oxidation states as critical for the overall activity in the catalyst^[2]. To investigate Mn-Co mechanistic interactions on the catalyst surface, well-defined Co(0001) single crystals serve as model systems, ideally under FTS relevant conditions^[3,4].

Mn (0-30 Å) was deposited onto Co(0001) single crystal varying the Mn:Co ratio. Surface chemical structure characterization was performed with lab-based X-ray

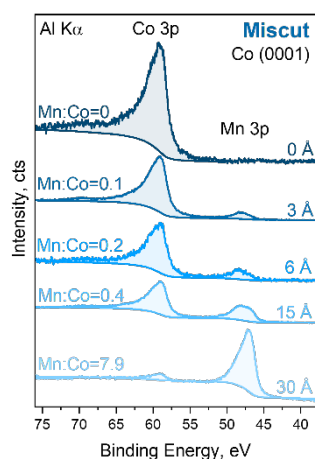


Fig. 1: Co 3p and Mn 3p shallow core level spectra of the studied Mn/Co(0001) samples

Photoelectron Spectroscopy (XPS). Scanning Tunnelling Microscopy (STM) complementary revealed surface structural changes upon Mn deposition. A selected sample was further investigated using Near Ambient Pressure (NAP-)XPS and X-ray Absorption Spectroscopy (NAP-XAS) in Oxygen, Hydrogen and Syngas (H_2+CO) atmosphere at the CAT endstation of the Energy Material In-situ Laboratory (EMIL) located at the BESSY II light source in Berlin. Here we report on oxidation state changes (see Fig. 1) of Mn and Co along with the chemical speciation of C and O containing compounds based on the respective 1s spectra. We discuss the influence of Mn on the surface chemistry of Co(0001) single crystals and how these results can be transferred to powder FT catalysts.

References: [1]: Moodley, D., et al. *Catalysis for a Sustainable Environment*, (2024), 73–116 [2]: Tucker, C.L., et al. *Journal of Catalysis*, 411, 97-108, (2022) [3]: Weststrate, C.J. et al. *Nat Commun*, 11, 750, (2020). [4]: van Helden, P., et al. *Catalysis Today*, 261, 48-59, (2016).