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Towards CO_2 hydrogenation: A combined (NAP-)XPS and DFT study on In_2O_3(111) model catalysts

Content

In_2O_3-based catalysts have shown high activity and selectivity for CO_2 hydrogenation to methanol. The origin of this high performance is, however, still under debate. To improve the understanding of the surface chemistry of In_2O_3, we studied the reactivity of an In_2O_3(111) single-crystalline film [1] and investigated the adsorption of CO_2 on In_2O_3(111) in a combined X-ray photoelectron spectroscopy (XPS) and density-functional theory (DFT) study.

Different surface terminations of In_2O_3(111) have been reported in the literature [2,3]. We have investigated the effect of these different surface terminations on the adsorption of CO_2 on the In_2O_3(111). The experiments show that the CO_2 adsorption is hindered on the hydroxylated surface compared to the stoichiometric and the reduced surface. This shows that the hydroxyl groups block the CO_2 adsorption. The CO_2 appears to adsorb as a HCOO on all surface terminations. The required hydrogen is believed to originate from residual H_2 or water in the experimental chamber.

Additionally, we studied the effect of the pressure gap on this system (Figure 1). NAP-XPS measurements showed the formation of a new chemical species at 1 mbar CO_2 that might originate from CH_2O. Furthermore, the addition CO to the CO_2 and H_2 gas mixture appears to cause the formation of O-CH_3 groups, indicating that CO in the syngas mixture might be crucial for CO_2 hydrogenation over In_2O_3 catalysts.

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