Influence of water pre-treatment on 2-propanol oxidation on Co_3O_4: A comparative study on model surfaces and powder catalysts

J. S. Smyczek[1], P. Hubert[1], H. Scheele[2], S. Najafishirtari[2], M. Behrens[2], S. Schauermann[1]

[1]Institute of Physical Chemistry, Kiel University, 24118 Kiel, Germany
[2]Institute of Inorganic Chemistry, Kiel University, 24118 Kiel, Germany

E-Mail presenting authors: smyczek@pctc.uni-kiel.de, hubert@pctc.uni-kiel.de, hscheele@ac.uni-kiel.de

In this study we investigated the influence of water on 2-propanol oxidation over a model Co_3O_4(111)/Au(111) catalyst under UHV conditions and its powder counterpart under technologically relevant conditions.

Following the rigorous surface science approach, we examined the interactions of H_2O/D_2O and 2-propanol with the Co_3O_4(111)/Au(111) surface by a combination of scanning tunnelling microscopy (STM), low energy electron diffraction (LEED), infrared-reflection-adsorption-spectroscopy (IRAS) and molecular beam techniques. The obtained microscopic-level information was then correlated with the gas-phase 2-propanol conversion on powder catalysts pre-treated with water.

Specifically, we show by IRAS and STM that a pre-treatment with H_2O/D_2O at 573 K leads to formation of large amounts of OH/OD-groups accompanied by structural changes of the catalytic surface. On this hydroxylated surface, 2-propanol was spectroscopically found to form both the desired dehydrogenation product acetone as well as the reaction intermediate propenoxy species in significantly higher amounts than on pristine Co_3O_4(111)/Au(111) or after a H_2O/D_2O pre-treatment at 180 - 200 K. For the spinel cobalt oxide powder catalyst, mostly exhibiting (111) facets, the 2-propanol oxidation can proceed via a low temperature (LT, 400-450 K) and a high temperature (HT, >460 K) pathway.[1] We demonstrated for powdered catalysts that their pre-treatment with water at 573 K specifically increases the activity of the LT pathway. This promotional effect sensitively depends on the pre-treatment temperature and the water exposure.

Thus, pre-treatment with water of both model and powdered catalysts was found to positively affect the 2-propanol conversion to acetone, which can be preliminarily linked to the enhanced formation of hydroxyl groups.

[1] S. Anke, *et al.*, *ACS Catal.* **2019**, *9*, 5974-5985. DOI: 10.1021/acscatal.9b01048