

Crystallography in energy applications

C. Weidenthaler

¹Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
e-mail: weidenthaler@mpi-muelheim.mpg.de

The energy transition requires the implementation of sustainable energy carriers. Hydrogen is one of these options, but the storage is still a challenge. Ammonia, NH₃, is intensively investigated as a suitable candidate as an H₂ storage medium and is already used for heavy-duty transportation systems. The efficient splitting of NH₃ into H₂ and N₂ for fuel cell applications requires the development of catalysts where supported transition metals are one amongst others.

To understand the function of a catalyst, it is inevitable to use in situ/operando techniques in addition to ex-situ analytics. This contribution presents a combination of different in situ techniques that were used to investigate structure-property relationships of several types of Co- and Ni-based catalysts supported on different oxides such as La₂O₃, Al₂O₃, and MgO. In addition to in situ X-ray diffraction experiments, X-ray total scattering and X-ray absorption methods reveal structure changes of the catalysts and the supports on different lengths scales from bulk to the atomic scale. In addition to the results obtained from structure studies, the reduction behaviour, surface chemistry, and catalytic activities will be included to the overall discussion.

For Co-based catalysts supported on Al₂O₃, it could be shown that a significant fraction of the Co catalysts reacts with Al₂O₃ and forms catalytically inactive CoAl₂O₄ (Weidenthaler et al. 2022). The Co content in the spinel cannot be compensated by higher metal loadings. Alumina is known to prevent sintering and a re-dispersion of metallic Co after the reaction was observed. However, the disadvantage of its tendency to form inactive cobalt aluminates predominates.

The second system, Co on basic La₂O₃ support, forms in situ during NH₃ cracking from a LaCoO₃ pre-catalyst. The structural transformation from LaCoO₃ to the catalysts via several intermediate phases was monitored by means of operando X-ray diffraction experiments. The catalytically active metallic Co neither reacts with La₂O₃ nor re-disperses after the reaction. The conversion for Co on La₂O₃ is comparable to the most active Co on Al₂O₃ catalyst, despite having multiple higher Co-loading.

The third system involves Ni on MgO, which shows a clear dependence of the catalytic conversion on the activation process and the associated structural changes.

Weidenthaler C, Schmidt W, Leiting S, Ternieden J, Kostis A, Ulucan TH, Budiyanto E (2022): In-situ investigations of Co@Al₂O₃ ammonia decomposition catalysts: The interaction between support and catalyst. - Chem Cat Chem 14, e202200688