A combined NAP-XPS and NAP-STM study on 2D MoS_2-based catalysts for hydrodeoxygenation of organic feedstocks

L. Mohrhusen, Aarhus/DK, M. Hedevang, Aarhus/DK, J. Lauritsen, Aarhus/DK,
Interdisciplinary Nanoscience Center (iNano), Aarhus University, 8000 Aarhus, DK.

For the technological utilization of sustainable feedstocks such as pyrolysis oils from biomass, oxygen removal via hydrodeoxygenation (HDO) is one of the most essential steps.[1] Metal-promoted MoS_2-based catalysts are well-established for hydrode-sulphurization (HDS) of crude oil components, and thus a promising material for HDO catalysts.[2-4] This is already proven technology for simple feedstocks such as vegetable oils, but more complex compounds with high oxygen content and multiple oxygen functionalities such as bio-oils remain challenging, and thus gain increasing interest.

In contrast to the established use in (virtually oxygen free) HDS, the sulphide catalyst will be exposed to water or organic oxygenates in the herein desired HDO process. Thus, in the presence of oxygen, sulphur atoms may be partially exchanged. Thereby, active sites can become blocked, which triggers strong catalyst degradation on the long term. [5,6]

To gain an atomistic understanding of such processes, herein two-dimensional MoS_2 particles on Au (111) surfaces exposed to H_2 and/or oxygenate containing atmospheres were investigated combining microscopic (scanning tunneling microscopy (STM), see fig. 1) and spectroscopic insights (photoelectron spectroscopy (XPS)) under various conditions mimicking HDO from UHV level to the near-ambient-pressure regime (few mbar, NAP-STM, NAP-XPS).

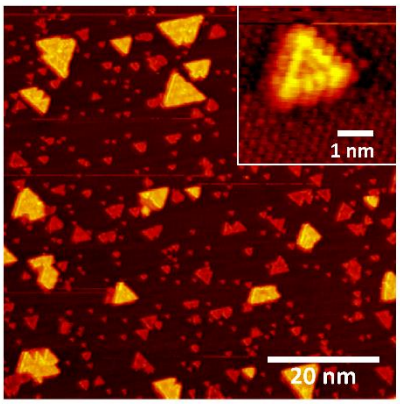

Figure 1: Scanning tunneling micrograph of 2D MoS_2 nanoparticles on a Au (111) support. The inset shows an atomically resolved individual particle.

Literature:

[1] T. M. H. Dabros et al. *Prog. Energy Combust.* Sci. **68**, 268 – 309 (**2018**).
[2] A. S. Walton et al. *J. Catal.* ***308***, 306 – 318 (**2013**).
[3] S. Grønborg et al. *Nat. Comm.* ***9,*** 2211 (**2018**).
[4] N. Salazar et al. *Nat. Comm.* ***11***, 4369 (**2020**).
[5] A. Gaur et al. *ACS Catal.* ***9***, 2568 – 2579 (**2019**).
[6] S. Grønborg et al. *2D Mater.* ***6***, 045013 (**2019**).