

Atomically resolved STM imaging of molecular adsorption on MoS₂ nanocatalysts

J. V. Lauritsen¹

¹Interdisciplinary Nanoscience Center, Aarhus University

The scanning tunneling microscope (STM) has proven to be phenomenally successful in resolving the real-space, atomic-scale structure of the surfaces and supported nanostructures. A distinct advantage of the STM for catalysis studies is the capability to image single, adsorbed molecules while they interact with the catalytically active nanoclusters. This opens the opportunity to experimentally pinpoint and characterize the atomic-scale nature of the catalytically active sites, and in particular address the questions related to size- and morphology-dependent catalytic properties, i.e. the observation that certain cluster sizes or certain defect sites on nanoclusters may be more active. In this contribution I will discuss STM observations of molecular adsorption on MoS₂ nanoclusters synthesized on a gold model substrate, which serve as a surface science model system for the very important group of hydrotreating catalysts used to produce transport fuels with ultra-low sulfur contents. Using the STM we have successfully elucidated the atomic-scale structure of these catalysts and revealed an interesting size-dependent structure and chemistry of MoS₂ [1,2]. The STM studies have been used successfully to shed light on the particular role of sterical hindrance by imaging the sites that preferentially display a chemical bonding to S-containing probe molecules of the dibenzothiophene (DBT) family, which are the major unreactive species in crude oil. We observe a very strong variation in the interaction strength and type depending on the MoS₂ cluster size (1–3nm) and edge structures, which suggest that improvement in catalytic activity and selectivity may be possible by tailoring on the cluster size [1,2].

[1] Lauritsen et al., *Nature Nanotechnology* 2, 53 (2007).

[2] Tuxen et al., *ACS Nano* 4, 4677 (2010).