# Atomic insights into hydrodesulfurization

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# Stellingen

**behorend bij het proefschrift**

**"Atomic Insights into Hydrodesulfurization"**

1. The atomic structure of 2D $CoS_2$ sheets proposed by Kibsgaard et al. is incorrect. 2D $CoS_2$ is a transition metal dichalcogenide (TMDC) with an S-Co-S layered structure. *(J. Kibsgaard et al., Restructuring of Cobalt Nanoparticles Induced by Formation and Diffusion of Monodisperse Metal-Sulfur Complexes, Phys. Rev. Lett. 100, 116104; chapter 3)*

2. Galhenage et al. have incorrectly interpreted that the elongated nanoparticles formed on the $TiO_2$(110) surface in their experiments are those of $MoS_2$. Their results can be explained by the spreading and restructuring of Mo oxide nanoparticles and the absence of sulfur in their XPS spectra. *(Galhenage et al., $MoS_2$ Nanoclusters Grown on $TiO_2$: Evidence for New Adsorption Sites at Edges and Sulfur Vacancies, J. Phys. Chem. C 2019, 123, 7185−7201)*

3. It is suggested by Kibsgaard et al. that the morphologies of $MoS_2$ slabs observed in their experiment are completely representative of those in a hydrodesulfurization (HDS) catalyst. This is not correct as the high temperature and the low surface coverage used in their synthesis procedure does not fully replicate the industrial HDS catalyst synthesis conditions. *(Kibsgaard et al., Scanning tunneling microscopy studies of $TiO_2$-supported hydrotreating catalysts: Anisotropic particle shapes by edge-specific $MoS_2$–support bonding, Journal of Catalysis 2009, 263, 1, 98-103)*

4. Šarić et al. incorrectly assume that the atomic structure of the Co-substituted S edges in their density functional theory (DFT) calculations is not influenced by the organosulfur molecules. *(Šarić et al., Modeling the adsorption of sulfur containing molecules and their hydrodesulfurization intermediates on the Co-promoted $MoS_2$ catalyst by DFT, Journal of Catalysis 2018, 358, 131-140)*

5. Under industrially-relevant conditions, the atomic structure of a Co-promoted $MoS_2$ HDS model catalyst is greatly influenced by the strong interaction between the organosulfur molecules and the edges of the Co-promoted $MoS_2$ nanocluster. *(chapter 6)*

6. The Co atoms present in the S edges of a Co-promoted $MoS_2$ nanocluster are in a kinetically trapped state. *(chapter 6)*

7. In order to synthesize a model catalyst for HDS which sufficiently represents a complex industrial catalyst, it is important to closely replicate the industrial catalyst synthesis conditions by selecting an industrially-relevant support, precursor, temperature of synthesis and sulfur saturation. *(chapter 4,5,6)*

8. The formation of the Co-promoted S edges in $MoS_2$ nanoclusters is not affected by the kinetically-hindered sulfidation of Co and Mo oxide nanoparticles. *(chapter 4)*

9. Transition metals without a layered structure in the bulk can also form single-layered TMDC sheets when provided with a suitable support. *(chapter 3)*

10. In order to understand the atomic world, theoreticians and experimentalists need to work together.

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