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## **Imaging complex model catalysts in action: From surface science towards industrial practice using high-pressure scanning tunneling microscopy**

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# Stellingen

behorend bij het proefschrift

## *“Imaging Complex Model Catalysts in Action”*

- I. The pressure gap is an oversimplified description of the difference between low-pressure experiments in vacuum systems and catalysis under genuine industrial conditions. The effects of the *combination* of high temperature and high pressure cannot be reproduced in vacuum experiments.  
*Chapters 1, 3, and 4 of this thesis*
- II. The nucleation density of metal oxide particles prepared by evaporation of metal in an oxygen atmosphere can reflect the interactions of the metal with the substrate rather than those of the metal oxide with the substrate.  
*Chapter 2 of this thesis*
- III. *Ab initio* thermodynamics predictions of the most stable phase of a catalyst can be applied to steady-state, i.e., non-equilibrium catalysis if the net forward rate is significantly lower than the absolute rate of each elementary step, except for the one that is rate determining, for which there is no such requirement.  
*Chapter 3 of this thesis*
- IV. *Ab initio* thermodynamics predictions of the Mo edge structure present on MoS<sub>2</sub> islands during the hydrodesulfurization reaction should take into account the possibility of hydrocarbon adsorption, even when one is only interested in the H or S edge coverages.  
*Chapter 3 of this thesis*
- V. Our understanding of catalysis at the atomic scale is mainly limited by the possibilities of the instruments used in chemical research.  
*Chapters 1, 3, and 5 of this thesis*
- VI. The structure proposed by Mehring *et al.* after preparation of a CH<sub>3</sub>S self-assembled monolayer on Au(111) in 1 mM dimethyl disulfide/ethanol has a lower coverage than that observed after preparation using 1×10<sup>-8</sup> mbar dimethyl disulfide. This violates basic thermodynamics.  
*Mehring et al. “The structural formation of methylthiolate SAMs on Au(111) for short deposition times from solution”, Appl. Surf. Sci. 256, 7265–7269 (2010)*

- VII. Bollinger *et al.* and Lauritsen *et al.* incorrectly calculated the entropy- and heat capacity-related contributions to the hydrogen chemical potentials corresponding to experimental and industrial conditions. As a result, they wrongly assigned the most stable phase under industrial hydrodesulfurization conditions implied by their data: 50%S-50%H instead of 50%S.  
*Bollinger et al., "Atomic and electronic structure of MoS<sub>2</sub> nanoparticles", Phys. Rev. B, 67, 085410 (2003)*  
*Lauritsen et al. "Atomic-scale insight into structure and morphology changes of MoS<sub>2</sub> nanoclusters in hydrotreating catalysts", J. Catal. 221, 510-522 (2004)*
- VIII. The structural response of single crystals towards gas environments, particularly those with strongly adsorbing molecules, is often more complex than that of nanoparticle catalysts, due to the presence of long-range phenomena that are absent on the nanoparticles.  
*Navarro et al., "In situ observation of self-assembled hydrocarbon Fischer-Tropsch products on a cobalt catalyst", Nat. Chem. 8, 929-934 (2016)*  
*Thostrup et al., "CO-induced restructuring of Pt(110)-(1x2): Bridging the pressure gap with high-pressure scanning tunneling microscopy", J. Chem. Phys. 118, 3724-3730 (2003)*
- IX. The general assumption that the hydrodesulfurization reaction on the Mo edge of MoS<sub>2</sub> proceeds via the formation of vacancies in the 50%S edge is unjustified.  
*Moses et al. "The hydrogenation and direct desulfurization reaction pathway in thiophene hydrodesulfurization over MoS<sub>2</sub> catalysts at realistic conditions: A density functional study" J. Catal. 248, 188-203 (2007)*
- X. If one were to take a scientific approach to choosing a career path after obtaining ones PhD, one would not become an academic researcher.

Rik Mom  
Leiden, 29 juni 2017