Understanding the surface structure of catalysts and 2D materials at the atomic scale

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Propositions

accompanying the thesis

"Understanding the Surface Structure
of Catalysts and 2D Materials
at the Atomic Scale"

1. Metallic two-dimensional CoS_2 with a structure analogous to TiS_2 can be formed on gold, even though no layered bulk analogue exists. *Chapter 4 of this thesis*

2. The characteristic PtO_2 surface oxide stripes arrange in a spoke-wheel-like shape during the initial stages of Pt(111) surface oxidation if the degree of surface oxidation is too low for the stripes to fully cover the surface. *Chapter 5 of this thesis*

3. At room temperature, NO can prevent surface roughening of Rh(100) by CO, since NO binds much stronger to the rhodium surface and thus blocks CO adsorption sites. *Chapter 6 of this thesis*

4. Atomistic thermodynamics is able to bridge the "gap" between zero-pressure, zero-temperature (electronic) structure calculations and *in situ* experiments for minimal additonal computational cost, which greatly aids in the interpretation of experimental results. *Chapters 5 & 6 of this thesis*

5. Comparison between this work and the work of Ataca et al. shows that substrate interactions are important, not only in experimental, but also in theoretical studies of 2D materials. *C. Ataca et al., Journal of Physical Chemistry C 2012, 116, 8983–8999*

6. Atomistic models of surface structures obtained by scanning tunneling microscopy combined with chemical intuition can be good starting points for further investigation with theoretical techniques.
M.A. van Spronsen et al., Nature Communications 2017, 8, 429.

7. Contrary to the findings of Novák et al. on supported rhodium nanoparticles, the results presented in this thesis show that NO does not promote, but instead, inhibits degradation of the Rh(100) surface by CO at room temperature. This indicates there is a key difference between studies on rhodium single crystals and rhodium nanoparticles for this reaction.
E. Novák et al., Applied Catalysis A: General 1997, 149, 89-101

8. When comparing theoretical and experimental results, a researcher should be acutely aware of the inherent limitations of both the experimental and theoretical techniques employed, even if it is not their particular area of expertise, to ensure that the comparison is meaningful.

9. A scientist can devise more calculations in an hour than a supercomputer can solve in seven years.

10. The most important thing you need for scanning tunneling microscopy (STM) is patience. The second most important thing is coffee.

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