Exploring structure dependencies of gas-surface interactions with curved single crystals

Auras, S.V.

Propositions (Stellingen)

accompanying the thesis

"Exploring structure dependencies of gas-surface interactions with curved single crystals"

1. Curved crystal surfaces host a continuous range of surface structures with variable site compositions. They can be employed in surface physics, surface chemistry, and material science to unravel structural effects of chemical behavior or electronic and material properties. As of yet, curved surfaces are, however, under-utilized.

2. Whereas step-step interactions have a distinct effect on terrace width distributions on Pt(111) vicinals, these interactions do not significantly change facet distributions along kinked {210} step edges. (Chapter 3)

3. Different step-types on Pt(111) react differently towards H_2 dissociation. Curved crystal surfaces are a useful tool to reveal these subtle effects, making it possible to define reaction cross-sections for H_2 dissociation at different sites. (Chapter 4)

4. The equilibrium shape of vacancy islands can be used to identify the surface chirality of, e.g. of kinked *fcc* (111) vicinal surfaces. (Chapter 5)

5. Curved crystals allow to extrapolate chemical reactivities (in the case of linearity with step density) towards "defect-free" flat surfaces, e.g. (111), thus facilitating comparison with theoretically calculated reactivities. (Chapter 5)

6. The influence of step edges on water nucleation and desorption varies drastically for Ag(111) and Ag(001) vicinal surfaces, due to differences in terrace geometry, rather than step-type. (Chapter 6)

7. Proper preparation of curved crystal surfaces can present an unexpected challenge and should be confirmed by thorough surface characterization, ideally combining several surface analysis methods.

8. Model catalysts and simplified chemical environments are highly beneficial in order to understand the fundamentals of chemical reactions on surfaces.

9. Chiral metal surfaces, e.g. on dome-shaped single crystals, have great potential to study enantioselective chemical reactions and reaction mechanisms in a heterogeneously catalyzed system. (B. Karagoz, M. Payne, A. Reinicker, P. Kondratyuk, and A. J. Gellman *Langmuir* 2019, *35*, 16438-16443.)

10. An anxious mind can easily find endless possibilities of impending catastrophe in a UHV laboratory.

11. Being able to gather new results, grow deeper understanding, and create further knowledge as a scientist, is a great privilege and should not be taken for granted.