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Surface-structure dependencies in catalytic reactions

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Propositions

Accompanying the thesis:

Surface-structure dependencies in catalytic reactions

- 1) Ultra-high vacuum (UHV), theoretical, and electrochemical studies complement each other in the search for better and cheaper catalyst materials in the future. UHV can form a bridge between theory and real catalysis (chapter 1 of this thesis).
- 2) Systems with Pd and Pt single crystals have been studied extensively in the last decades, yet are still not completely understood. New studies still shine new light on the mechanisms and interactions, sometimes yielding unexpected results.
- 3) Dissociation dynamics of oxygen on low Miller indices of Pd are distinctly different, even though similar trends in reactivity are observed for these surfaces (chapter 3 of this thesis).
- 4) The near absence of incident energy, surface temperature, and incident angle dependencies make it difficult to interpret the data of oxygen sticking on Pd(100) (chapter 3 of this thesis).
- 5) Not only a higher surface temperature and/or incident energy can be beneficial in obtaining a large oxygen coverage on the Pd(100) surface. If the temperature is low enough, additional molecules can adsorb on patches of atomic oxygen on Pd (chapter 4 of this thesis).
- 6) Defect sites are thought to be more active in bond breaking and making reactions (M.T.M. Koper, *Nanoscale*, 2011, 3, 2054). The D/Pt(977) surface (with 8-atom wide (111) terraces!) does not resemble the infinite D/Pt(111) surface (chapter 6 of this thesis). Therefore, the presence of steps should be taken into account more often in theoretical, UHV, and electrochemical studies.

- 7) When step sites are taken into account, the step type is usually neglected. However, on Pt surfaces with (111) terraces, the (100) step type is not the same as the (110) step type (chapter 5 of this thesis). The type of the steps should be taken into account as well in the different studies.
- 8) Good fine mechanical and electronics departments are indispensable in UHV-based research, where some of the lab equipment is even older than the PhD student.
- 9) Pingpong balls are very helpful in visualizing and understanding the processes that are taking place on the surface.
- 10) Molecules larger than H_2 and the presence of step sites are considered a challenge in theoretical studies. In UHV studies, molecules with more than 4 atoms are considered a challenge, molecules containing more than two carbon atoms are considered highly undesirable.
- 11) Chocolate (cake) may not actually solve your problems, nevertheless, it does help.

Angela den Dunnen

Leiden, December 9 2015