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Structure dependence of molecular reactions on surfaces

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Citation

Cao, K. (2018, October 11). *Structure dependence of molecular reactions on surfaces*. Retrieved from <https://hdl.handle.net/1887/66120>

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Cover Page



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Title: Structure dependence of molecular reactions on surfaces

Issue Date: 2018-10-11

Propositions

Accompanying the thesis

Structure dependence of molecular reactions on surfaces

1. Using surface science techniques, well-defined surface structures and simple molecules is a good way to study the mechanisms of catalytic reactions.
2. H_2/D_2 dissociation on Pt(111) is a model system that has been studied abundantly. Nevertheless, azimuth dependent sticking coefficients are unknown and for proper benchmarking of theory such data is required (Ghassemi et al., Chem. Phys. Lett. 683 (2017) 329).
3. Measuring and publishing all relevant parameters is highly important. First it is required for proper comparison of data. Second it saves time when trying to reproduce earlier work (chapter 3 and 5 of this thesis).
4. Besides the average energy of a molecular beam, the energy distribution is an important parameter. It may affect the reactivity significantly and make results apparently different from earlier ones (our data in chapter 4 with Rettner et al., J. Chem. Phys. 94 (1991) 7499) (Díaz et al., Science 326 (2009) 832).
5. Generally, reactivity is higher on a stepped surface than on a flat surface. Anomalously, a stepped Cu(211) surface is less reactive than flat Cu(111) for hydrogen dissociation (chapter 4 of this thesis).
6. Using curved single crystals, the materials gap in catalysis can be overcome.
7. Highly accurate data on the role of step density in molecule surface interactions are usually obtained by studying a series of single crystals with different step densities. Curved crystals allow to get more accurate data more quickly.

8. The cleaning procedure is important to a single crystal experiment, but it is often overlooked (chapter 5 of this thesis).
9. Sometimes a chemical probe is more sensitive to the surface structure than a physical probe (chapter 5 of this thesis).
10. For O₂ sticking on Pt, step facets show a preference for molecules being aligned parallel to their surfaces (chapter 6 of this thesis).
11. Good mechanical and electronic departments are necessary in a UHV laboratory.