Catalysis on high-index platinum surfaces

Computational study of the catalytic activity of high-index platinum surfaces

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In Short

- Heterogeneous catalysis
- DFT calculations
- Pt nanoparticles
- high-index platinum surfaces
- methanol oxidation and decomposition

The main challenges of the catalysis are to investigate and improve efficient and environmentally friendly processes. This can be realized by changing the composition of the chemical process or by tuning the shape of the catalyst itself. [1–3] The Pt nanoparticles as catalysts for instance show different catalytic reactivity by varying the surface shape and structure. [4] It has been established, that the higher density of atomic steps and kinks leads to more active sites on the surface. This might lead to an increasing reactivity for these stepped platinum surfaces.
The main focus of our research is to analyze the dependence of the catalytic reactivity and selectivity of the industrially relevant reactions, such as methanol decomposition and methanol oxidation, on the surface structure of Pt nanoparticles. The different stepped and kinked high index Pt surfaces provide thereby a lot of active sites for these reactions, thus detailed insight in the reaction mechanisms can be obtained. The theoretical calculations are performed using the exchange-correlation functional PBE [5] implemented in the Vienna ab initio simulation package (VASP). [6]The analysis of the adsorption sites, adsorption geometries and the favorable reaction pathways of the investigated reactions are the main objective of this research. Moreover, surface coverage with different species and influence of metallic Substituents, as Pd and Au, in the surface will be considered.

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https://www.uni-oldenburg.de/tc-kluener

More Information

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Project Partners

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