Water-Related Adsorbates on Stepped Platinum Surfaces

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Propositions

accompanying the thesis

Water related adsorbates on regularly stepped platinum surfaces

1. The adsorption properties of water related adsorbates on regularly stepped platinum surfaces as obtained from density functional theory calculations can be used to semi-quantitatively explain most temperature programmed desorption traces on these surfaces.
Chapter 2 of this thesis

2. Water adsorption geometries surrounding the (100)-type step edge present on Pt(533) show significantly more variety than the structures predicted for the Pt(111) surfaces, with favorable structures containing sizes ranging from 4 to 7-membered rings.
Chapter 3 of this thesis

3. Water adsorption along the (111)-type step edge of Pt(553) will only prefer one ring-size, namely the tetragonal ring, due to a strong templating effect of the underlying platinum surface.
Chapter 4 of this thesis

4. The exact high-coverage hydrogen adsorption geometries and energies prove crucial for explaining previously not understood temperature programmed desorption traces from the Pt(553) surface.
Chapter 5 of this thesis

5. The distinct lack of clear understanding of the local solvation environment of electrochemical reactions is one of the main deficits of the current computational hydrogen electrode approach in theoretical electrochemistry.

6. Temperature Programmed Desorption experiments can give very good, but no final, evidence for adsorption structures on surfaces.

7. Long and short-range interactions between adsorbates play a crucial role for the realized adsorption structures on (stepped) surfaces

8. Regularly stepped surfaces can give well-defined insight into the most simple defect type, namely the edge sites of nano-particles, however other defect types, such as kinks and corners, also need attention in order to arrive at a full understanding of the reactivity under realistic conditions.

9. Experiment without Theory is (educated) guesswork, while Theory without Experiment is simply pointless.