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The role of water in hydrogen electrocatalysis

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Citation

Ledezma Yanez, I. D. (2016, June 9). *The role of water in hydrogen electrocatalysis*. Retrieved from <https://hdl.handle.net/1887/40161>

Version: Not Applicable (or Unknown)

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Title: The role of water in hydrogen electrocatalysis

Issue Date: 2016-06-09

Propositions

accompanying the thesis:

“The role of water in hydrogen electrocatalysis”

1. The hydrogen oxidation and evolution reactions in acetonitrile are mediated by (trace amounts of) water. This observation is extensible to several other non-protic solvents.

(Chapter 2 of this thesis)

2. The first electron transfer step is the rate-determining step for the hydrogen evolution in acetonitrile solutions on gold and platinum. The mechanism points out the relevance of solvent reorganization in the hydrogen adsorption step.

(Chapter 3 of this thesis)

3. The kinetics of hydrogen adsorption are affected by the strength of the interfacial electric field because it influences the energetic barrier for the water reorganization during the charge transfer.

(Chapter 4 of this thesis)

4. The energetics of the reorganization of interfacial water is a molecular descriptor of the hydrogen evolution kinetics.

(Chapter 4 of this thesis)

5. A better description of the influence of intermediate states in the kinetics of electrocatalytic reactions can be achieved by understanding the role of the solvent.

6. Spectroscopic studies pertaining to the influence of cations in electrocatalytic processes are overestimated, in the frame of solvent-cation interactions. A better approach would be the modeling by molecular dynamics.

7. The mind is the only place where we are entirely free.