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In silico study of reaction mechanisms and design principles for water oxidation catalysts

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Stellingen

behorende bij het proefschrift

***In silico* study of reaction mechanisms and design principles for water oxidation catalysts**

1. Metadynamics is essential for a genuine modelling of chemical reactions. (*This thesis, Chapter 2*)
2. The conjecture that proton management is essential for good water oxidation catalysis is now provided with a solid understanding for a specific molecular paradigm. (*This thesis, Chapter 3*)
3. The finding in the modelling, that a destructive route also can provide a productive intermediate, offers a promising handle for rational *in silico* design of better catalysts. (*This thesis, Chapter 3*)
4. Without explicit solvent environment in the AIMD simulation it is neither possible to reproduce accurately the water oxidation reaction pathway, nor to obtain the right intermediates. (*This thesis, Chapter 4*)
5. The aromatic ring involved in π -cation interaction in a mono-nuclear WOC can play the role of an electronic charge buffer, thereby facilitating the electronic steps in the catalytic cycle. (*This thesis, Chapter 4*)
6. In contrast to common belief that the proper free energy change for the complete water oxidation cycle requires an improved treatment of the oxygen molecule, it is sufficient to include solvent effects for the water molecule. (*This thesis, Chapter 5*)
7. Operation of photosystem II in with four equal steps of 1.23 V is only plausible when the ligand exchange requires zero free energy. (*This thesis, Chapter 5*)
8. The best inspiration comes with a cappuccino cup and a nice live jazz concert.
9. In every workplace there are two bosses: the office holder, and the coffeemaker.
10. Theoreticians and experimentalists are like day and night, and computationalists are the dawn.

Leiden, December 2012

José Luis Vallés Pardo