

Accelerating the photocatalytic water splitting in catalyst-dye complexes Shao, Y.

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Propositions

Belonging to the thesis entitled "Accelerating the Photocatalytic Water Splitting in Catalyst-dye Complexes"

- 1. O–O bond formation in water oxidation critically depends on antiparallel spin alignment of unpaired electrons on the WOC and dye. *Chapter 2, this Thesis*
- 2. Solvent rearrangement plays a significant role in facilitating the photocatalytic water oxidation reaction.

 Chapter 2, this Thesis
- 3. Tuning the proton chemical potential near the catalytic active site is able to accelerate the rate-limiting O–O bond formation.

 Chapter 3, this Thesis
- 4. Tunable resonant coupling between electronic and nuclear motions can enhance the rate of O–O bond formation.

 Chapter 4, this Thesis
- 5. Probably spin conservation over the catalyst–dye motif and its oxygen product facilitates O–O bond formation.

 Chapter 5, this Thesis
- 6. A complete story returned in a scientific article should be supported by sufficient macroscopic and microscopic evidences, and computational tools can make it happen.
- 7. It happens in scientific research that you start and continue with a faulty logic but end up with an exact answer to your initial question.
- 8. It is of practical importance for humankind to convert "funds" from the sun into chemically useful forms to support their daily lives rather than only high impact factor articles.
- 9. If you cannot focus on writing during the day, especially in the times of Corona, try it at night when the whole world falls asleep.
- 10. If it is not good then it is not the end.