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Computational Modelling of Singlet Fission

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Stellingen

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Computational Modelling of Singlet Fission From the static picture to fission dynamics

door Meilani Wibowo

 An ultrafast phenomenon such as singlet fission coexists with nonadiabatic processes. This urges computational chemists to go beyond the static picture provided by the timeindependent Schrödinger equation within the Born-Oppenheimer approximation.

(This thesis, Chapters 4 and 5)

- 2. Geometry relaxation in the excited state is a key parameter controlling the overall singlet fission rate, and hence, it should be taken into account in our simulations.
- 3. An integrative approach to interpreting the very complex behaviour of chemical processes is very useful but hard to implement. However, this approach can be split into a number of simple associated approaches providing insightful information.
- 4. When the exact solution is not available and only best estimates are obtained, determining a good set of reference values is not undemanding.
- Because we cannot know everything about everything, therefore we should at least know a little about everything. For it is better to know something about everything than to know everything but only about one thing.

- 6. Having a clear-cut objective is important. Acknowledging the limitation of our theoretical models is also important. These two will help us to be more careful on answering the question and solving the problem at hand.
- 7. All scientific works would not be possible without all bureaucracy and paper works.
- 8. While we are progressing to implement gender equality in many sectors, sometimes we still forget to give equal opportunity to everyone regardless of age, race, nationality, religion, physical appearance, and sexual orientation. Everyone is unique and deserves equal opportunity.
- 9. A double PhD degree programme allows one to see two different worlds with one goal.
- 10. Leaving the comfort zone is the first step to challenge oneself.