Theoretical Modelling of the Singlet Fission Process

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Propositions

accompanying the dissertation

THEORETICAL MODELLING OF THE SINGLET FISSION PROCESS
FROM THE GAS PHASE TO THE EFFECT OF THE ENVIRONMENT

by

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1. The protocol described in Chapter 1 of this thesis can be used for the proper identification of novel singlet fission molecules.
2. The higher levels of theory (NOCI and AIFDEM) presented in Chapters 1 and 2 of this thesis are not meant for high throughput screening of dimer dispositions.
3. Benchmarking of time-dependent density functional theory against high-level excited-state methods must be done beyond the comparison of solely excitation energies and oscillator strengths. (Chapter 4 of this thesis)
4. Supervision of students by PhD candidates should not be taken lightly. We are training future professionals, therefore the level of involvement and compromise should be at the same level as doing scientific research.
5. Presentation skills must be a mandatory course for any PhD curriculum. Scientists should be able to deliver properly and concisely a scientific concept to any broad or specialised audience in an attractive manner.
6. Nowadays, efforts must be made to include the effect of the environment (at any affordable level of theory) when studying the singlet fission process. Even though the gas phase dimer model has shown its utility to study the process, this is not a realistic picture. (Chapter 5 of this thesis)