Propositions

accompanying the dissertation

Nonorthogonal configuration interaction to study electron and excitation energy transfer

by

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1. Of the methods available today, nonorthogonal configuration interaction (NOCI)-Fragments gives the most chemically intuitive picture of electron and excitation transfer processes occurring between molecular fragments. [This thesis]

2. The creation of a reduced common molecular orbital basis can be extended to other methods involving nonorthogonal molecular orbital sets, as a general procedure to reduce computational effort in evaluating Hamiltonian matrix elements. [Chapter 3]

3. The active space decomposition (ASD)-CASSCF procedure introduced by Parker and coworkers [J. Chem. Phys. 139, 021108 (2013)] is not a viable replacement of the NOCI method. The main advantage of the use of nonorthogonal orbitals can be seen when charge transfer states also need to be described on an equal footing.

4. A model for excitation transfer in singlet fission that is based on a localized description of the excitation gives sufficiently reliable values of the electronic coupling matrix element. A more involved delocalized description is not necessary. [Chapter 5]

5. The important results of research on alternative energy that are obtained by performing a large volume of calculations on supercomputers outweigh by far the negative aspects related to the high power consumption involved. This is of relevance in the future where our society will have more dependence on data and computational models.

6. Singlet fission has the potential to improve the photo-conversion efficiency of organic solar cells by a considerable extent. Yet, organic photovoltaics can never be the first choice solar cell material of the future as the level of cost effective production and photo-conversion efficiency provided by silicon or perovskite based solar cells is hard to match. Singlet fissionable materials used in conjunction with silicon is an interesting alternative to look into. [J. Phys. Chem. Lett. 11, 8703−8709 (2020)]

7. Evaluation of material properties of sufficiently large molecular systems to a higher accuracy will not be possible with the help of only classical computers. A quantum computer will be required to carry out at least a part of this calculation thereby giving an exponential speedup for that part of the calculation.

8. In today's silicon age, the growing number of jobs predominantly in the computation and engineering sector does not imply that people working in other sectors are rendered jobless soon, it merely implies that there will be a shift in type of jobs people do in the future.