

Singlet Fission: H₂ dimer model system

Singlet fission (SF), a process whereby one high energy singlet exciton is converted into two lower energy triplet excitons, is an excited state phenomenon with a potential impact on the efficiency of inexpensive organic solar cells [1,2]. In this process high energy singlet exciton, resultant from the absorption of a high energy photon, is converted into two triplet exciton which increase the efficiency of single junction solar cell. In principle, we can increase the efficiency limit to 42%, which is about a quarter more than conventional (Shockley–Queisser limit on efficiency, 33%) solar cell. It is observed to occur spontaneously in some organic materials where the energy of the singlet exciton, E_s , is approximately twice the energy of the triplet exciton, E_T . However, the dynamical mechanism of this phenomenon is not fully understood and a complete microscopic theory of singlet fission is lacking. A four-electron four-orbital model is a simple model to understand the mechanism of singlet fission for the transition from an initially excited intramolecular singlet state, S_1 , to the multiexciton triplet-triplet state, T_T . In this work we considered H₂ dimer as a model and try to comprehend the SF mechanism.

References:

- (1) M. B. Smith, J. Michl, Singlet Fission. *Chem. Rev.*, 110, 6891–6936 (2010).
- (2) M.B. Smith, J. Michl, Recent Advances in Singlet Fission. *Annu. Rev. Phys. Chem.*, 64, 361–368 (2013).

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