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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, Es, is approximately twice the energy of the triplet exciton, ET. 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, S1, to the multiexciton triplet-triplet state, TT. 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).

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