

Singlet Fission

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Singlet fission is a photophysical process in which a singlet excited molecule shares some of its energy with a nearby ground state molecule to produce two triplet excited molecules. It is of potential interest for solar energy conversion since it offers an increase of the maximum theoretical efficiency of a solar cell from the Shockley-Queisser limit of $1/3$ to nearly $1/2$.

The detailed mechanism of singlet fission is still only poorly understood. The biggest obstacle to its practical utilization is the tiny number of materials that are known to perform the process efficiently. None of them appear to be very practical. Our efforts focus on the use of concepts of quantum chemistry for the development of simple general structural rules for new materials in which singlet fission will occur rapidly and will produce a 200% triplet yield. We shall address both the problem of identifying suitable chromophores and the problem of positioning them relative to each other in an optimal way for an effective interaction.