

Electronic structure of substituted BODIPY dyes : Application to singlet fission

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Singlet fission (SF) is a spin-allowed conversion of a singlet state to two triplet states which has the potential to enhance the efficiency of single-junction solar cells [1,2]. To enable singlet fission, the energy of the singlet exciton should be larger than twice the energy of triplet exciton ($E(S_1) > 2 E(T_1)$). Very few classes of polyenes and biradicals meet the energy criteria. Recently biradical systems containing the boron-nitrogen pairs received interest as potential candidates for potential singlet fission enabled molecules [3,4]. In this contribution we present electronic structure of BODIPY (4,4-difluoro-4-bora-3a-4a-diaza-s-indacene) dyes and the effect of substitution on alpha, beta and meso positions in the SF process.

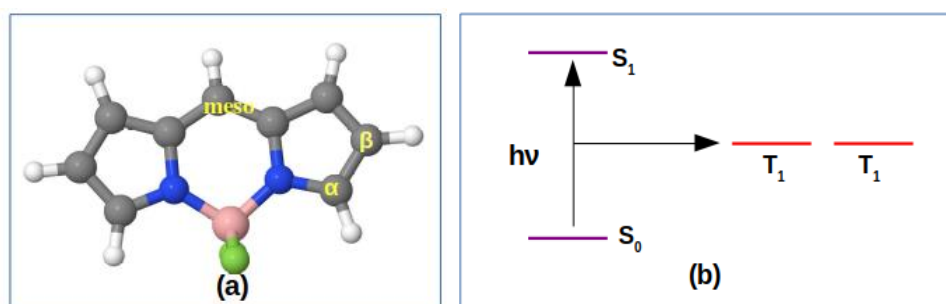


Figure : Singlet Fission (a) Structure of BODIPY where α , β and meso positions are represented in yellow colour (b) Generation of two triplets from one single exciton.

1. (a) M. B. Smith; J. Michl; *Chem. Rev.* **110** 6891 (2010). (b) Smith, M. B.; Michl, J. *Annu. Rev. Phys. Chem.* **2013**, *64*, 361-386.
2. M. C. Hanna; A. J. Nozik; *J. Appl. Phys.* **100** 074510 (2006).
3. S. M. Barbon; J. T. Price; U. Yogarajah; J. B. Gilroy; *RSC Adv.* **5** 56316 (2015).
4. E. Pradhan; J. N. Bentley; C. B. Caputo; T. Zeng; *ChemPhotoChem* **4** 5279 (2020).