Acenes and their fluorinated derivatives as model systems for singlet heterofission

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To overcome the so called Shockley-Queisser limit in photo voltaic cells, the process of singlet fission[1,2] is of high interest in experimental and theoretical studies. By generation of two triplet excitons from one singlet exciton, one can achieve better conversion efficiencies. Therefore the aim is to understand the process of bi-exciton generation and to design new model systems with better singlet fission rates.
The process can be described by the following simplified scheme:

$$\mathrm{S_1} + \mathrm{S_0} \rightleftharpoons {}^1\mathrm{(TT)} \rightleftharpoons \mathrm{T_1} + \mathrm{T_1}$$

To make the process exoergic, the singlet excitation energy has to be higher than twice the triplet excitation energy. Optimally the process should be close to be isoergic to have small energy losses and high singlet fission rates.
Additionally the recombination of the two generated triplets to another triplet exciton has to be suppressed. That can be achieved if the following two conditions are fulfilled.

$$\mathrm{E(S_1)} \geq 2\ \mathrm{E(T_1)}$$
$$\mathrm{E(T_2)} > 2\ \mathrm{E(T_1)}$$

Rather than singlet homofission, which takes place in the bulk of molecular crystals like pentacene and generates twice the same triplet exciton, this study focuses on singlet heterofission[3]. Here we discuss energy level matching and the aspect of coupling matrix elements for singlet heterofission.

References

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