Electronic coupling calculations for a potential singlet fission chromophore

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The singlet fission process converts an excited singlet state into two (local) triplets that are coupled into a singlet (^{1}TT). This process exploits a high-energy photon to generate multiple electron-hole pairs that are capable for charge separation, which ultimately can improve the efficiency of organic solar cells. For an efficient singlet fission process, one has to ensure that for the chromophore the condition of $E(T_2) > E(S_1) \cong 2E(T_1)$ is met in order to have a significant rate [1]. In the Fermi's golden rule approximation, the singlet fission rate depends on the electronic coupling between the initial and final states and the density of final states. Here, we describe the calculation of the electronic coupling based on a nonorthogonal configuration interaction approach and the effect of intra molecular vibrations on this coupling [2,3]. This approach will be applied to a potential singlet fission chromophore, the biradicaloid molecule (see Figure 1), which has been previously reported to fulfil the energetic condition [4].

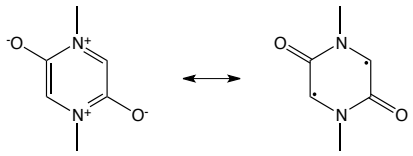

Figure 1. The resonance structures of the biradicaloid molecule

References

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