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Title: Effect of Nanoscale Confinement on Ultrafast Dynamics of Singlet Fission in TIPS-Pentacene

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Abstract:

Singlet fission (SF) is a phenomenon for the generation of a pair of triplet excitons from anexcited molecule in singlet electronic state interacting with another adjacent molecule in its ground electronic state. By increasing the effective number of charge carriers and reducing thermal dissipation of excess energy, SF is promised to enhance light-harvesting efficiency for photovoltaic applications. While SF has been extensively studied in thin films and crystals, the same has not been explored much within a confined medium. Here, we report the ultrafast SF dynamics of triisopropylsilylethynyl pentacene (TIPS-Pn) in micellar nanocavity of varying sizes (prepared from TX-100, CTAB, and SDS surfactants). The nanoparticles with a smaller size contain weakly coupled chromophores which are shown to be more efficient for SF followed by triplet generation as compared to the nanoparticles of larger size which contain strongly coupled chromophores which are less efficient due to the presence of singlet exciton traps. Through these studies, we delineate how a subtle interplay between short-range and long-range interaction among chromophores confined within nanoparticles, fine-tuned by the curvature of the micellar interface but irrespective of the nature of the micelle (cationic or anionic or neutral), play a crucial role in SF through and generation of triplets.

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