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"Ultrafast Singlet Fission (SF) dynamics of 9,10-bis(phenylethynyl)anthracene in solution : A Ultrafast Raman Loss Study"

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Abstract:

Singlet Fission (SF) produces correlated triplet pair from photoexcited singlet exciton via electronic coupling between singlet exciton and triplet pair state. In solution, the process is diffusion controlled dictated by the diffusional collision of singlet exciton with ground state molecules. The singlet fission process can overcome Shockley-Queisser limit as two charged particle generates and hence can provide greater solar cell efficiency. In this article, we have studied the singlet fission process of 9,10-Bis(phenylethynyl) anthracene (BPEA) in solution phase to understand the diffusion controlled collisional singlet fission process. We have observed the singlet fission process is mediated by multiexcitonic triplet pair state formation over picosecond timescale. Three intermediate species has been recognized via Transient Absorption (TA) spectroscopy. Ultrafast Raman Loss Spectroscopy (URLS) showed large structural rearrangement mainly in the anthracene moiety region during multiexciton formation followed by energy relaxation on the triplet surface with 20 ps timescale.

In the excited state, the TA spectra of hot multiexcitonic state overlapped with TA spectra from the moderately allowed electronic state dictated by Pseudo Jahn-Teller Effect (PJTE). Probing this mixed electronic region of the TA by URLS shows quantum interference of Raman polarizabilities of two electronic origins.

References and Notes:

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