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The Non-Adiabatic dynamics of Singlet Fission in Polyacenes[1]

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Singlet fission involves the splitting of a single excitation into two coupled triplet excitations and is manifested in an increasing range of aromatic crystals and amorphous thin films. If the energy of the lowest triplet state is one half (or less) of the first singlet excited state, as it is for tetracene or pentacene and their derivatives, singlet fission may occur between two adjacent chromophores. Since there is no change in the overall spin state of the system, singlet fission can be exceptionally fast, occuring on the fs – ps range. If the triplets can diffuse away from the fission site they are available for harvesting as a dissociated carriers with up to two charge carrier pairs per absorbed photon. The possibility of recovering excess energy above the material band gap (in this case determined by the triplet energy) when a higher energy photon is absorbed has led to great recent interest in exploiting this process for increased efficiency solar energy harvesting. The nature of the electronic couplings between the chromophores, intermediate electronic configurations, and the role of entropy in the spin-allowed primary fission event have all come under great scrutiny. Results from a series of femtosecond spectroscopy experiments on a variety of amorphous thin films, nanoparticles and isolated acene dimer compounds will be presented that shed light on the electronic intermediate states key to the efficiency and speed of this process.

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