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Characterizing the multiexciton fission intermediate in pentacene through 2D spectral modeling[1] ROEL TEMPELAAR, DAVID REICHMAN, Columbia University — Singlet fission, the molecular process in which a singlet excitation splits into two triplet excitons, holds promise to enhance the photoconversion efficiency of solar cells. Despite advances in both experiments and theory, a detailed understanding of this process remains lacking. In particular, the nature of the correlated triplet pair state (TT), which acts as a fission intermediate, remains obscure. Recently, 2D spectroscopy was shown to allow for the direct detection of the extremely weak optical transition between TT and the ground state through coherently prepared vibrational wavepackets in the associated electronic potentials. Here, we present a microscopic model of singlet fission which includes an exact quantum treatment of such vibrational modes. Our model reproduces the reported 2D spectra of pentacene, while providing a detailed insight into the anatomy of TT. As such, our results form a stepping stone towards understanding singlet fission at a molecular level, while bridging the gap between the wealth of recent theoretical works on one side and experimental measurements on the other.

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