Singlet fission is a process unique to molecular photophysics that splits one spin-singlet exciton into two spin-triplet excitons. Incorporated into a solar cell, it has the potential to boost efficiencies beyond the single-junction Shockley-Quiesser limit of 31%. For the process to be practically relevant, however, the currently limited set of efficient materials available needs to be expanded considerably. To this end, much work has been done to establish guidelines for optimal chromophore structure and packing. Because singlet fission is a multi-step process, involving the formation, separation, and decoherence of a spin-correlated triplet pair intermediate, progress toward developing molecular packing guidelines has been slow and complicated. Most work, for example, has focused on better understanding and optimizing only the first step of the process, i.e., triplet pair formation. In this talk, I will discuss our efforts to develop molecular packing guidelines that simultaneously promote high triplet pair yields and long lifetimes—both essential parameters for efficient triplet harvesting. I will first describe our work elucidating the mechanism of singlet fission in solids (i.e., nanoparticles and films) of pentacene derivatives using transient absorption spectroscopy, which has brought renewed attention to two critically overlooked steps, namely, triplet pair separation and decay. I will then present several examples illustrating how molecular packing in various crystalline and amorphous-phase pentacene derivative solids simultaneously governs the yield and lifetime of triplet pairs, which in turn control overall triplet yields. This work represents an important advance toward establishing molecular packing guidelines for efficient triplet harvesting.

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