Singlet Fission for Photovoltaics: Search for New Materials

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The photophysical process of singlet fission in a solid organic material converts a singlet exciton into two triplet excitons and can be thought of as the inverse of triplet-triplet annihilation. A combination of a thin layer of singlet-fission capable material with a thin layer of ordinary photovoltaic material promises to offer an upper limit of theoretical photovoltaic efficiency approaching 1/2, well above the usual Shockley-Queisser limit of 1/3, yet at a comparable cost, because it does not require current matching. The immediate objective in singlet fission research is finding a material that meets all the usual criteria for photovoltaics, especially long-term stability, but also provides a 200% triplet exciton yield. The search can be divided into identifying a suitable chromophore, assuring its favorable packing in the solid, and transporting all charges generated at a suitable interface to electrodes. We shall describe the current understanding of the fairly complicated mechanism by which singlet fission takes place and the main competing processes that can thwart the desired quantitative generation of two triplet excitons, with emphasis on theory and time-resolved spectroscopy. We shall provide a few examples from our own work, which involves collaborating teams in Colorado in the USA and in Prague in the Czech Republic.