# Toward New Materials for Singlet Fission: Structural Design Rules

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Singlet fission generates two triplet excitations from one singlet excitation in a dimer, aggregate, or solid, and promises to increase the efficiency of inexpensive single-junction solar cells. In the best case, using a layer of a singlet fission sensitizer and a layer of an ordinary sensitizer but applying no current matching requirement, it would increase the theoretical efficiency from the Shockley-Queisser limit of 1/3 to nearly 1/2. Unfortunately, the number of materials known to perform singlet fission efficiently is tiny and most are related to the notoriously air-sensitive hydrocarbons, tetracene and pentacene. In order to meet the numerous conditions that will be imposed on a practical singlet fission material, we consider it important to formulate structural design rules for materials that perform singlet fission efficiently. We shall outline how this can be accomplished using simple quantum chemical models. We proceed in two steps: (i) choice of chromophores, where we present promising structures of a new type related to indigo, and (ii) choice of the spatial relation between chromophores, where we present the results of an exhaustive optimization of the six-dimensional spatial relation of two ethylene molecules.
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