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Effect of co-crystallization on singlet fission efficiency in pentacene derivatives XIAOPENG WANG, Carnegie Mellon University, SAMUEL SANDERS, LUIS CAMPOS, Columbia University, MATTHEW SFEIR, Brookhaven National Laboratory, NOA MAROM, Carnegie Mellon University — Singlet fission (SF), the conversion of one singlet exciton into two triplet excitons, may lead to a twofold increase in the efficiency of organic photovoltaics. Since SF has been observed in crystalline pentacene, this material has drawn interest both experimentally and theoretically. Recently, it has been shown that SF efficiency in rubrene may be improved by modifying the crystal packing [CrystEngComm 18, 7353 (2016)]. Here, we study the effect of co-crystallization with small molecule H-bond donors on SF efficiency in pentacene derivatives. Five co-crystals are synthesized and their photoluminescence (PL) and absorption spectra are measured. First-principles calculations based on many-body perturbation theory (MBPT) are then employed to study their excitonic properties. By combining experiment and theory, we demonstrate that excitonic properties, including singlet-triplet gaps, exciton binding energies, and exciton localization, are significantly modulated in pentacene co-crystals. Consequently, co-crystallization becomes an effective strategy for improving SF efficiency in molecular crystals of organic semiconductors.

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