Electron Transfer from Triplet State of TIPS-Pentacene Generated by Singlet Fission Processes to CH₃NH₃PbI₃ Perovskite

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After singlet fission was first discovered in 1965 as a way to explain delayed fluorescence in anthracene crystals, singlet fission research received much attention in an attempt to circumvent the Shockley–Queisser limit in photovoltaic devices because each of the two triplet excitons generated by singlet fission processes can produce electrons after dissociation at the interface. For this reason, many research groups have made strenuous efforts to find new materials exhibiting singlet fission processes. However, only a few examples of solar cells sensitized by singlet fission processes have been reported. Moreover, the conversion of high-energy singlets into pairs of low-energy triplets via singlet fission processes in light-harvesting devices does not generally yield a high power conversion efficiency because solar cell materials possess intrinsically low power conversion efficiencies.

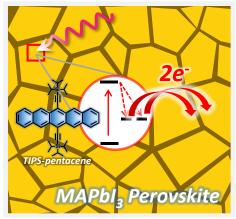


Figure 1. Illustration of electron transfer from triplet state of TIPS-pentacene generated by singlet fission processes to MAPbI₃ perovskite in TIPS-pentacene/MAPbI₃ perovskite bilayer film

To address this issue, we investigated electron-transfer dynamics between TIPS-pentacene as a singlet fission material and CH₃NH₃PbI₃ (MAPbI₃) perovskite nanocrystals as an electron acceptor material to reveal the applicability of singlet fission processes in the perovskite solar cell (Fig. 1). The perovskite photovoltaics was triggered by the development of long-term stable solid-state perovskite solar cell, which have drawn considerable attention in recent years as promising materials that can be used to develop high performance photovoltaic devices at a low cost. Moreover, their high absorption coefficient, tunable band gap, low temperature processing, and abundant elemental constituents provide numerous advantages over most thin-film absorber materials.^[2] In addition, TIPS-pentacene has a high singlet fission yield and hole mobilities in the solid state.^[3] Therefore, the target systems seem to be ideally suited for highly efficient solar cells sensitized by singlet fission processes.

Through the observation of the shorter fluorescence lifetime in TIPS-pentacene/MAPbI₃ perovskite bilayer film (5 ns) compared with pristine MAPbI₃ perovskite film (20 ns), we verified electron-transfer processes between TIPS-pentacene and MAPbI₃ perovskite. Additionally, direct observation of initial rise dynamics with a time constant of 1.1 ps in the decay profiles supports the fact that singlet fission processes occur in TIPS-pentacene/MAPbI₃ perovskite bilayer film. Moreover, TIPS-pentacene cation band in the TA spectra indicate the existence of electron transfer from TIPS-pentacene to MAPbI₃ perovskite in TIPS-pentacene/MAPbI₃ perovskite bilayer film. Finally, it was fully verified that the electron transfer is attributed to the triplet state of TIPS-pentacene generated by singlet fission processes through the analysis of TA decay profiles and the intensity ratio between 500 and 525 nm in TA spectra of TIPS-pentacene/MAPbI₃ perovskite bilayer film. This is the first study, to the best of our knowledge, showing the electron-transfer dynamics between TIPS-pentacene and MAPbI₃ perovskite, which can be applied to perovskite solar cells to improve solar cell efficiency. Therefore, we think that our results can provide useful information on the design of solar cells sensitized by singlet fission and the fabrication of new types of perovskite solar cells in the future.

References:

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