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Uncovering Singlet Fission in TIPS-tetracene Crystals

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Abstract

Singlet fission in organic semiconductors is a promising concept that can be used to increase the efficiency of solar photovoltaic cells. Upon light absorption a singlet exciton ($S = 0$) is created, which splits into two triplet excitons ($S = 1$), via an intermediate triplet-pair state ($S = 1 \otimes S = 1$). This carrier-multiplication process potentially reduces the thermalization losses hampering solar power conversion efficiency.

We identify several sharp triplet-pair peaks in the low temperature (1.4 K) photoluminescence (PL) spectrum of high-quality TIPS-tetracene (5,12-bis(triisopropylsilylethynyl)tetracene) single crystals. Using magnetic fields up to 30 T, we are able to tune the $S = 1$ and $S = 2$ triplet-pair states into resonance with the $S = 0$ triplet-pairs, resulting in a drastic reduction of the PL intensity at resonant magnetic fields [1]. The position of the resonances permits the determination of the exchange coupling constant of the triplet-pair state $J = 0.44$ meV. The triplet-pair emission displays a characteristic vibrational spectrum and is found to disappear above 2.4 K, which is attributed to the thermal activation of triplet-pair dissociation via the triplet-pair quintet states ($S =2$) [2]. Most remarkably, we find that the 1.4 K triplet-pair PL decay time exceeds 10 ms, indicating that in the absence of thermal dissociation the triplet-pairs can have a very long lifetime [2]. Finally, the PL reduction at the resonant magnetic fields can be as large as 90%, much more than the maximum of 50% anticipated before [1]. PL decay time measurements in an applied magnetic field show that this is a dynamic effect, as the decay time decreases at the resonant field strengths. Our results pave the way for a detailed (time-resolved) study of the properties of triplet-pairs and the singlet fission process.

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References

[1] Bayliss et al., Proc. Nat. Acad. Sci 115, 5077, DOI: 10.1073/pnas.1718868115 (2018)

[2] Stern et al., Nature Chemistry 9, 1205–1212, DOI: 10.1038/nchem.2856 (2017)

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