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Understanding Singlet and Triplet Excitons in Acene Crystals from First Principles TONATIUH RANGEL GORDILLO, SAHAR SHARIFZADEH, Lawrence Berkeley Natl Lab, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY NEATON, Lawrence Berkeley Natl Lab and Department of Physics, UC-Berkeley — Singlet fission, a process in which two triplet excitons are formed from a singlet exciton, has the potential to increase the solar cell efficiencies above 100%. Efficient singlet fission has been reported in larger acene crystals, such as tetracene and pentacene, in part attributable to their low-lying triplet energies. In this work, we use many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation approach to compute quasiparticle gaps, low-lying singlet and and triplet excitations, and optical absorption spectra across the entire acene family of crystals, from benzene to hexacene. We closely examine the degree of localization and charge-transfer character of the low-lying singlets and triplets, and their sensitivity to crystal environment, and discuss implications for the efficiency of singlet fission in this systems. This work supported by DOE and computational resources provided by NERSC.

Tonatiuh Rangel Gordillo
Lawrence Berkeley Natl Lab

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