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Effects of molecular packing in organic crystals on singlet fission with ab initio many body perturbation theory[1] JONAH HABER, Dept. of Physics, University of California Berkeley, CA, USA, SIVAN REFAELY-ABRAMSON, Molecular Foundry, Lawrence Berkeley National Lab; Dept. of Physics, University of California Berkeley, CA, USA, FELIPE H. DA JORNADA, STEVEN G. LOUIE, Dept. of Physics, University of California Berkeley; Materials Sciences Division, Lawrence Berkeley National Lab, CA, USA, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab; Dept. of Physics, University of California Berkeley; Kavli NanoScience Institute, Berkeley, CA, USA
— Multi-exciton generation processes, in which multiple charge carriers are generated from a single photon, are mechanisms of significant interest for achieving efficiencies beyond the Shockley-Queisser limit of conventional p-n junction solar cells. One well-studied multiexciton process is singlet fission, whereby a singlet decays into two spin-correlated triplet excitons. Here, we use a newly developed computational approach to calculate singlet-fission coupling terms and rates with an ab initio Greens function formalism based on many-body perturbation theory (MBPT) within the GW approximation and the Bethe-Salpeter equation approach. We compare results for crystalline pentacene and TIPS-pentacene and explore the effect of molecular packing on the singlet fission mechanism.

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