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Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs XIAOPENG WANG, Tulane University, TAYLOR GARCIA, STEPHEN MONACO, Pennsylvania State University, BOHDAN SCHATSCHNEIDER, California State Polytechnic University, Pomona, NOA MAROM, Tulane University — Singlet fission, the down-conversion of one singlet exciton into two triplet excitons, has been recently observed in molecular crystals of rubrene. The orthorhombic form of rubrene is the most stable in ambient conditions. However, rubrene has two additional known polymorphs, a triclinic form and a monoclinic form. To investigate the relative stability of the three polymorphs under different temperature and pressure conditions we use dispersion-inclusive density functional theory (DFT) with the pairwise Tkatchenko-Scheffler (TS) method and the many-body dispersion (MBD) method. Many-body perturbation theory is then employed to study the effect of crystal structure on the electronic and excitonic properties. Band structures are calculated within the GW approximation, where G is the one-particle Green's function and W is the screened Coulomb interaction, and optical properties are calculated by solving the Bethe-Salpeter equation (BSE). We find that crystal packing affects the band gaps, band dispersion, optical gaps, singlet-triplet gaps, and exciton localization in the three polymorphs of rubrene. Singlet fission efficiency may thus be improved by modulating the crystal packing.

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