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On the Possibility of Singlet Fission in Crystalline Quaterrylene

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Singlet Fission (SF), the spontaneous down-conversion of a singlet exciton into two triplet excitons centered on neighboring molecules, is a promising route to improving organic photovoltaic (OPV) device efficiencies by harvesting two charge carriers from one photon. However, only a few materials have been discovered that exhibit SF, most of which are acene derivatives. Recently, there has been a growing interest in a different chemical family of rylenes as potential SF materials. We use many-body perturbation theory in the GW approximation and the Bethe-Salpeter equation (BSE) to investigate the possibility of SF in crystalline quaterrylene. Based on comparison to known and predicted SF materials with respect to the energy conservation criterion (E_S-$2E_T$) and the percent charge transfer (%CT) character of the singlet exciton, crystalline quaterrylene is a promising candidate for SF.