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Can Singlet Fission Enhance the Performance of Organic Solar Cells?[1] J.A. MUNOZ, K. ARYANPOUR, S. MAZUMDAR, Dept of Physics, Univ of Arizona — The high efficiency of pentacene-fullerene (Pc-C_{60}) donor-acceptor solar cells has been ascribed to singlet fission, which generates two spin triplet excitons that each undergo ionization to give two pairs of electrons and holes [1,2]. For triplet ionization to give charge generation, the charge-transfer exciplex in the Pc-C_{60} heterostructure should be energetically below the the molecular triplet state in Pc.Our initial calculations show that this is not a plausible scenario. We propose an alternate mechanism for the relatively high efficiencies of solar cells constructed from donors such as Pc, based on correlated-electron configuration interaction calculations [3] of ground state and photoinduced charge-transfer.

[1] Wilson M. W. B.; et al., J. Am. Chem. Soc, v133, 31, 11830-11833 (2011)
[2] Rao A.; et al., J. Am. Chem. Soc, v132, 36, 12698-12703 (2010)
[3] Yi Y.; Coropceanu V.; Br??das J. L.; J. Am. Chem. Soc, v131, 43, 15777-15783 (2009)

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