



# Triphenylamine-Based Push-Pull $\sigma$ -C60 Dyad As Photoactive Molecular Material for Single-Component Organic Solar Cells: Synthesis, Characterizations, and Photophysical Properties

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A push-pull  $\sigma$ -C60 molecular dyad was synthesized via Huisgen-type click chemistry and used as photoactive material for single-component organic solar cells. Steady-state photoluminescence (PL) experiments of the dyad in solution show a significant quenching of the emission of the push-pull moiety. Spin-casting of a solution of the dyad results in homogeneous and smooth thin films, which exhibit complete PL quenching in line with ultrafast photoinduced electron-transfer in the solid state. Spectroelectrochemistry reveals the optical signatures of radical cations and radical anions. Evaluation of the charge carrier mobility by space-charge limited current measurements gives an electron-mobility of  $\mu_e = 4.3 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , ca. 50 times higher than the hole-mobility. Single-component organic solar cells yield an open-circuit voltage  $V_{oc}$  of 0.73 V and a short-circuit current density of 2.1 mA  $\text{cm}^{-2}$ ; however, a poor fill factor FF (29%) is obtained, resulting in low power conversion efficiency of only 0.4%. Combined transient absorption (TA) and time-delayed collection field (TDCF) experiments show mostly ultrafast photon-to-charge conversion and a small component of diffusion-limited exciton dissociation, revealing the presence of pure fullerene domains. Furthermore, a strong field dependence of charge generation is observed, governing the device fill factor, which is further reduced by a competition between extraction and fast recombination of separated charges.

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