

Article

Understanding of Photophysical Processes in DIO Additive-Treated PTB7:PC₇₁BM Solar Cells

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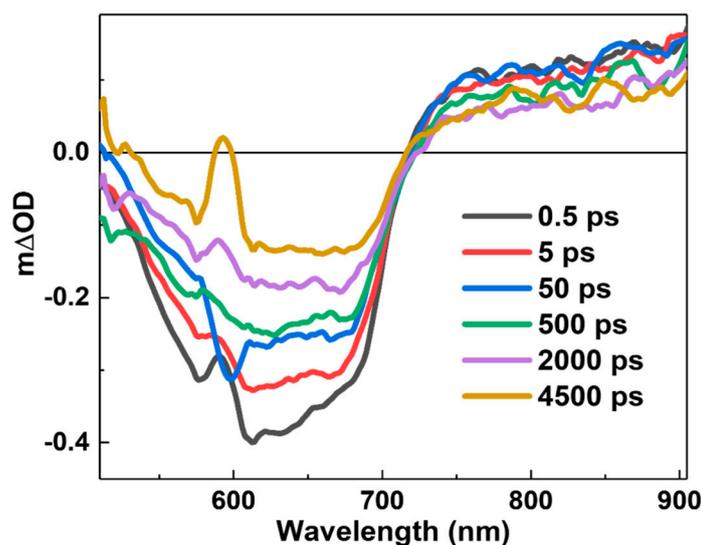


Figure S1. TA spectrum of PTB7:PC₇₁BM film without DIO treatment at indicated delay times after 600 nm excitation with an excitation fluency of 1.16×10^{13} photon·cm⁻²·pulse⁻¹.

Table S1. Fitting parameters of TA kinetics traces in Figure 7c.

Sample	A	τ (ps)
PTB7:PC ₇₁ BM	0.62	7793.11 ± 920.99
DIO-treated PTB7:PC ₇₁ BM	0.66	24891.16 ± 6002.03

S1. Calculation of Coulomb binding energy

The electric field can be calculated by considering the thickness of active layer in neat PTB7 device (~90 nm) and external bias (10 V):

$$E = \frac{U}{d} = \frac{10}{90} \left(\frac{\text{V}}{\text{nm}} \right) = 1.11 \times 10^8 \left(\frac{\text{V}}{\text{m}} \right). \quad (1)$$

Assuming the external electric field just overcomes the Coulomb attraction between the positive and negative charge of the charge pairs:

$$E = \frac{e}{4\pi\epsilon_0\epsilon_r r^2} \quad (2)$$

where E is the external electric field, e is the elementary charge, ϵ_0 is the vacuum permittivity constant (8.85×10^{-12} F/m), and ϵ_r is the ensemble-averaged dielectric constant of the film ($\epsilon_r = 3$) [1]. The distance between electron-hole r can be calculated as 2.1 nm.

Coulomb binding energy of PTB7 exciton, E_b , can be the estimated as:

$$E_b = \frac{e^2}{4\pi\epsilon_0\epsilon_r r} = 0.23 \text{ (eV)}. \quad (3)$$

Reference

1. Hughes, M.P.; Rosenthal, K.D.; Ran, N.A.; Seifrid, M.; Bazan, G.C.; Nguyen, T.-Q. Determining the Dielectric Constants of Organic Photovoltaic Materials Using Impedance Spectroscopy. *Adv. Funct. Mater.* **2018**, *28*, 1801542. <https://doi.org/10.1002/adfm.201801542>.