

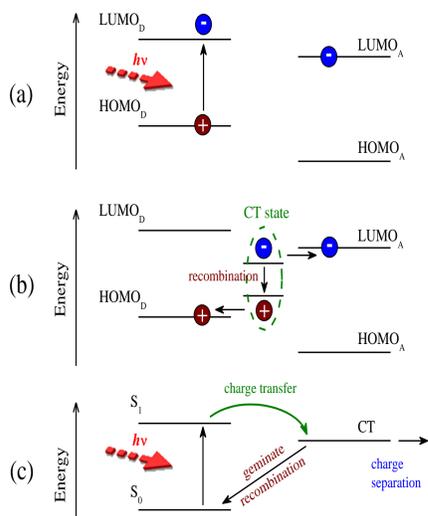
Effect of microadditives on morphology, stability and number of charge carriers in a solar cell based on P3DDT/PC₆₁ BM.

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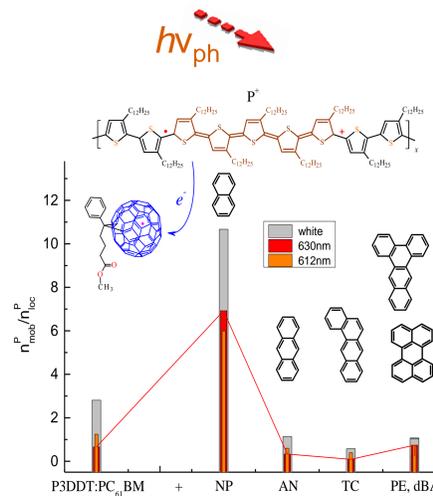
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INTRODUCTION

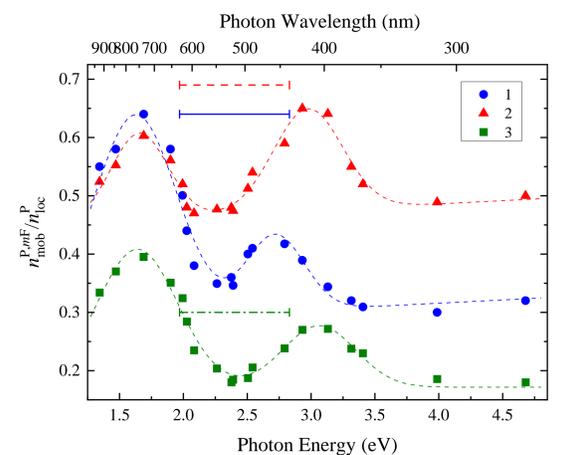
One of the important tasks of organic photovoltaics is to optimize the morphology of composites to achieve balanced transport of charge carriers and increase the efficiency of solar energy conversion. The fundamental problem of photovoltaic elements based on organic polymers is the formation of energetically deep spin traps in them due to the disorder and heterogeneity of polymer matrices. The improvement of conducting properties in organic photovoltaic systems can be achieved by modifying them with various carbon allotropes, for example, nanotubes, graphene, as well as small 2D hydrocarbon molecules [1]. The use of such molecules with conjugate and flat structure as additives should enhance the intermolecular π - π interaction in the composite and, thus, improve its ordering and energy-transforming properties.



SPIN CONCENTRATIONS

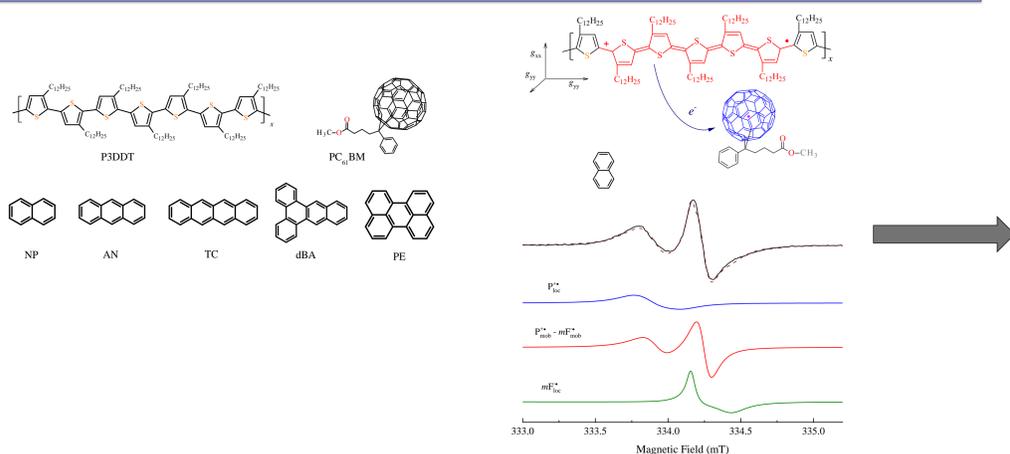


Effective concentration of spins excited in the initial P3DDT:PC₆₁BM composite without phenyl molecules ($N_{ph} = 0$) and BHJ doped with naphthalene (NP, $N_{ph} = 2$), anthracene (AN, $N_{ph} = 3$), tetracene (TC, $N_{ph} = 4$), perylene (PE, $N_{ph} = 5$), and dibenzanthracene (dBA, $N_{ph} = 5$) up to the level $y = 0.06$ illuminated by photons of the white light at $T = 77$ K.



Concentration ratio ($n_{mob}^{(P,mF)}/n_{loc}^P$) obtained for the composite P3DDT:PC₆₁BM before (1) and after doping up to level $y = 0.06$ with naphthalene, P3DDT:PC₆₁BM/NP (2), and anthracene, P3DDT:PC₆₁BM/AN (3), respectively, upon steady-state illuminated as function of photon energy $h\nu_{ph}$. The corresponding parameters obtained for the samples illuminated by white light are shown by horizontal solid, dashed, and dash-dotted lines.

SPIN ENSEMBLES



Effective LEPR spectra of the composite P3DDT:PC₆₁BM/NP_{0.06} irradiated by white light with $T_c = 5000$ K at $T = 77$ K. Sum spectrum and its terms due to localized polarons, P_{loc}^{+} , radical pairs, $P_{mob}^{+} \leftrightarrow mF_{mob}^{-}$, and immobilized methanofullerene, mF_{loc}^{-} .

MAGNETIC PARAMETERS OF SPECTRA

Spectra' fitting allows us to obtain separately all magnetic resonance parameters for all spin ensembles stabilized and/or photoinitiated in BHJ:

✓ Landé g -factor

$$g = g_0 + \frac{A}{\hbar\omega_1} \coth\left(\frac{\hbar\omega_1}{2k_B T}\right)$$

✓ EPR line width

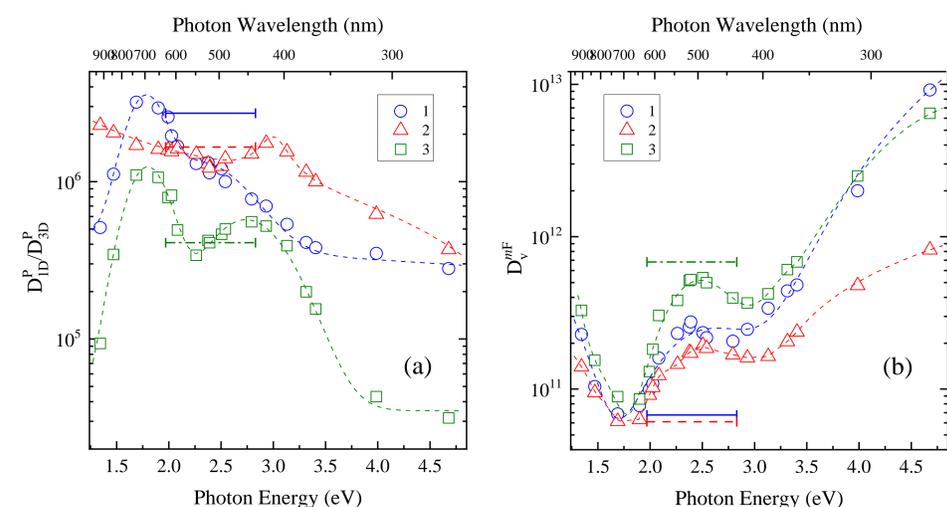
$$\Delta B_{pp} = \Delta B_{pp}^0 + \Delta B_{pp}^{dd} n_i \exp\left(\frac{E_a}{k_B T}\right) + \Delta B_{pp}^{ex} n_i \exp\left(-\frac{E_a}{k_B T}\right)$$

✓ Spin relaxation & dynamics

$$T_1^{-1}(\omega_e) = \langle \omega^2 \rangle [2J(\omega_e) + 8J(2\omega_e)]$$

$$T_2^{-1}(\omega_e) = \langle \omega^2 \rangle [3J(0) + 5J(\omega_e) + 2J(2\omega_e)]$$

DYNAMIC PARAMETERS OF SPINS



Anisotropy of polaron dynamics D_{1D}^P/D_{3D}^P (a) and coefficient of vibrational/librational diffusion D_v^{mF} of methanofullerene radical anions mF_{mob}^{-} (b) photoinitiated in the composite P3DDT:PC₆₁BM before (1) and after its doping with naphthalene (2) and anthracene (3) molecules up to level $y = 0.06$ at $T = 77$ K and different photon energy $h\nu_{ph}$.

References

1. V.I. Krinichnyi, E.I. Yudanov, N.N. Denisov, V.R. Bogatyrenko, Synth. Met., 267 (2020) 116462.

CONCLUSIONS

The effect of additives on the processes of formation, separation, transfer and recombination of charge carriers in organic photovoltaic systems was studied by light-induced EPR (SEPR) and optical IR-view-UV spectroscopy in a wide range of temperatures and photon energy in P3DDT:PC₆₁BM. The addition of two-dimensional planar molecules (about 6% by weight) with an optimal π -structure to the bulk heterojunction polymer:fullerene P3DDT/PC₆₁BM increases its ordering/crystallinity by enhancing the π - π interaction between layered stacks of macromolecules. This eliminates the selectivity of spin charge carriers to photon energy and changes the mechanism of their transfer to the electrodes, as well as increases the stability of spin charge carriers photoinitiated in a composite doped with anthracene or naphthalene molecules by more than 2 and 5 times, respectively. An increase in the crystal phase leads to a significant decrease in the number of spin traps, an increase in the concentration and stability of mobile spin charge carriers and their interaction with the lattice medium. The change in the mechanism of charge transfer to the electrodes is due to the fact that the charge in the amorphous phase is carried mainly by polarons along polymer chains, and in the more crystalline phase charge transfer between the two-layer stacks of the sample structure prevails.

Acknowledgements

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