LEPR STUDY OF NON-FULLERENE SOLAR CELLS ON THE PBDB-T: IT-M BASE POLYMER COMPOSITES

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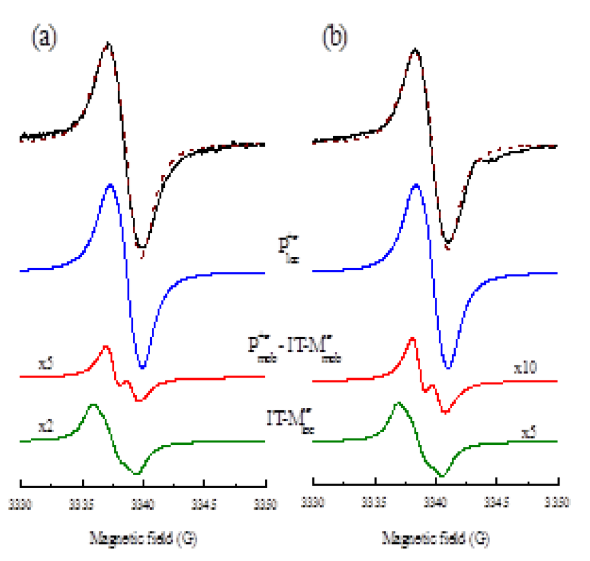
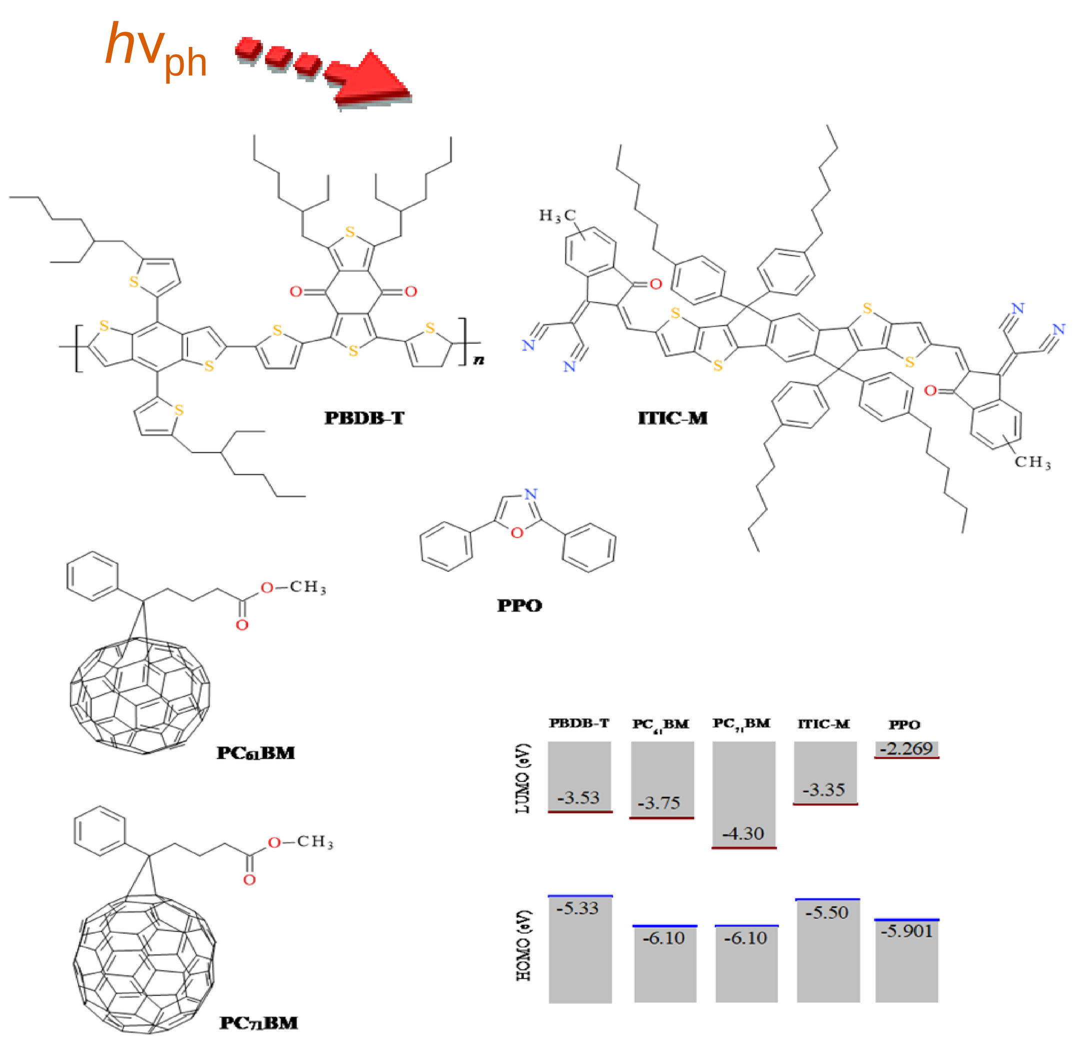
Introduction



We present a light-induced EPR (LEPR) study of photoinitiation, relaxation, and recombination of charge carriers initiated by achromatic /white and mono-chromatic (with a photon energy of 1.34-3.41 eV) light in the PBDB-T-based photovoltaic systems with IT-M counterions.

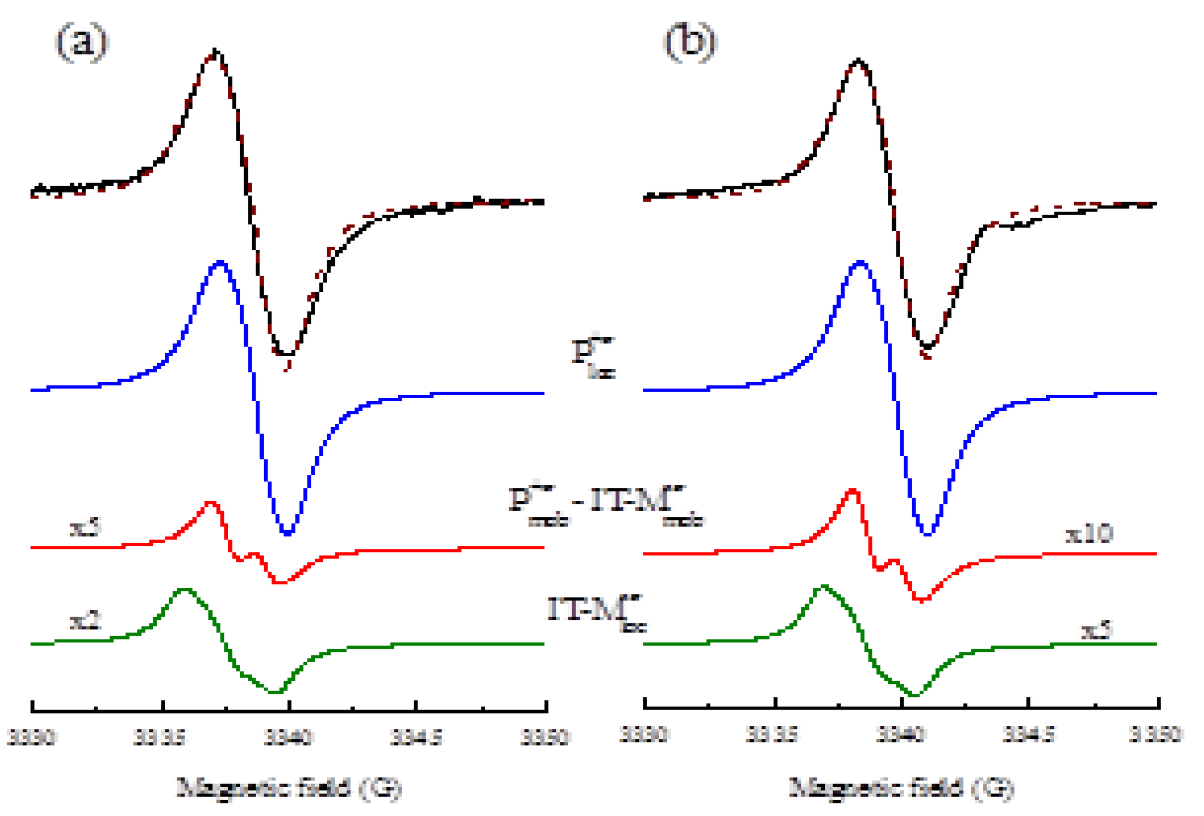
Because fullerenes absorb only a part of the solar irradiation spectrum, the light power conversion efficiency (PCE) of respective polymer:fullerene bulk heterojunctions (BHJ) cannot reach high values. This sparked the development and research of a new generation of non-fullerene electron-accepting molecules for more efficient organic photonics properties [1]. The paramagnetic nature of charge carriers determines the spin-assistant character of all processes occurring in such systems. These processes become dependent not only on the structure and morphology of a sample but also on the number, energetic depth, and spatial distribution of spin traps in its BHJ as well as on the energy and density of the initiated phonons [2].

Spin Ensembles



Schematic structures of the (PBDB-T), (PC61BM), (PC71BM), and 3,9-bis(2-methylene-((3-(1,1-dicyanomethylene)-6/7-methyl)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC-M, IT-M), and 2,5-diphenyloxazole (PPO) used for preparation of polymer composites. LUMO and HOMO data taken from Refs. [3].

Spin Composition



Calculation of individual and sum EPR spectra of spin charge carriers stabilized and photoinitiated in different spin systems.

Spin Parameters

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

- ✓ Landé g-factor

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

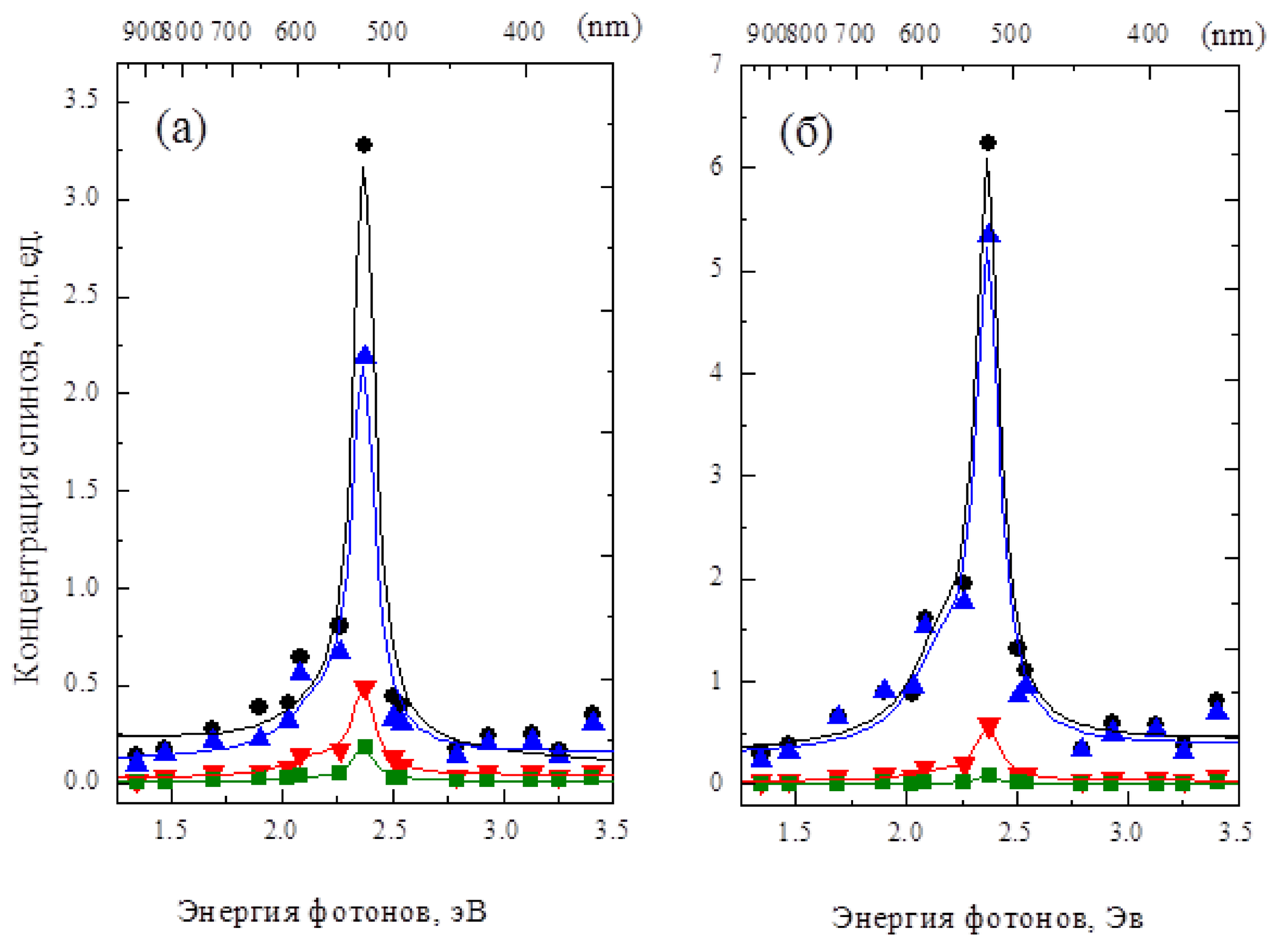
- ✓EPR line width

$$\delta(\Delta\omega) = \frac{\pi t_{1D}^2 n_g(T)}{\hbar\sqrt{\frac{E_r k_B T}{\pi}}} \cdot \frac{\exp\left(-\frac{E_r}{4k_B T}\right)}{1+\left[\frac{3J_{ex}}{2t_{1D}^2}\sqrt{\frac{E_r k_B T}{\pi}}\exp\left(\frac{E_r}{4k_B T}\right)\right]^{-2}}$$

- ✓Spin dynamics

Носители зарядов	g_{zz}	g_{yy}	g_{xx}	g_{iso}	ΔB_{pp}^X	ΔB_{pp}^Y	ΔB_{pp}^Z	ΔB_{pp}^{iso}
P^+	2.00327	2.00224	2.00146	2.00232	1.42	1.58	1.42	1.47
$IT\text{-}M^-$	2.00401	2.00304	2.00170	2.00292	1.56	1.70	1.56	1.61
PBDB-T: IT-M/PPO	2.00403	2.00299	2.00176	2.00293	1.57	1.73	1.57	1.62

Spin-Photon Correlations



Dependence of effective spin concentration and its contributions due to mobile and immobilized charge carriers on the frequency of incident photons at 77K. a) - PBDB-T:IT-M ; b) - PBDB-T:IT-M/ PPO

Conclusions

The paper presents the results of an LEPR study of a new organic photovoltaic composite with a non-fullerene acceptor PBDB-T:IT-M. The parameters of the LEPR spectra of all spin charge carriers, both localized and mobile, arising in the composite under the action of light, were determined. The dependence of the spin concentration of all localized and mobile charge carriers on the photon energy shows an extreme increase in the region of 2.37 eV, which coincides with the band gap of the PBDB-T:IT-M polymer composite. The introduction of microadditives of the photoactivator 2,5-diphenyloxazole (PPO) into the system improves the morphology of the composite due to a more intense π - π interaction between the components. These interactions contribute to an growth of the exchange interaction between them and stabilize the number of spin charge carriers, mainly localized in the energy traps of the polymer matrix. The exchange interaction in the composite between polymers and PPO leads to a twofold increase in the number of spins in the energy region close to the band gap of the composite.

References

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2. Krinichnyi, V. I.; Yudanova, E. I.; Denisov, N. N.; Bogatyrenko, V. R., J. Phys. Chem. C 2019, 123, 16533-16545.
3. Li, S.; Ye, L.; Zhao, W.; Zhang, S.; Mukherjee, S.; Ade, H.; Hou, J., Adv. Mater. 2016, 28, 9423-9429.

Acknowledgements

This work was performed with financial support from the Russian Foundation for Basic Research, Grant No. 18-29-20011-mk according the State Assignment, No. AAAA-A19-119032690060-9.