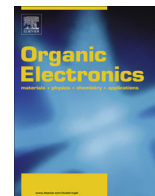




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## Computation of full polymer-based photovoltaic nanodevices using a parametrized field-based multiscale solar-cell approach

Sergii Donets, Anton Pershin, Stephan A. Baeurle\*

*Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany*

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### ABSTRACT

Polymer electronics has the power of revolutionizing the world of printable flexible electronics through reducing the production costs of large-scale nanoelectronic applications. However, performance and stability of such devices are still generally low compared to their inorganic counterparts, rendering the development of novel multiscale experimental- and theoretical-investigation techniques necessary, to increase the understanding of the causes for performance losses under operation conditions. To this end, we introduce in this paper a novel parametrized field-based multiscale algorithm, which permits to study effects of chemical details, like e.g. inter-mixing of the donor- and acceptor-components and/or photodegradation, on the photovoltaic performance of polymer-based solar-cell nanodevices with sizes of technological relevance. By comparing its results with the ones of atomistic particle-based solar-cell calculations, we demonstrate that the parametrized field-based approach provides a reasonable value for the internal quantum efficiency of a polyfluorene-based blend heterojunction, used for parametrization of the exciton dissociation and charge transfer rates. Moreover, we show that its combination with a modified version of the transfer-matrix method allows the inclusion of the influence of the optical absorption of the individual device components, like e.g. the electrodes and/or nanophases from the photoactive layer, into the algorithm. This full-device solar-cell approach enables us to determine values for the external quantum efficiency of several polymer blend morphologies in good agreement with experimental measurements. Finally, the latter study also reveals, in concordance with experimental observations, that reducing charge-carrier losses is more important than reducing exciton- and photon-losses for optimizing the performance of solar-cell devices.

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### 1. Introduction

Polymer nanodevices have attracted considerable attention in the past decade for large-scale applications, because of their low fabrication costs as well as favorable physical characteristics, such as light weight and high mechanical flexibility [1,2], conferring them high potential for modern societies in the field of energy, information and communication [3]. Examples of polymer electronic devices include polymer solar cells (PSCs) [4–7], polymer light-emitting diodes (PLEDs) [8–11], polymer field-effect transistors [12,13], polymer data storage [14] and energy storage devices [15]. The number of applications continue to grow as the technology mature, offering in many cases new electronic functionalities not available in inorganic devices. Promising examples of novel characteristics in polymer devices, which might be integrated within nanocircuits, are e.g. memory effects [16], charge storage capabilities of nanocapacitor arrays [17] and negative differential

resistance behavior [16,18]. However, the integration of these new device functionalities within electronic nanocircuits frequently poses considerable challenges for material scientists, because a detailed understanding of their underlying mechanisms is in most cases still lacking [16]. Moreover, some types of polymer nanodevice applications are affected by low device efficiencies [19,20] and/or degradation processes [21], limiting their usefulness compared to their inorganic counterparts. For instance, in case of PSCs the photoelectric conversion efficiency currently reaches a maximum of around 9–11% [22–24], which is still too low for a wide range of commercial applications.

The causes for the low power conversion efficiency of PSCs have primary been associated with loss phenomena of the elementary particles, occurring during the photovoltaic process, such as photon loss, exciton loss and charge carrier loss [25]. Their complex relationship and strong dependence on the structural-dynamical characteristics of the photoactive material have been investigated in various recent experimental [26–29] and theoretical studies [17,30–34]. For example, photon losses can be caused by the reduced absorption of the semiconducting polymer material in a

\* Corresponding author.

E-mail address: [stephan.baeurle@chemie.uni-regensburg.de](mailto:stephan.baeurle@chemie.uni-regensburg.de) (S.A. Baeurle).

specific part of the solar spectrum. This problem can be alleviated by using multi-junction solar-cell constructions, which represent an effective way to harvest a broader range of the solar spectrum by connecting two or more solar cells with different absorption bands in series [22,24], or using ternary blend solar cells [35]. Another source of photon losses can result from optical interference effects, induced by the transmission and reflection of the light at the device interfaces, causing that a fraction of the photons will be lost for the subsequent process of exciton generation [36]. In order to get a better understanding of the light propagation in such heterogeneous multi-layer systems, Hoppe et al. [36] performed optical modeling using the transfer-matrix method, to quantify optical losses and gains within thin film polymer-fullerene bulk-heterojunction devices. They demonstrated for a polymer blend solar cell, consisting of poly(2-methoxy-5-(3,7-dimethyloctyloxy)-1,4-phenylenevinylene) (MDMO-PPV) and [6,6]-phenyl C<sub>61</sub> butyric acid methyl ester (PCBM), that a thickness of 90 nm for the photoactive layer is optimal and in good agreement with experimentally optimized devices. Moreover, in case of a blend, composed of regioregular poly(3-hexylthiophene-2,5-diyl) (P3HT) and PCBM, they showed that post-production treatments lead to an increase in the optical absorption in the photoactive layer of more than 40%, which demonstrates that optical gains can play an important role for enhancing the efficiency of solar-cell devices. Yan et al. [37] used the transfer-matrix method, to determine the exciton generation profiles of a poly(9,9'-dioctylfluorene-co-bis-N,N'-(4-butylphenyl)-bis-N,N'-phenyl-1,4-phenylenediamine) (PFB)-poly(9,9'-di-*n*-octylfluorene-co-benzothiadiazole) (F8BT) bilayer solar-cell device, and introduced them into dynamic Monte Carlo (DMC) simulations, to investigate the influence of annealing on the device performance. They found that the decrease in device performance with annealing is partly due to a decrease in the electron- and hole-mobilities in the respective nanophases as well as a decrease in the separation probability of interfacial electron-hole pairs, induced by an increased structural disorder at the donor-acceptor (DA) interface. From the experimental point of view, Bavel et al. [38] showed through transmission-electron-microscopy measurements on thermally annealed P3HT-PCBM films of different thickness that the nanoscale organization of a morphology is more crucial for a high efficiency of solar-cell devices than absorption alone. They obtained the best device performance using moderately thick photoactive layers of about 100 nm, characterized by a high overall crystallinity of P3HT and the enrichment of P3HT as well as PCBM close to the hole- and electron-collecting electrodes, respectively. Thicker films of about 200 nm absorbed more light, but showed less favorable morphological organization in the photoactive layers, due to a lower crystallinity of P3HT especially near to the hole-collecting electrode, and as a result produced poorly functioning solar-cell devices. This work demonstrated that, besides light absorption, also other elementary steps of the photovoltaic process, such as exciton dissociation, charge transport and charge collection, may play a critical role in the device performance. To optimize the nanoscale morphology of photovoltaic devices, Xia and Friend [29] highlighted the importance of the fabrication process by showing on polyfluorene-based blends that improving the fine-scale phase separation through inkjet printing (IJP) technologies leads to a factor two of enhancement in the external quantum efficiency (EQE) with regard to blends prepared with spin-coating (SC). From the theoretical side, we have recently demonstrated that nanoscale morphology optimization can be realized by using our recently developed field-based multiscale solar-cell algorithm [17,32], which relies on the coupling of a mesoscopic field-theoretic approach, to generate the nanoscale morphology of the polymer system under consideration, with a suitable DMC algorithm, to

model the elementary photovoltaic processes. Using this algorithm, we investigated the influence of structural characteristics and different device conditions on the exciton-generation- and charge-transport-efficiencies of a nanostructured polymer blend at different stages of the phase-separation process [32]. In this study we found that the disjunction of continuous percolation paths leads to the creation of dead ends, resulting in charge carrier losses through charge recombination. Moreover, we observed that defects are characterized by a low exciton dissociation efficiency (EDE) caused by a high charge accumulation, counteracting the charge generation process. From these observations, we concluded that both the exciton- and charge-carrier-loss-phenomena are responsible for the dramatic decrease in the internal quantum efficiency (IQE) of the polymer blend heterojunction. In two very recent theoretical works we demonstrated by introducing a novel particle-based multiscale solar-cell algorithm that not only the visible nanoscale morphology, but also the chemical composition of the nanophases needs to be taken into account and optimized, to enhance the performance of solar cells [33,34]. In the first study [33] our results revealed that inter-mixing of the electron-donor (D) and -acceptor (A) type of monomers in a lamellar-like PFB-F8BT blend causes that the major part of the charge generation and charge transport takes place within the bulk of the nanophases in agreement with the experimental measurements of Coffey and Ginger [28] and not, as commonly believed [27], at the DA interfaces. Moreover, we found that keto-defects on the fluorene moiety of the F8BT phase, induced by photo-oxidation, lead to the keto-induced trapping of electrons on the same polymer chain, resulting in a deterioration of the overall electron transport efficiency in the F8BT phase of the polymer solar cell. In the second study [34] we applied the particle-based multiscale solar-cell algorithm and investigated the effect of random tapering on the photovoltaic properties of lamellar-like PFB-F8BT-diblock-copolymer systems. These simulation results revealed that inserting a tapered middle block with optimal length at the chemical junctions between the D- and A-blocks of the diblock copolymers leads to a maximum in the IQE, accompanied by a significant increase of the EDE and only a moderate deterioration of the charge transport efficiency (CTE). In conclusion, these latter studies demonstrated that the chemical composition of the domains can also be a crucial factor, which needs to be considered for enhancing the photovoltaic performance of solar-cell nanodevices.

Our goal in this paper is to investigate the influence of chemical details and optical absorption on the device performance of full polymer solar-cell nanodevices of large system size at low computational costs. To this end, we introduce a novel parametrized field-based multiscale solar-cell approach, which extends the conventional field-based solar-cell approach by parametrizing the processes associated with exciton dissociation as well as charge transport depending on the segmental composition of the photoactive layer. For its validation, we apply the so-called parametrized field-based approach on PFB-F8BT blends and compare the results to data from conventional field-based- and atomistic-particle-based-solar-cell calculations. With our new simulation algorithm, we aim to demonstrate that the parametrization procedure permits to correctly take into account effects from chemical details, like e.g. inter-mixing of the D- and A-components and/or photodegradation, in field-based solar-cell calculations. To include the optical absorption of the various device components, like e.g. the electrodes and individual nanophases of the photoactive layer, into the algorithm, we couple it in a subsequent step with a modified version of the transfer-matrix method, which allows to determine the external quantum efficiencies of polymer blend nanodevices of different degree of phase separation. Using this full-device algorithm, our objective is to explore the impact of

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