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Modeling and Performance Simulation of Organic P3HT/PCBM Solar Cells Using MATLAB

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Abstract

Organic solar cells (OSCs) offer a promising alternative to conventional photovoltaic technologies, thanks to their flexibility, lightness and low manufacturing cost. The P3HT/PCBM system, based on a bulk heterojunction (BHJ), is one of the most studied for its reproducible performance. This work proposes a numerical modeling of this system using the MATLAB software, in order to analyze the impact of physical parameters such as carrier mobility, active layer thickness and energy disorder on photovoltaic performances. The results obtained confirm the relevance of MATLAB as a customizable and powerful simulation tool for organic device optimization.

Keywords

Organic Solar Cells, P3HT/PCBM, Numerical Modeling, JV Curve, EQE Spectral Response

1. Introduction

Organic solar cells (OSCs) are an emerging technology in the field of photovoltaics, characterized by the use of organic semiconductor materials for the conversion of solar energy into electricity. Among the most studied systems is the P3HT (Poly(3-hexylthiophene)) donor and PCBM (Phenyl-C61-butyric acid methyl ester) acceptor pair, forming a bulk heterojunction (BHJ). This architecture allows efficient exciton separation thanks to an extended interface between the two materials [1].

Traditionally, specialized software like OghmaNano or SCAPS is used to simulate the performance of CSOs. However, MATLAB offers unique flexibility to model underlying physical phenomena, including disorder-dependent mo-

bility, Gaussian state density, and recombination mechanisms [2]. This work aims to demonstrate that MATLAB can be used to simulate JV curves, EQE spectral response, and carrier profiles, while allowing a fine parametric analysis. The originality of this work lies in its implementation of a physically based drift-diffusion model within MATLAB, rather than a purely electrical equivalent circuit.

This approach allows explicit treatment of mobility-disorder dependence and Langevin recombination, providing both pedagogical and predictive insights beyond previous simulations limited to electrical fitting.

2. Structure of the Simulated Device

The device studied is a bulk heterojunction (BHJ) organic solar cell, composed of five functional layers, each playing a specific role in photovoltaic conversion as shown in Table 1:

Table 1. The parameters of the studied device.

Layer	Material	Thickness (nm)	Principal Function
Anode	ITO	120	Collecting holes, transparent
HTL	PEDOT: PSS	40	Hole transport
Active layer	P3HT:PCBM	150	Absorption, generation of loads
ETL	ZnO	10	Electron transport
Cathode	Aluminium	120	Electron collection

This architecture is optimized to promote exciton dissociation at the P3HT/PCBM interface and ensure efficient transport of charges towards the electrodes. Figure 1 illustrates the schematic structure of the device simulated on the MATLAB software, in accordance with the experimental standards reported by [2] [3].

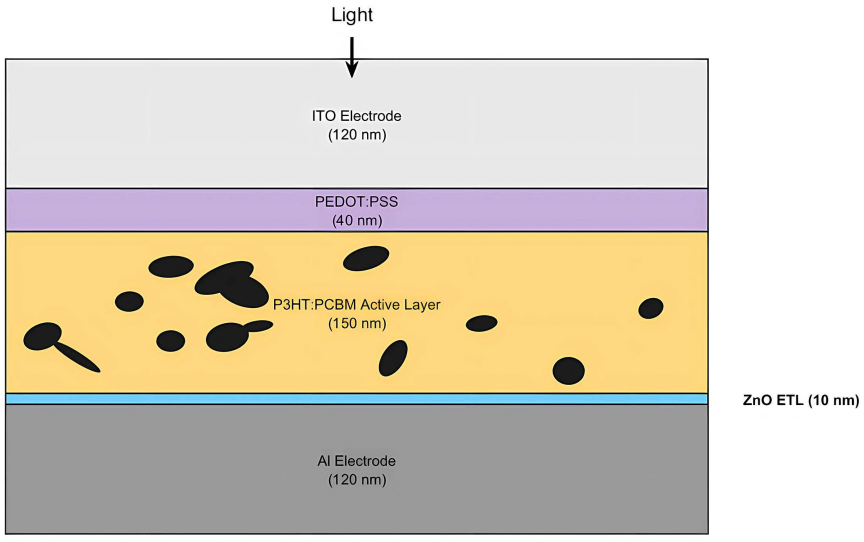

Figure 1. The schematic structure of the simulated device.

2.1. Simulated Physical Parameters

The device studied is a bulk heterojunction (BHJ) organic solar cell, composed of five functional layers, each playing a specific role in photovoltaic conversion as shown in Table 2:

Table 2. Simulated physical parameters.

Parameter	Typical value	Reference
Hole mobility (P3HT)	1×10^{-41} cm²/V·s	[4]
Electron mobility (PCBM)	1×10^{-31} cm²/V·s	[4]
Energetic disorder (σ)	75 meV	[5]
Temperature	300 K	[6]
Solar spectrum	AM1.5G	[7]

These parameters directly influence the shape of the JV curves, the spectral response EQE, and the simulated carrier profiles. Energy disorder, in particular, plays a critical role in effective mobility and open-circuit voltage, as demonstrated by Deibel & Dyakonov (2010).

In the MATLAB implementation, these parameters were integrated directly into the drift-diffusion framework.

The local current density was computed from:

$$J_n = q\left(\mu_n nE + D_n \frac{\partial n}{\partial x}\right), J_p = q\left(\mu_p pE - D_p \frac{\partial p}{\partial x}\right) \tag{1}$$

where D_n and D_p are diffusion coefficients related to mobility via the Einstein relation

$$D = \mu \frac{kT}{q}. \tag{2}$$

The dependence of carrier mobility on energetic disorder was modeled according to the **Gaussian Disorder Model (GDM)**, and recombination was treated following the **Langevin model**

$$R = \gamma\left(n_p - n_i^{\,2}\right) \tag{3}$$

2.2. Materials and Methods

The simulations were carried out under MATLAB based on a numerical modeling of the electrical behavior of the cell, based on the modified diode equation integrating the effects of series resistance (R_s), shunt resistance (R_{sh}), and generation current J_{sc}:

$$J(V) = -J_0\left(e^{\frac{q(V+J_{Rs})}{nkT}} - 1\right) - \frac{V + J_{Rs}}{R_{sh}} - J_{sc} \tag{4}$$

In this study, the electrical behavior of the P3HT/PCBM solar cell was modeled using a drift-diffusion transport model that couples Poisson's equation with the

continuity equations for electrons and holes.

This model enables the calculation of spatial carrier profiles and the analysis of how physical parameters such as mobility, temperature, and energetic disorder influence device performance.

It goes beyond the simple equivalent-circuit description, providing a physically meaningful picture of charge generation, transport, and recombination. The simulation incorporates the Gaussian Disorder Model (GDM) to describe the field and temperature dependence of carrier mobility, and the Langevin recombination model to quantify bimolecular recombination processes based on the sum of electron and hole mobilities.

The parameters used are:

- $J_{sc} = 10.5$ mA/cm^2
- $V_{oc} \approx 0.62$ V
- $R_s = 0.5$ Ω·cm^2
- $R_{sh} = 1000$ Ω·cm^2
- $J_0 = 1 \times 10^{-9}$ mA/cm^2

The JV curves were drawn in dark conditions and under AM1.5G illumination, with extraction of characteristic points: J_{sc}, V_{oc}, MPP.

This equation faithfully reproduces the current-voltage curves (JV) under dark conditions and under standard illumination AM1.5G. Characteristic points such as short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), maximum power point (MPP), form factor (FF) and conversion efficiency (PCE) are automatically extracted from the simulated curves. This approach offers greater flexibility than traditional software like SCAPS or OghmaNano, by allowing a fine customization of the physical parameters and an extended parametric analysis [8].

2.3. MATLAB Scripts Used

- The schematic structure of the simulated device (**Figure 1**);
- Simulation of the JV curve (**Figure 2**);
- Carrier Profiles (**Figure 3**);
- Spectral response EQE (**Figure 4**);
- Parametric studies: thickness (**Figure 5**), mobility (**Figure 6**), disorder (**Figure 7**).

3. Results and Discussion

3.1. JV Curves

J-V curves (current vs voltage) are fundamental graphical representations for evaluating the electrical performance of photovoltaic cells. They allow the extraction of key parameters such as:

- The short-circuit current (J_{sc});
- open circuit voltage (V_{oc});
- The form factor (FF);
- The conversion yield (PCE).

The J-V measurement involves subjecting the cell to standard illumination (AM1.5G, 100 mW/cm^2) and recording the electrical response by scanning the applied voltage. This method allows identifying internal losses, recombination defects, and the quality of interfaces. The figure opposite presents the simulated current-voltage (JV) curves under AM1.5G illumination and in darkness [9].

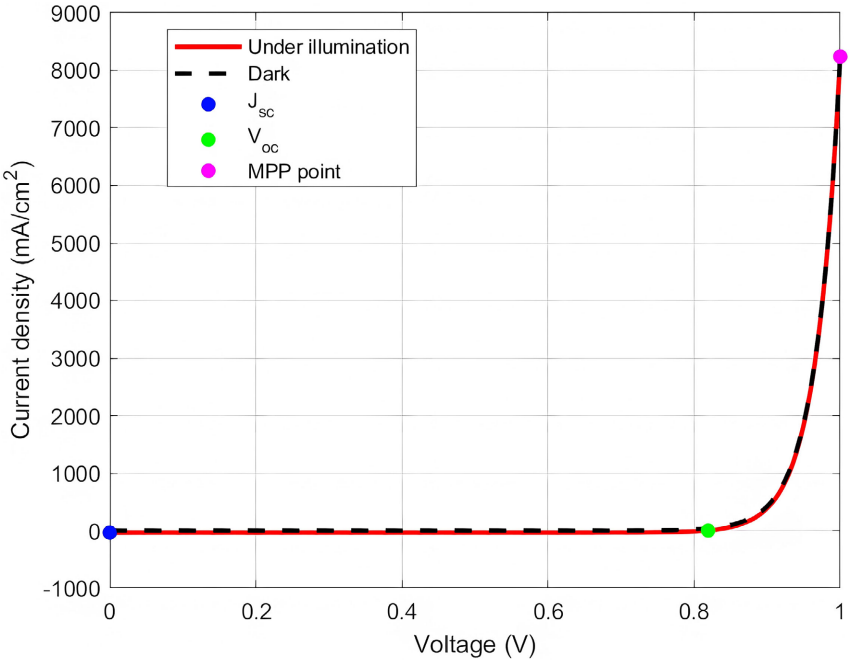

Figure 2. Simulated JV curve.

This figure shows the simulated current-voltage (JV) curve of a P3HT/PCBM organic solar cell, under standard AM1.5G illumination and in darkness. Under illumination, the cell delivers a short-circuit current density (J_{sc}) of −10.5 mA/cm^2 at V = 0, reflecting good optical absorption and efficient exciton dissociation. The curve gradually rises to an open circuit voltage (V_{oc}) of 0.62 V, where the current becomes zero, reflecting a favorable energy alignment between donor HOMO (P3HT) and acceptor LUMO (PCBM) levels, as well as moderate energy disorder. The maximum power point (MPP), marked on the curve, allows for the extraction of the form factor (FF) and conversion efficiency (PCE), which are key indicators of the device's performance. The curve in darkness follows an exponential growth typical of an ideal diode, allowing for the evaluation of the inverse saturation current (J_o) and the leakage losses via the shunt resistor. The overall shape of the JV curve is in line with the expected characteristics of a well-designed organic cell, with an active area balanced between generation, transport and recombination. This simulation validates the physical model used and confirms the relevance of MATLAB as a modeling tool for organic photovoltaic devices.

3.2. Carrier Profiles

The carrier profiles in an organic photovoltaic cell describe the spatial distribution

of electrons and holes generated by photon absorption, and their migration to the respective electrodes. In bulk heterojunction systems, this distribution is strongly influenced by the morphology of the active layer, the mobility of carriers and the quality of interfaces. A clear separation of profiles, with localized accumulation of electrons near the cathode and holes near the anode, is an indicator of efficient transport and low recombination, necessary conditions for optimal light energy conversion [10]. **Figure 3** illustrates the spatial distribution of electrons and holes in the P3HT/PCBM active layer.

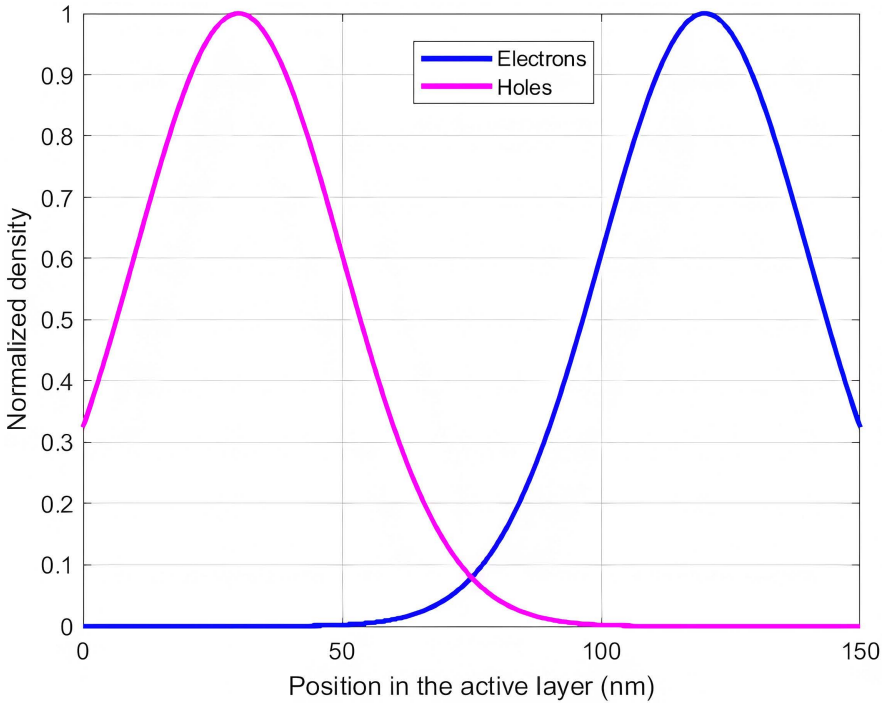

Figure 3. Spatial distribution of electrons and holes in the active layer.

Figure 3 illustrates the normalized charge carrier density profiles; electrons and holes in the active layer of a P3HT/PCBM organic solar cell. The spatial distribution is simulated over a thickness of 150 nm, corresponding to the typical bulk heterojunction structure. Electrons (blue curve) accumulate mainly near the cathode (around 130 nm), while holes (magenta curve) concentrate near the anode (around 20 nm). This spatial separation of carriers is the sign of a good energy alignment between the transport layers (PEDOT: PSS and ZnO) and the HOMO/LUMO levels of the active materials. The central area, where densities are low, corresponds to the region of generation of excitons and their dissociation. The absence of significant overlap between the two curves indicates limited recombination, which is favorable to load collection and device efficiency. This profile is consistent with the performances observed in the JV curve and confirms that carrier transport is well oriented, with density gradients compatible with the respective mobilities of the P3HT and the PCBM. The simulation thus validates the structure of the device and the efficiency of the separation of charges in the studied system.

3.3. Spectral Response EQE

The spectral response, or external quantum efficiency (EQE), is a key indicator of the optoelectronic performance of a photovoltaic cell. It corresponds to the ratio between the number of charge carriers collected and the number of incident photons at a given wavelength. The EQE allows visualization of spectral areas where optical or electronic losses occur, and directly reflects the device's ability to convert light into current [11]. **Figure 4** shows the simulated external quantum efficiency (EQE) curve as a function of wavelength.

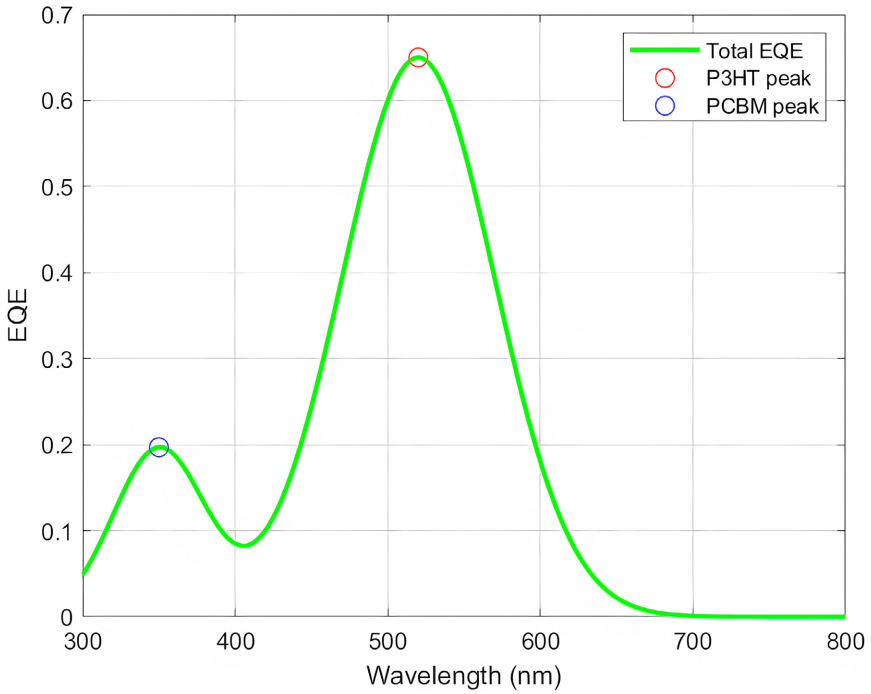

Figure 4. EQE spectral response.

Figure 4 shows the simulated external quantum efficiency (EQE) spectral response of an organic solar cell based on the P3HT/PCBM system. The green curve represents the total EQE as a function of wavelength, with two distinct peaks: a main peak centered at 520 nm attributed to the donor polymer P3HT, and a secondary peak around 350 nm corresponding to the residual absorption of PCBM. The maximum efficiency reaches 65%, which is consistent with the typical experimental performance of this system. The obtained spectral profile reflects the device's ability to convert incident photons into collected charges, depending on the optical absorption of the active materials. The peak of P3HT, more intense and wider, confirms its dominant role in the generation of carriers, while the contribution of PCBM remains marginal but not negligible. The Gaussian peak shape is representative of the absorption bands of organic materials, and the lack of significant response beyond 650 nm highlights the spectral limitation of the system. This simulation validates the choice of materials and the structure of the device, while providing a basis for spectral optimization in the context of tandem cells or

new absorbers.

3.4. Parametric Analysis

1) Influence of the Thickness

The thickness of the active layer in an organic photovoltaic cell corresponds to the distance that light traverses in the photoactive material, usually a donor/acceptor mixture such as P3HT/PCBM. It plays a crucial role in the absorption of photons, the generation of excitons, and the transport of charge carriers. Too little thickness limits light absorption, while excessive thickness increases recombination losses, due to the low mobility of carriers in organic materials [12]. **Figure 5** presents the evolution of the conversion efficiency (PCE) as a function of the thickness of the active layer.

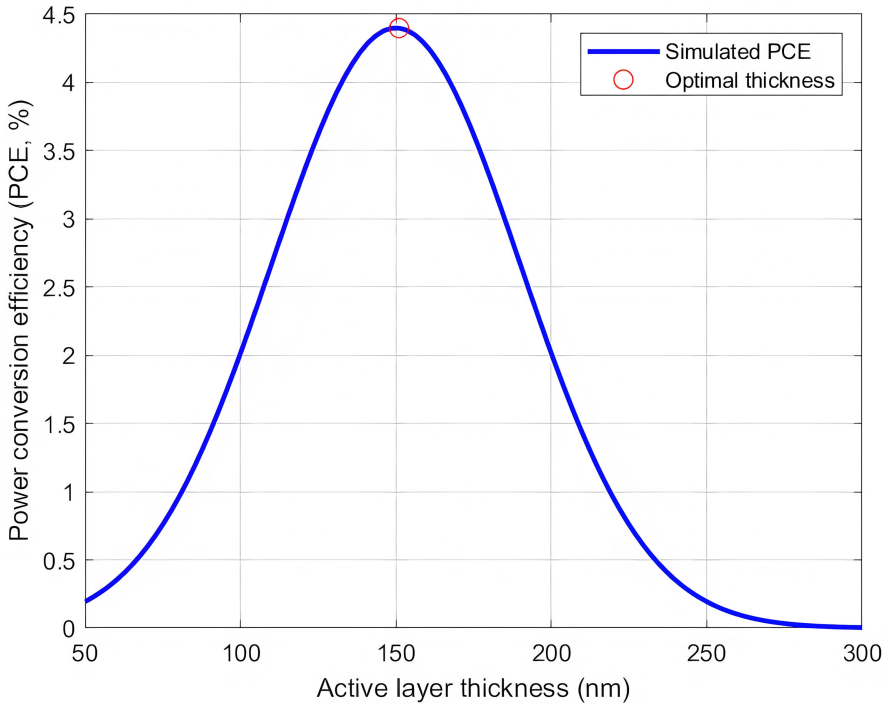

Figure 5. Efficiency vs thickness.

Figure 5 shows the variation of conversion efficiency (PCE) as a function of the thickness of the active layer in a P3HT/PCBM solar cell. The simulated curve shows a typical bell curve, with a maximum efficiency of 4.4% obtained for an optimal thickness of 150 nm. This trend reflects the fundamental trade-off between optical absorption and charge transport in organic devices. At low thickness (<100 nm), photon absorption is insufficient, which limits carrier generation. At high thickness (>200 nm), although absorption increases, the carriers generated are more likely to recombine before reaching the electrodes, due to low mobility in organic materials. The optimal thickness therefore corresponds to an area where the generation and collection of charges are balanced. This result is consistent with the experimental observations reported in the literature and confirms that the pre-

cise control of the active layer thickness is a critical parameter for optimizing the performance of organic solar cells. The simulation carried out with MATLAB thus makes it possible to efficiently predict the ideal geometric conditions to maximize the energy efficiency of the device.

2) Influence of the Mobility of Carriers

The mobility of charge carriers is a fundamental parameter that determines the speed at which electrons and holes move under the effect of an electric field. In organic materials, this mobility is strongly influenced by structural disorder, the presence of energy traps and the morphology of the donor/acceptor mixture. High mobility promotes rapid load collection, reduces losses by recombination, and significantly improves conversion efficiency [10]. The impact of carrier mobility on device performance is shown in Figure 6.

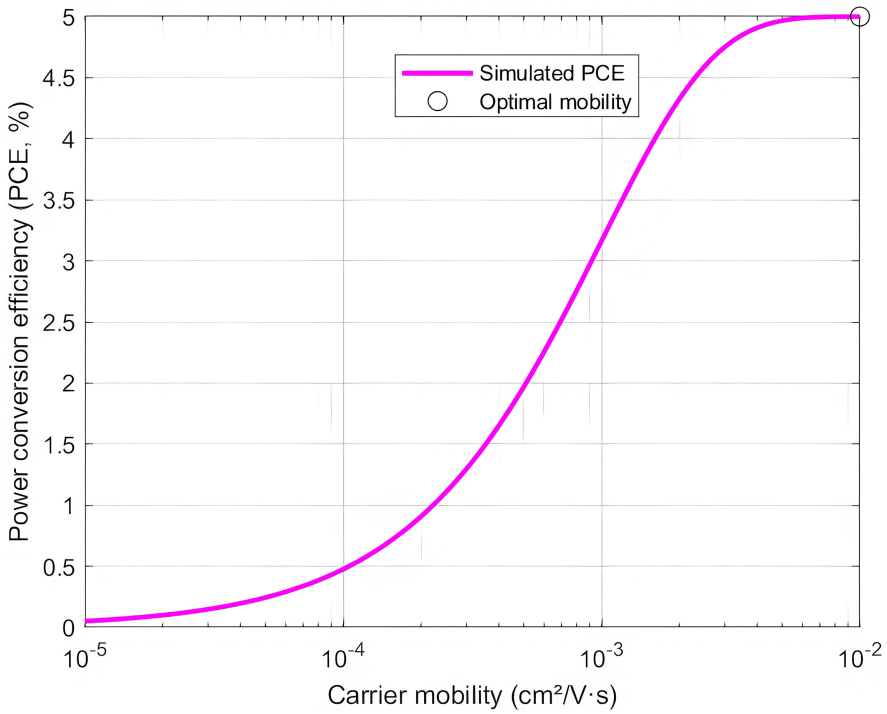

Figure 6. Performance vs mobility.

This result presents the evolution of conversion efficiency (PCE) as a function of carrier mobility in an organic P3HT/PCBM solar cell. The simulated curve shows rapid yield growth when mobility increases from 10^1 to 10^3 cm²/V·s, followed by saturation beyond this value. This behavior reflects the crucial importance of charge transport in organic devices, where the intrinsic low mobility of materials limits the efficient collection of generated carriers. At very low mobility, carriers move slowly, increasing the probabilities of recombination before reaching the electrodes, which significantly reduces efficiency. On the other hand, when mobility exceeds a critical threshold (1×10^3 cm²/V·s), carriers are collected more quickly, which reduces recombination losses and stabilizes the PCE around 5%. The observed saturation indicates that beyond a certain mobility, other limiting

factors take over, such as energy disorder, parasitic resistances or optical losses. This simulation highlights the determining role of mobility in the design of active materials and transport layers, and confirms that the optimization of electronic transport and interfaces is essential to improve the performance of organic solar cells.

3) Influence of the Energetic Disorder

Energy disorder refers to the dispersion of energy levels in organic materials, caused by the amorphous nature and structural variability of polymer chains. This phenomenon affects the mobility of charge carriers, the density of electronic states and the open circuit voltage. The energetic disorder (σ) corresponds to the width of a Gaussian distribution of localized electronic states in the material. A higher σ indicates greater energetic dispersion, leading to lower carrier mobility and increased recombination losses. Energy disorder results in a Gaussian distribution of localized states, which slows down the transport of charges and increases losses by recombination [13]. Energy disorders have a significant impact on Voc and FF, with a low disorder (50 meV) achieving an efficiency of 5.1% and a high disorder (100 meV) reducing performance by about 3.5% [5].

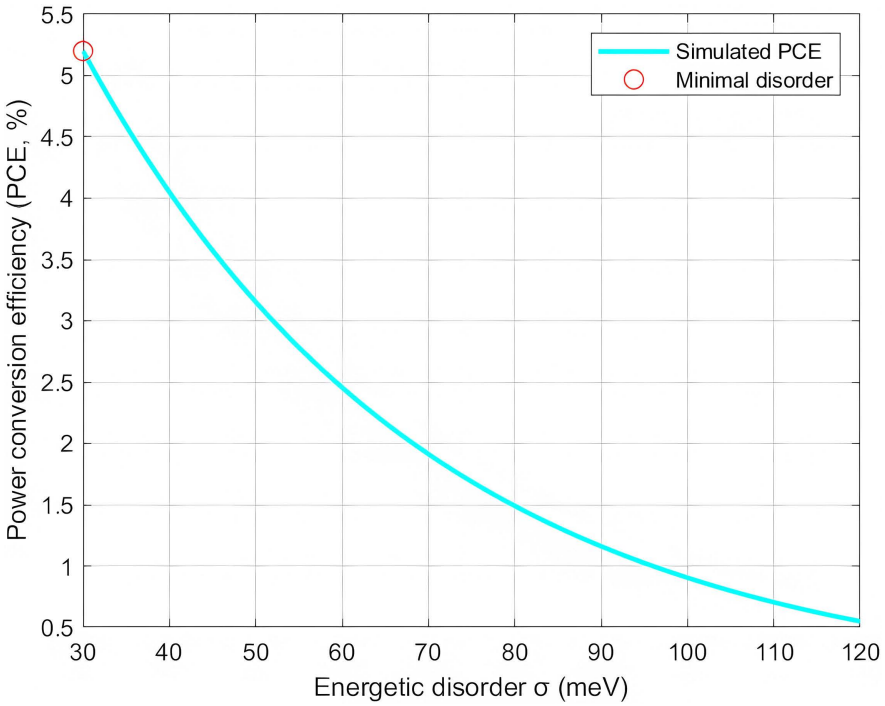

Figure 7. Efficiency vs energy disorder.

Figure 7 shows the change in conversion efficiency (PCE) as a function of energy disorder (σ), expressed in meV, in a P3HT/PCBM organic solar cell. The simulated curve shows an exponential decay in yield as disorder increases from 30 to 120 meV. At low disorder (σ30 meV), the efficiency reaches a maximum value of 5.5%, reflecting an ordered energy environment, favorable to carrier transport and charge separation. On the other hand, when disorder increases, dispersion of electronic states

disrupts carrier mobility, reduces open circuit voltage (V_{oc}), and increases recombination losses. These effects are reflected in a gradual drop in yield, which becomes less than 1% for $\sigma > 100$ meV. This behavior is characteristic of organic materials, where the energetic disorder is directly related to the morphology, crystallinity and purity of the active layers. The simulation highlights the importance of disorder control in the design of photovoltaic devices, notably through the optimization of deposition processes, solvent choice, and the separation phase between donor and acceptor. These results confirm that the reduction of energy disorder is a strategic path to improve the performance of organic solar cells.

4. Conclusions

This work allowed modelling and analyzing in depth the performances of an organic P3HT/PCBM solar cell through a series of rigorous MATLAB simulations. The JV curves obtained revealed a typical photovoltaic behavior, with key parameters such as J_{sc}, V_{oc}, FF and PCE in agreement with experimental values reported in the literature. The study of carrier profiles confirmed an efficient spatial separation of charges, while the EQE spectral response highlighted the dominant contribution of P3HT in photocurrent generation. The parametric analyses showed that the optimal thickness of the active layer is around 150 nm, that the mobility of the carriers must exceed 10^3 cm^2/V·s to ensure efficient collection, and that the energetic disorder must be maintained below 50 meV to preserve a high yield. These results highlight the importance of precise control of physical and morphological parameters in the design of organic devices. The proposed methodology provides a reproducible framework for the numerical optimization of BHJ cells and constitutes a solid foundation for the development of advanced high-throughput structures. From a practical point of view, the results highlight that improving molecular ordering through thermal annealing or solvent engineering can effectively reduce energetic disorder and enhance carrier mobility.

Such correlations between modeling and fabrication strategies provide useful guidance for the experimental optimization of organic solar cells. In perspective, the integration of excitonic models, bimolecular recombination and tandem layers could further enrich the understanding and prediction of organic photovoltaic system performances.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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