

Modeling and Simulation of an Organic Photovoltaic Cell: ITO/MoO₃/CARAPA/PCBM/Alq₃/Al with SCAPS

Donafologo Soro^{1*}, Adama Sylla², Aboudramane Gbané², Bamba Abdoulaye Franck³, Julia Mari Guaita⁴, Amal Bouich⁴, Siaka Toure², Bernabé Marí⁴

¹Département des Sciences et Technologie, Ecole Normale Supérieure (ENS) d'Abidjan, Abidjan, Côte d'Ivoire

²LASMES Laboratory (Laboratory of Material Sciences Environment and Solar Energy), Université FHB D'Abidjan-Cocody, Abidjan, Côte d'Ivoire

³Unité de Formation et de Recherche Sciences Technologiques, Université de Man, Man, Côte d'Ivoire

⁴Departament de Física Aplicada-IDF, Universitat Politècnica de València, València, Spain

Email: donafologosoro@yahoo.fr

How to cite this paper: Soro, D., Sylla, A., Gbané, A., Franck, B.A., Guaita, J.M., Bouich, A., Toure, S. and Marí, B. (2024) Modeling and Simulation of an Organic Photovoltaic Cell: ITO/MoO₃/CARAPA/PCBM/Alq₃/Al with SCAPS. *Modeling and Numerical Simulation of Material Science*, **14**, 79-96.

<https://doi.org/10.4236/mnsms.2024.143005>

Received: June 17, 2024

Accepted: July 28, 2024

Published: July 31, 2024

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Abstract

Renewable energies are of major interest due to their inexhaustible and clean nature, with minimal impact on the environment. Numerous technological pathways exist in this field, each distinguished by the materials used and their implementation principles. However, the cost-efficiency ratio remains a significant challenge for researchers. Currently, organic materials are gaining popularity due to their relatively low cost. However, their performance, particularly in terms of conversion efficiency, still requires improvements. This study focuses on optimizing the organic photovoltaic cell ITO/MoO₃/CARAPA/PCBM/Alq₃/Al using SCAPS. Several parameters were considered, such as layer thickness, recombination center density, and doping, to improve the cell's performance. The optimal parameters obtained include an efficiency of 3%, a fill factor of 81.67%, an open-circuit voltage of 1610 mV, and a short-circuit current of 2.28 mA/cm². The study also revealed that doping the phenyl-C61-butyric acid methyl ester (PCBM) layer has a significant impact on efficiency and short-circuit current, improving these parameters up to a certain point before causing degradation due to increased recombination. Furthermore, high doping of the tri (8-hydroxyquinoline) aluminum (Alq₃) layer improves performance up to a critical threshold, after which degradation is also observed. In contrast, doping the molybdenum trioxide (MoO₃) layer does not have a notable impact on cell performance. Regarding the thickness of the active Carapaprocera (CARAPA) and PCBM layers, non-optimal values lead to a decrease in per-

formance. Similarly, an optimal thickness of the Alq₃ layer significantly improves efficiency. These results highlight the importance of parameter optimization to maximize the efficiency of organic solar cells.

Keywords

Renewable Energie, Solar Cells, Simulation, Organic Materials, Performance

1. Introduction

Energy production constitutes a crucial issue for the coming decades. Indeed, the energy needs of industrialized societies continue to grow unabated, and developing countries will also require increasingly large amounts of energy to support their economic growth. Global energy consumption is constantly increasing. However, fossil resources, such as oil, are limited and will not be able to sustainably meet the world's energy needs. Consequently, the cost of energy is continuously rising, mainly due to increasing demand and the gradual depletion of raw materials [1]. This overconsumption of fossil resources presents another major danger. It alarmingly reduces the reserves available for future generations. Faced with these challenges, states are compelled to seek new methods of energy production and consumption to reduce their dependence on these non-renewable fuels. Furthermore, the massive use of fossil energies significantly contributes to the global warming of our planet due to the greenhouse gas emissions they generate [2]. This dual challenge, of resource depletion and environmental impact, underscores the urgency of transitioning to more sustainable and environmentally friendly energy sources. The consequences of using fossil energies, which result in considerable environmental impacts, impose an urgent search for alternative supply sources. Among the options that meet the criteria of cost, sustainability, and environmental respect, renewable energies stand out as an excellent compromise. These are inexhaustible resources derived from the sun, wind, water falls, earth's heat, and much more. Their exploitation is advantageous as it does not lead to pollutant emissions. Among these renewable energy sources, photovoltaic solar energy, which allows direct conversion of solar radiation into electricity, holds a prominent place in research and has been experiencing significant growth since the 1990s. Research in this field focuses on two main areas: increasing the efficiency of photovoltaic cells and reducing production costs [3]. To ensure the successful development of photovoltaic technologies, a thorough understanding of the materials used in component design is essential. Although currently less efficient in terms of yield compared to inorganic solar cells, organic solar cells offer significant advantages that position them as a promising alternative. Among these advantages are considerably lower production costs, simplified and adaptable manufacturing, and substrate flexibility, which opens the way to diverse and innovative applications, such as integration into textiles or curved surfaces. The intensification of research and innovations in the field of

organic solar cells could quickly make this technology competitive and viable on the market. For instance, studies on heterojunction structures in dye-sensitized solar cells, which are a type of organic cell, have shown yields ranging from 0.001% to 5% [4] [5]. Although these figures are still lower than those of inorganic technologies, they demonstrate significant potential for future improvements.

The main objective of the simulations conducted in this context is to establish precise correlations between the properties of the materials used and the performance of solar cells. This approach aims to optimize yields while reducing production costs. By focusing on optimizing parameters such as the thickness of active layers, defect density, and doping levels, it is possible to improve the conversion efficiency of organic solar cells. Research efforts are focused on identifying material configurations and manufacturing processes that maximize energy efficiency while maintaining low production costs. Organic solar cells also offer a unique opportunity to expand the applications of photovoltaic energy due to their flexibility and potential for integration into diverse and innovative materials. For example, they can be used in portable devices, photovoltaic textiles, or even integrated into building architecture in the form of films or transparent panels. Thus, this research and development approach could lead to significant advances in the field of organic solar cells, transforming an emerging technology into a sustainable and economically viable solution for renewable energy production.

It is in this context that the work of this research is situated, aiming to advance the understanding of materials and develop more efficient and affordable photovoltaic technologies for a cleaner and more sustainable energy future.

2. Theoretical Model

The SCAPS simulator solves the fundamental equations for structures containing up to seven semiconductor layers. It accounts for band-to-band (direct), Auger, and Shockley-Read Hall recombination mechanisms, different defect distributions, the work function of contacts, tunneling effects, and a variety of standard and other spectra (AM0, AM1.5D, AM1.5G). This program calculates energy bands, concentrations, and currents at a given operating point, the J - V characteristics, etc [6]. SCAPS opens with the “Action Panel” that allows various operations to be initiated. It enables the generation of various simulation curves, notably I - V, C - V, C - f curves, as well as the band diagram, carrier densities, and current densities.

The basic parameters used for the simulation of solar cells under irradiation are crucial for evaluating and improving their performance. These parameters include essential characteristics concerning acceptor (A) and donor (D) levels within the various layers of the cell. The acceptor levels (A) refer to electron trapping states that accept electrons, thereby creating holes, while the donor levels (D) refer to states that can donate electrons to the material. In specific layers

of the solar cell, such as the donor and acceptor layers, these levels play fundamental roles in the dynamics of charge generation and transport. **Table 1** provides a summary of the parameters used for the simulation. It presents a clear distinction between these parameters, identifying (A) for acceptor levels and (D) for donor levels. Moreover, it also includes an assessment of the defect levels associated with these states, which can significantly impact the solar cell's efficiency by influencing the recombination mechanisms of charge carriers. Precise identification and quantification of these acceptor and donor levels, as well as their respective defects, are of paramount importance. This allows for a deep understanding of the underlying mechanisms of the solar cell's operation. A detailed comprehension of these levels is essential to analyze the current performance of the cell, identify weak points, and formulate optimization strategies. Additionally, it enables accurate modeling of the cell's behavior under different radiation and environmental conditions, thereby facilitating the design of more efficient solar cells.

Table 1. Parameters used for the simulation.

	Properties of the Different Layers			
	MoO ₃	CARAPA	PCBM	Alq ₃
Epaisseur (μm)	0.100	0.100	1.5	0.050
Eg (eV)	3.0	2.48	2.85	2.80
X (eV)	3.0	3.12	3.4	3.12
S _r	3.5	3.5	3.0	3.0
N _c (cm ⁻³)	1.000E + 22	1.000E + 19	1.000E + 22	1.000E + 22
N _v (cm ⁻³)	1.000E + 22	1.000E + 19	1.000E + 22	1.000E + 22
S ^p , S ⁿ (cm/s)	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7
th	th	th	th	th
μ _n (cm ² /Vs)	1.620E + 1	2.000E-1	1.000E-3	1.400E-5
μ _p (cm ² /Vs)	1.620E + 0	2.000E-2	1.000E-4	2.000E-7
Doping (cm ⁻³)	1.000E + 20 (A)	1.000E + 20 (A)	2.000E + 15 (D)	1.000E + 16 (D)
Properties of Bulk Defects (Gaussian Distribution)				
N _t (cm ⁻³)	1.000E + 10 (D)	1.000E + 10 (D)	1.000E + 6 (A)	1.000E + 10 (A)
Mid-bandgap				
WGD/WDA (eV)	0.010	0.010	0.010	0.010
EGD/EGA (eV)	1.500	1.240	1.425	1.400
σ _n (Cm ²)	5.000E-13	5.000E-13	1.000E-15	1.000E-15
σ _p (Cm ²)	1.000E-15	1.000E-15	5.000E-13	5.000E-13
References				
	[11]	[12] [13]	[7] [8]	[9] [10]

3. Structure of the Organic Photovoltaic Cell

The chosen structure is a bilayer (or heterojunction) donor-acceptor (D-A) organic photovoltaic cell. This design helps to overcome some issues encountered with the Schottky structure (semiconductor/metal). Indeed, a D-A junction can be illuminated from either the ITO side or the metal side, especially if the layers are very thin. In practice, illumination is done from the ITO side, which trans-

mits nearly 80% of the light. **Figure 1** shows the structure of the simulated organic photovoltaic cell of type ITO/MoO₃/CARAPA/PCBM/Alq₃.

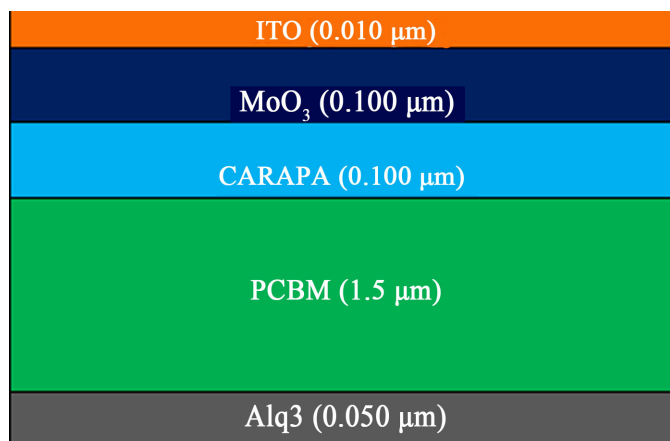


Figure 1. Structure of the organic photovoltaic cell.

4. Result and Discussion

4.1. Effect of Doping on CARAPA and PCBM Layers

Doping is a physical process that alters the intrinsic properties of a material by introducing specific impurities. We studied the impact of varying doping levels on the performance of different layers in the solar cell. The results obtained are illustrated in **Figure 2**, which shows the effect of doping on the CARAPA and PCBM layers. It indicates that the acceptor material, PCBM, can be lightly doped without significantly affecting the conversion efficiency. The efficiency remains nearly constant around 3% for doping levels ranging from 10^{13} cm^{-3} to 10^{16} cm^{-3} . At these doping levels, we achieved a fill factor of 81.3%, an open-circuit voltage of 1612.9 mV, and a short-circuit current of 2.28 mA/cm^2 . However, for doping levels exceeding 10^{17} cm^{-3} , a rapid decrease in short-circuit current is observed, accompanied by a decline in conversion efficiency, while the open-circuit voltage decreases more gradually. This efficiency decrease is attributed to increased recombination rates as dopant concentration increases in the PCBM layer, which acts as the electron acceptor layer [14]. These observations align with findings from other similar studies [15]. Regarding the CARAPA layer, the conversion efficiency varies slightly from 2.97% for doping at 10^{15} cm^{-3} to 3% at 10^{20} cm^{-3} , with a minimum of 2.87% at 10^{18} cm^{-3} . Thus, the extreme values of efficiency are comparable, suggesting that doping in the CARAPA layer can be reduced without compromising cell performance. The fill factor shows a similar trend to efficiency, ranging from 80% to 81.5% with a minimum of 77.3%. The short-circuit current remains nearly constant for all doping levels, while the open-circuit voltage decreases beyond doping levels of 10^{18} cm^{-3} . The open-circuit voltage (V_{oc}) depends on the Highest Occupied Molecular Orbital (HOMO) level of the electron-donating material and the Lowest Unoccupied Molecular Orbital (LUMO) level of the electron-accepting material [16]. Theoretically, V_{oc} is determined by

the difference between these energy levels. Therefore, an increase in dopant concentration in the donor material raises its HOMO level, leading to a reduction in open-circuit voltage V_{oc} [17].

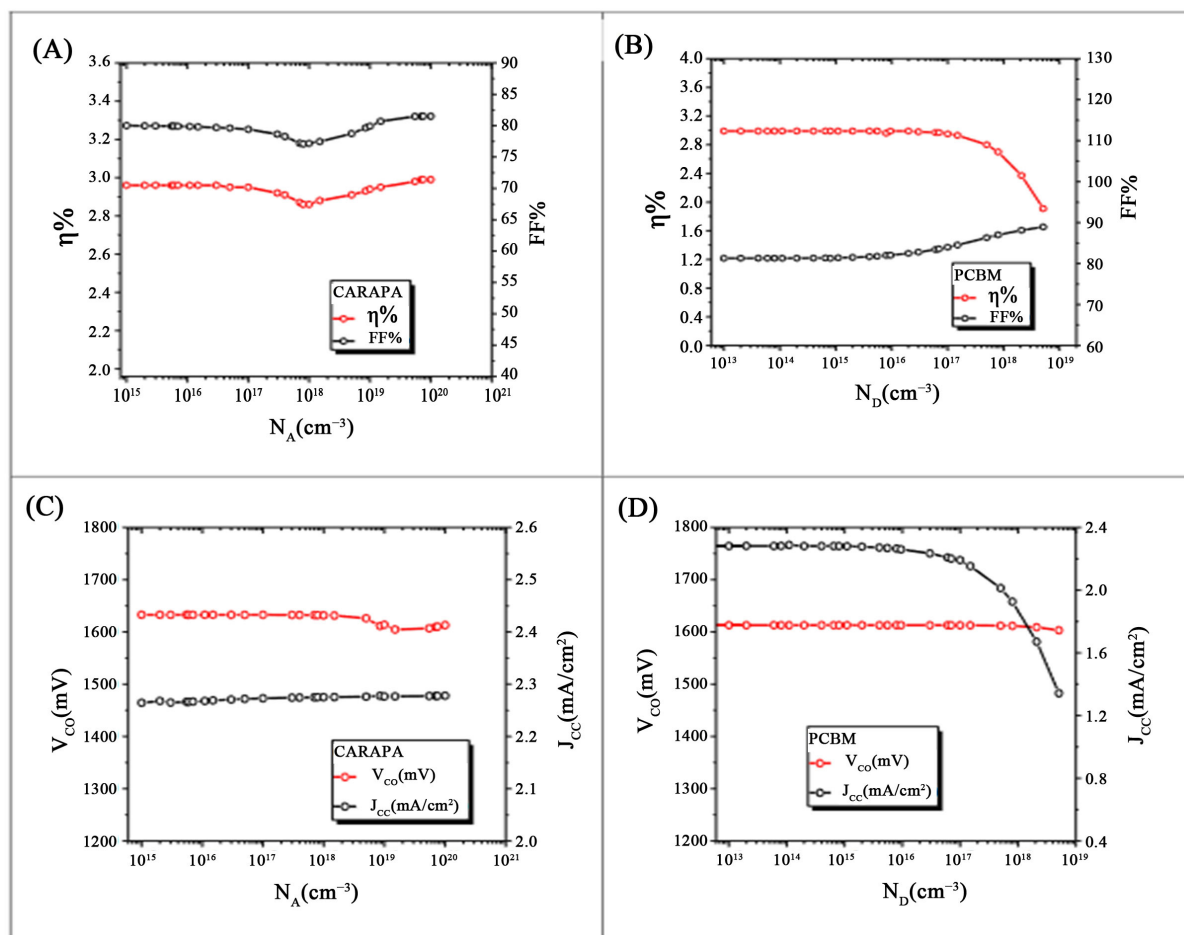


Figure 2. Efficiency and fill factor of the cell as a function of doping in CARAPA and PCBM layers: (A), (B) efficiency and fill factor. (C), (D) open-circuit voltage and short-circuit current.

4.2. Impact of Doping on the MoO_3 Layer

The study of doping effects on different layers of the solar cell revealed that the MoO_3 (molybdenum trioxide) layer exhibits a certain stability against doping variations. As illustrated in **Figure 3**, the characteristic parameters of the solar cell, such as conversion efficiency, open-circuit voltage (V_{oc}), and short-circuit current, do not undergo significant changes when the doping level of the MoO_3 layer is altered. This stability can be attributed to the inherent properties of MoO_3 , which often serves as a Hole Transport Layer (HTL) in photovoltaic devices, facilitating efficient hole transport without significantly contributing to recombination processes [18].

4.3. Impact of Doping on the Alq_3 Layer

In contrast, the Alq_3 (tris (8-hydroxyquinolino) aluminum) layer, used as an

Electron Transport Layer (ETL), shows increased sensitivity to doping. As shown in **Figure 3**, doping of the Alq₃ layer significantly influences the performance of the solar cell. Specifically, beyond a concentration of 10¹⁷ cm⁻³, increasing the doping level leads to a rapid improvement in the conversion efficiency of the solar cell. This improvement can be attributed to increased electrical conductivity of the Alq₃ layer, thereby facilitating electron collection and reducing the device's series resistance. However, it is important to note that excessive doping of the Alq₃ layer carries risks. A high concentration of dopants can increase the rates of charge carrier recombination, paradoxically reducing the overall efficiency of the solar cell. Indeed, a high dopant concentration creates recombination sites within the Alq₃ layer, where electrons and holes can recombine before reaching the electrodes, thereby reducing the short-circuit current and conversion efficiency.

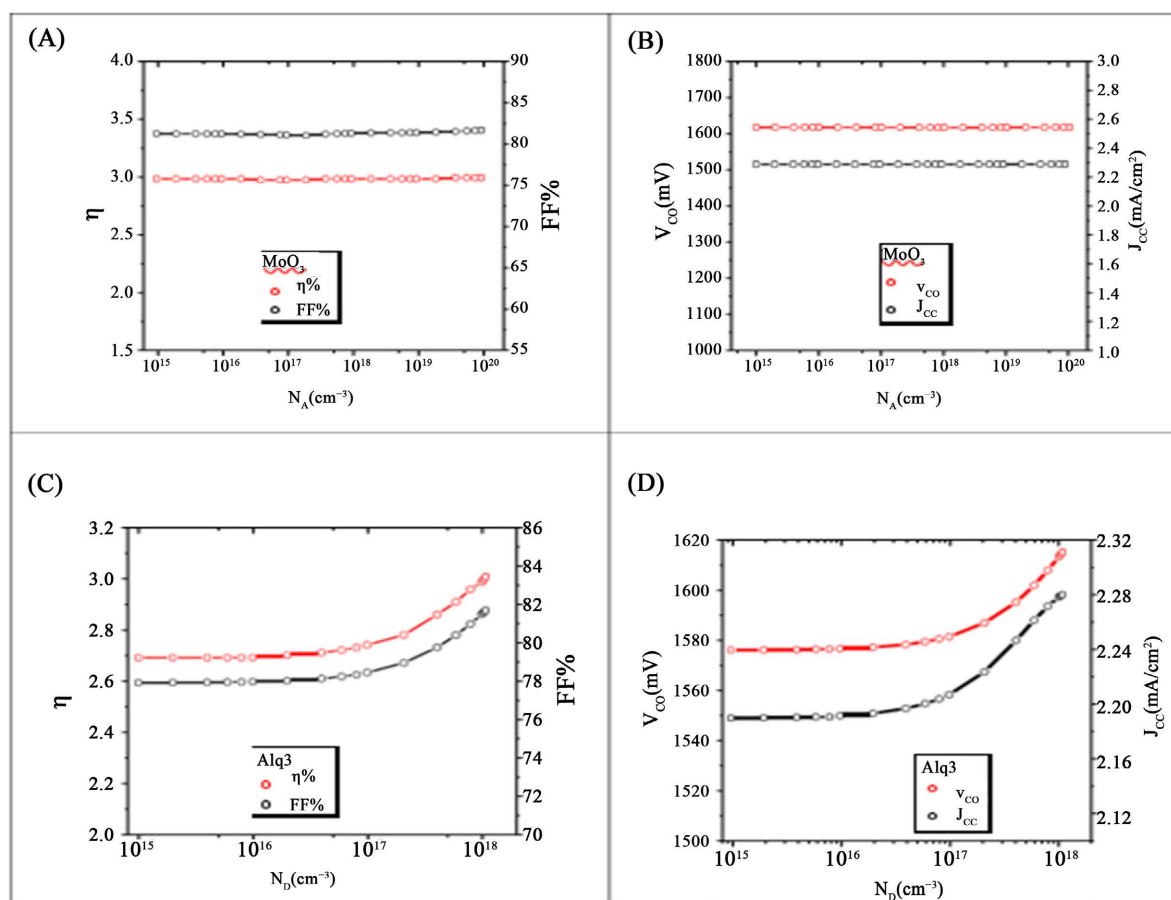


Figure 3. Efficiency and fill factor of the cell as a function of doping in MoO₃ and Alq₃ layers: (A), (B) efficiency and fill factor. (C), (D) open-circuit voltage and short-circuit current.

4.4. Role of the Alq₃ Layer

One of the key roles of the Alq₃ (tris (8-hydroxyquinolino) aluminum) layer in the structure of the solar cell is to facilitate electron collection by the back contact, typically composed of a metallic material such as aluminum. Alq₃ acts as a

buffer layer, enhancing compatibility between the active layers of the solar cell and the back contact. This layer also plays a crucial role in contributing to the formation of an ohmic contact at the interface, enabling efficient extraction of charge carriers without creating significant potential barriers. An ohmic contact is essential to minimize losses due to resistance at the contacts, thereby improving the overall efficiency of the solar cell. In conclusion, the analysis of doping in the MoO₃ and Alq₃ layers highlights distinct behaviors: while the MoO₃ layer remains stable and relatively unaffected by doping, the Alq₃ layer exhibits increased sensitivity, where fine optimization of the doping level is necessary to maximize efficiency without inducing recombination losses. These findings provide valuable insights for the development of more efficient solar cells and underscore the importance of precise management of doping levels in different layers of photovoltaic devices.

4.5. Effect of CARAPA and PCBM Active Layer Thicknesses

The impact of active layer thickness in an organic solar cell is a crucial factor that directly influences device conversion performance. In this section, we analyze how variations in the thicknesses of CARAPA and PCBM layers affect the performance parameters of the solar cell.

4.5.1. Impact of the Thickness of the CARAPA Layer

Figure 4 illustrates the effect of CARAPA layer thickness on various performance parameters of the solar cell. CARAPA, as a donor layer, plays a fundamental role in the generation and dissociation of excitons (bonded electron-hole pairs). Observations show that the thickness of this layer has no significant impact on the form factor (FF) and the short-circuit current (J_{sc}), which remain almost constant at around 81.7% and 2.8 mA/cm² respectively. These parameters are essential because the form factor measures how efficiently a solar cell converts light energy into electricity, and the short-circuit current represents the maximum flow of current generated by the cell under illumination. However, the open circuit voltage (V_{oc}) decreases with increasing thickness of the CARAPA layer. This reduction in V_{oc} leads to a reduction in conversion efficiency. The best conversion performance, with an efficiency of 3%, is obtained for a thickness less than 0.1 μm, accompanied by an open circuit voltage of 1613 mV. This relationship indicates that to optimize cell performance, the thickness of the CARAPA layer must be kept low, thus promoting better exciton dissociation and reduced recombination.

4.5.2. Impact of PCBM Layer Thickness

The PCBM layer, serving as the acceptor layer, plays a crucial role in collecting electrons generated by light absorption. Analysis shows that the thickness of the PCBM layer significantly influences the performance of the solar cell. As the thickness of this layer increases, the fill factor varies and the open-circuit voltage decreases slowly. In contrast, the short-circuit current decreases rapidly with in-

creasing thickness, reaching a maximum for a thickness of $0.1 \mu\text{m}$. This rapid decrease in J_{sc} with increasing PCBM layer thickness is problematic because the overall efficiency of the solar cell closely follows the short-circuit current evolution. The explanation for this phenomenon lies in the dynamics of electron-hole pair recombination. As the thickness of the PCBM layer increases, excitons must travel a longer distance to reach the region where they become majority carriers, thereby increasing the probability of recombination before reaching the junction. Indeed, increased thickness forces excitons to undergo multiple hops before being dissociated into free charges, which enhances recombination losses and reduces charge collection efficiency. This dynamic leads to a decrease in solar cell performance, despite an initial increase in efficiency for optimal thicknesses. In summary, the thickness of the CARAPA and PCBM active layers must be carefully optimized to maximize solar cell performance. Excessive thickness of the donor or acceptor layer can lead to significant losses due to charge carrier recombination, thereby reducing the overall efficiency of converting light energy into electricity. These findings underscore the importance of precise thickness management for the development of more efficient and sustainable solar cells.

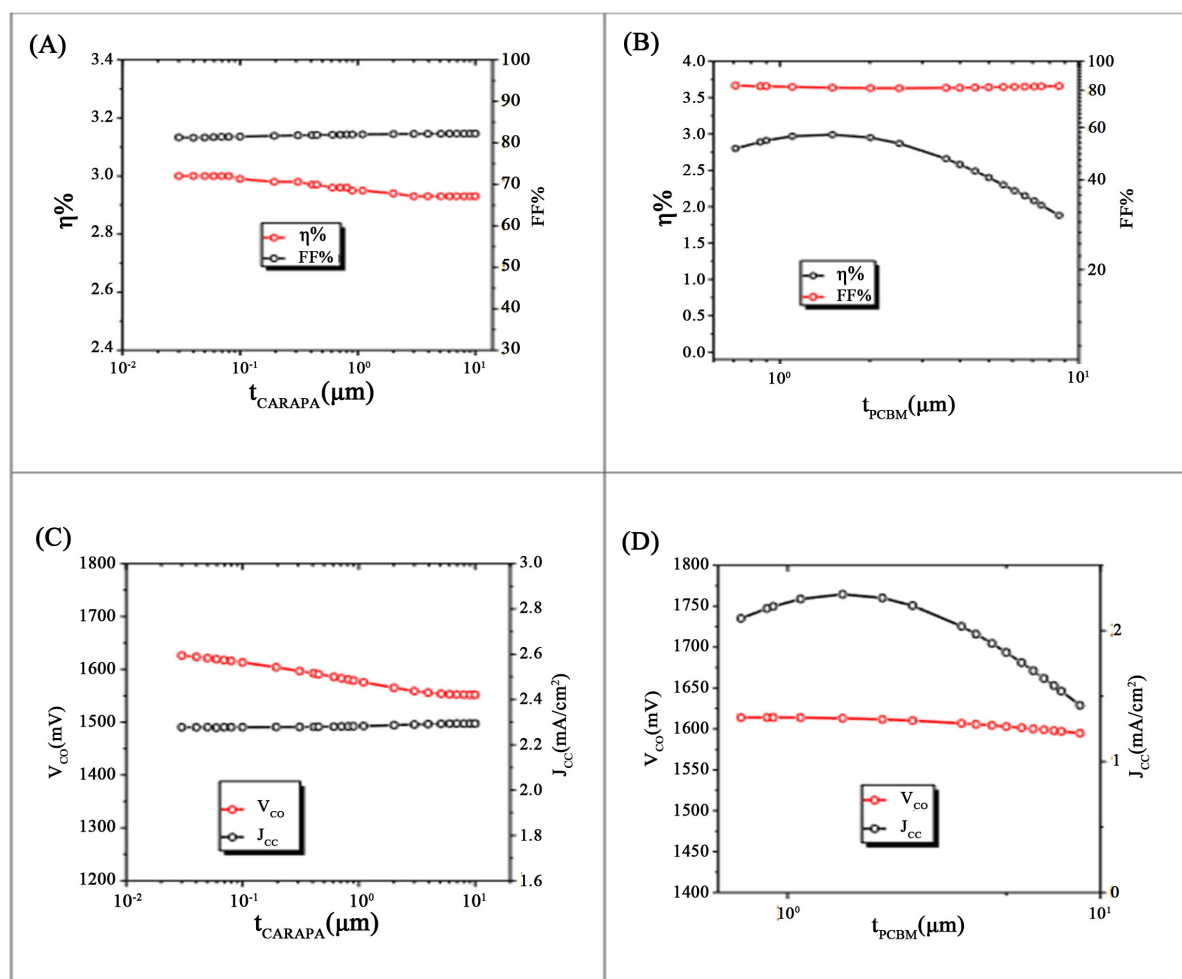


Figure 4. Efficiency and fill factor as a function of thickness of different layers PCBM (A), (C) CARAPA (B), (D).

4.6. Effect of MoO₃ and Alq₃ Layer Thickness

The thickness of MoO₃ and Alq₃ layers plays a crucial role in the overall performance of organic photovoltaic cells. These layers, acting as buffer layers and essential interfaces within the cell structure, directly influence the mechanisms of charge carrier collection and transport. **Figure 5** illustrates the impact of the thickness of these layers on the energy conversion efficiency of the solar cell.

4.6.1. Effect of MoO₃ Layer Thickness

The MoO₃ layer, typically used as a hole transport layer (HTL) or anodic buffer layer, is essential for facilitating the collection of holes (positive charge carriers) at the anode. However, simulations and experiments indicate that the thickness of the MoO₃ layer has no significant effect on the performance parameters of the solar cell. This lack of variability can be attributed to the primary function of the MoO₃ layer, which is to provide an adequate potential barrier for holes while minimizing losses due to recombination at the anode/active layer interface. The stability of performance despite thickness variations suggests that the MoO₃ layer is effective over a relatively wide range of thicknesses in ensuring efficient hole collection without compromising charge transport to the anode.

4.6.2. Effect of Alq₃ Layer Thickness

Unlike the MoO₃ layer, the thickness of the Tris (8-hydroxyquinolino) aluminum (Alq₃) layer, acting as a cathodic buffer and electron transport layer (ETL), shows a notable effect on the performance of the solar cell. Alq₃ is crucial for facilitating electron collection at the cathode and ensuring efficient ohmic contact, thereby minimizing contact losses. The results illustrated in **Figure 5** demonstrate that increasing the thickness of the Alq₃ layer improves the energy conversion efficiency up to an optimal thickness. Specifically, the cell efficiency increases with the thickness of the Alq₃ layer, reaching a maximum of 3% for a thickness of approximately 50 nm. This improvement is likely due to optimized electron collection and reduced non-radiative recombinations, allowing better charge carrier separation and an increase in short-circuit current density (J_{sc}). Beyond this optimal thickness of 50 nm, further increases in the Alq₃ layer thickness lead to a gradual decrease in the solar cell efficiency. This decline in performance can be attributed to several factors including increased charge losses, enhanced recombination, and imbalance in charge collection. Excessive thickness of the Alq₃ layer may introduce additional losses due to increased electrical resistance, hindering electron transport to the cathode. A thicker layer can promote recombination of electrons and holes before they are collected at their respective contacts, thereby reducing the overall efficiency of the cell. Excessive thickness of the Alq₃ layer may create an imbalance between electron and hole collection, disrupting energy level alignment and charge transport processes. These observations underscore the crucial importance of optimizing the Alq₃ layer thickness to maximize solar cell efficiency. Well-balanced thickness minimizes recombination and ensures efficient charge transport, contributing to high and stable pho-

to voltaic cell performance. In summary, the study of MoO₃ and Alq₃ layer thickness highlights the importance of engineering intermediate layers to enhance the performance of organic solar cells. While the MoO₃ layer demonstrates tolerance to thickness variations without significant impact, the Alq₃ layer requires precise optimization to achieve maximum performance, illustrating the complexity and necessity of careful design in photovoltaic device engineering for efficient energy conversion.

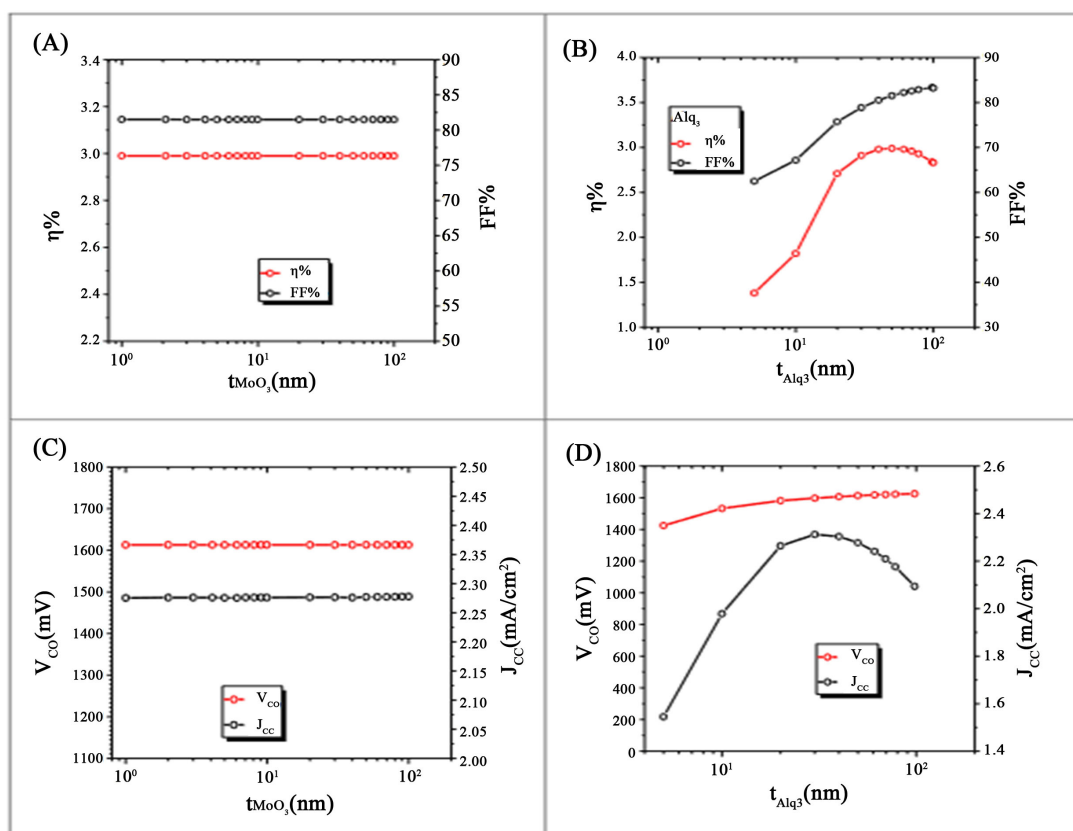


Figure 5. Open circuit voltage (V_{oc}) and short circuit current density (J_{sc}) as a function of layer thickness: Alq₃ (B), (D), MoO₃ (A), (C).

4.7. Impact of Defect Density in Active Layers CARAPA and PCBM

The efficiency of organic photovoltaic cells is closely linked to the quality of the materials used, particularly the defect density in the active layers. **Figures 6-7** illustrate how defect density influences solar cell performance in terms of short-circuit current (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and overall efficiency.

4.7.1. Effect of CARAPA Layer Thickness on Short-Circuit Current

For the CARAPA layer, our simulations show that the short-circuit current (J_{sc}) remains relatively constant despite variations in thickness. The J_{sc} value is approximately 2.28 mA/cm². This constancy suggests that the CARAPA layer is less sensitive to thickness variations in terms of charge collection. This can be

attributed to a low defect density, enabling efficient collection of charge carriers even when thickness varies.

4.7.2. Effect of PCBM Layer Thickness on Short-Circuit Current

In contrast, the thickness of the PCBM layer has a significant impact on the short-circuit current (J_{sc}). J_{sc} decreases significantly from 2.8 mA/cm² to 0.97 mA/cm² as the thickness increases. This marked decrease indicates that defects or traps within the PCBM layer hinder charge collection, thereby increasing non-radiative recombination of carriers. This results in reduced cell efficiency, as carriers generated by light do not effectively reach the cell contacts.

4.7.3. Influence of Trap Density

Trap density plays a crucial role in the performance of organic photovoltaic cells. For trap densities below 10⁹ cm⁻³, the characteristic parameters of solar cells such as efficiency, open-circuit voltage (V_{oc}), and fill factor (FF) remain relatively stable, regardless of the thickness of the active layers. This indicates efficient charge carrier collection and minimized recombination even with thickness variations. Beyond this critical trap density of 10⁹ cm⁻³, cell performance starts to degrade rapidly. The efficiency of photovoltaic cells decreases significantly: for PCBM, efficiency drops from 3% to 0.74%, while for CARAPA, it decreases from 3% to 2.35%. This decline is attributed to increased recombination in thicker active layers and a higher density of traps that capture charge carriers. Regarding open-circuit voltage (V_{oc}), for the PCBM layer, it decreases from 1612.9 mV to 1506.3 mV. Similarly, for the CARAPA layer, V_{oc} decreases from 1634 mV to 1237.7 mV. This reduction in V_{oc} indicates reduced charge separation efficiency and increased recombination, limiting the electric potential difference the cell can generate. Finally, the fill factor (FF), which reflects the quality of the I-V curve of the cell, also decreases with increased thickness and trap density. For PCBM, FF shows a drastic drop from 81.7% to 12.45%, whereas for CARAPA, FF initially increases slightly to 82.5% before decreasing to 80.3%. These variations indicate that while CARAPA is less sensitive to thickness variations, overall material quality remains a crucial factor for cell efficiency. These trends were expected, as increased trap density and thickness of active layers intensify non-radiative recombination processes, thereby reducing solar cell efficiency. The simulations conducted align well with observed behaviors in real devices, confirming the validity of our approach. In the case of PCBM, an increase in thickness and trap density results in a substantial reduction in charge collection, thereby decreasing efficiency from 3% to 0.74%. This reduction is largely due to increased recombination in the thicker active layer, hindering a significant fraction of charge carriers from contributing to electrical current. For CARAPA, although efficiency also decreases from 3% to 2.35% and V_{oc} drops from 1634 mV to 1237.7 mV, the decline is less pronounced compared to PCBM. This observation can be explained by lower sensitivity to defects and more effective charge separation in the CARAPA layer. The fill factor (FF) similarly shows variations, reflecting the impact of material quality on overall cell performance.

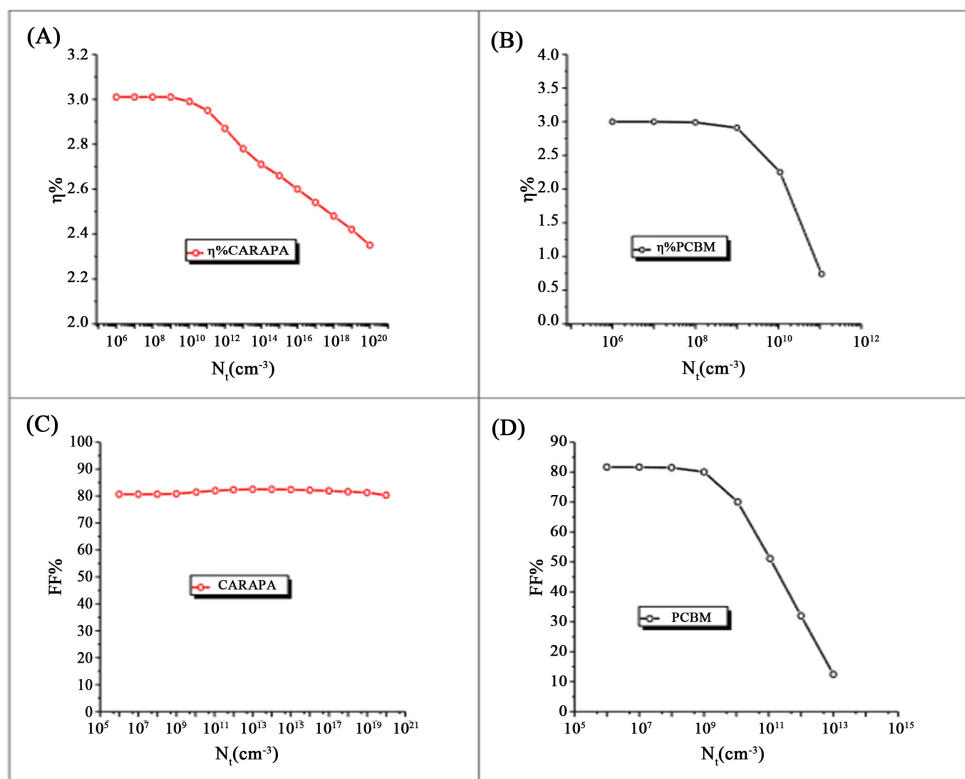


Figure 6. (A), (B) Efficiency and (C), (D) fill factor as a function of the thickness of the active layers CARAPA and PCBM.

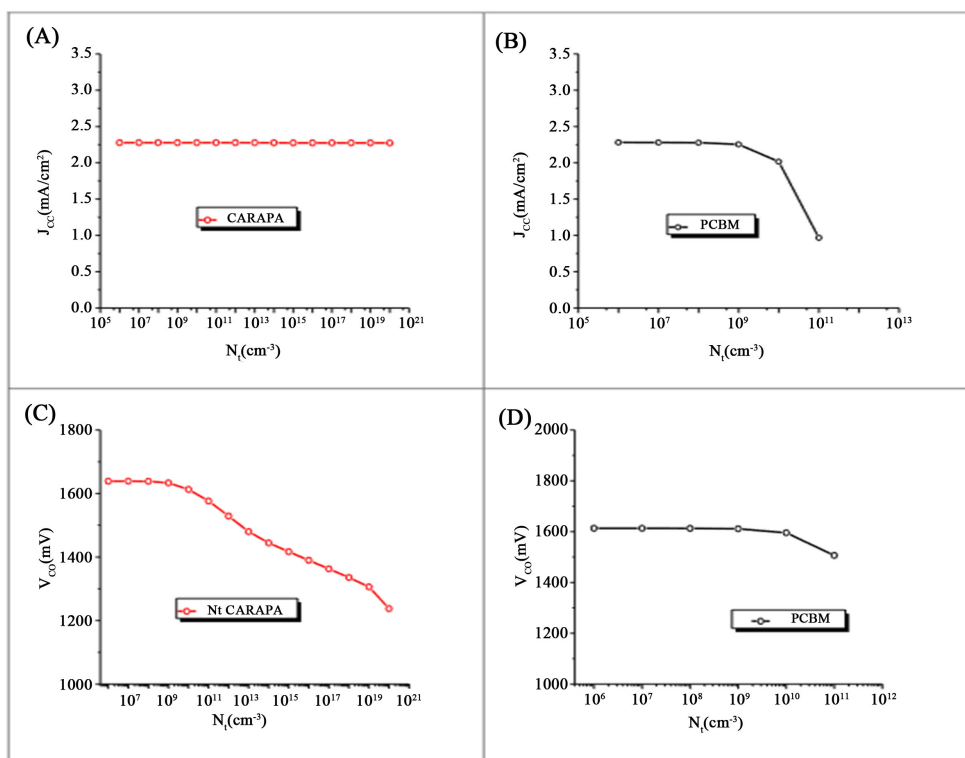


Figure 7. (A), (B) Short-circuit current and (C), (D) open-circuit voltage as a function of the thickness of the active layers CARAPA and PCBM.

4.8. Influence of Defect Density in MoO₃ and Alq₃ Layers

The study of defect density in the materials layers used in organic photovoltaic cells is crucial for understanding and optimizing their performance. **Figures 8** and **9** depict the effects of defect density on the electrical characteristics and efficiency of the solar cell, specifically in the MoO₃ (molybdenum trioxide) and Alq₃ (tris (8-hydroxyquinolino) aluminum) layers.

4.8.1. Effects on MoO₃ Layer

The MoO₃ layer serves as a window or buffer layer in the photovoltaic cell, facilitating charge carrier transport while minimizing non-radiative recombination. **Figure 8** shows that the thickness of this layer does not significantly impact the fill factor (FF) and short-circuit current (J_{sc}), which remain relatively stable. These parameters exhibit negligible variations, with the short-circuit current around 2.3 mA/cm² and a fill factor of approximately 81.7%. However, defect density within this layer has a notable effect on other essential parameters. When the defect density in the MoO₃ layer exceeds 10¹² cm⁻³, a degradation in cell performance is observed. The Open-Circuit Voltage (V_{oc}) decreases from 1610.3 mV to 1469.6 mV. This reduction can be attributed to increased non-radiative recombination within the MoO₃ layer, limiting the potential difference generated by the cell. An increased defect density acts as recombination centers, reducing charge separation efficiency and consequently V_{oc}. Similarly, the solar cell efficiency decreases from 3% to 2.75%. This decline is primarily due to the decrease in V_{oc} and increased energy losses caused by recombination. A high defect density leads to decreased efficiency in converting photons into usable charges, thereby reducing overall efficiency. These results highlight the importance of controlling defect density in the MoO₃ layer to maintain high solar cell performance.

4.8.2. Effects on Alq₃ Layer

The Alq₃ layer serves as an electron transport and collection layer, playing a crucial role in efficiently extracting charge carriers from the cell. **Figure 9** shows that defect density within this layer significantly impacts key parameters of the photovoltaic cell. When the defect density exceeds 10⁹ cm⁻³, the efficiency drops drastically from 3.05% to 1.89%. This decline is attributed to increased carrier recombination within the Alq₃ layer, reducing charge collection efficiency and increasing energy losses. A high defect density creates trapping centers for charge carriers, preventing a significant portion of electrons and holes from contributing to the output current. The fill factor (FF) decreases significantly, dropping from 81.9% to 67.13%. A decrease in FF indicates a deterioration in the I - V curve of the cell, signaling increased resistive losses and recombination. This degradation shows that defects in the Alq₃ layer negatively impact interface quality and contact rectification, reducing cell efficiency. The short-circuit current also decreases from 2.30 mA/cm² to 1.72 mA/cm². This decrease is due to reduced collection of light-generated charge carriers. Defects act as recombina-

tion sites, reducing carrier mobility and lifetime, thereby limiting the amount of current available at the cell interface. Unlike the MoO₃ layer, the Voc in the Alq₃ layer slightly increases from 1612 mV to 1642 mV with increased defect density. This increase may seem counterintuitive but could be related to a reduction in radiative recombination in the layer, leading to an increase in potential difference. However, this improvement in Voc does not offset other performance losses caused by defects.

4.8.3. Analysis and Implications

These results clearly show that defect density in the MoO₃ and Alq₃ layers has differentiated impacts on the performance of organic photovoltaic cells. While the MoO₃ layer exhibits moderate sensitivity to defects, the Alq₃ layer is much more affected by variations in defect density, resulting in significant decreases in efficiency, fill factor, and short-circuit current.

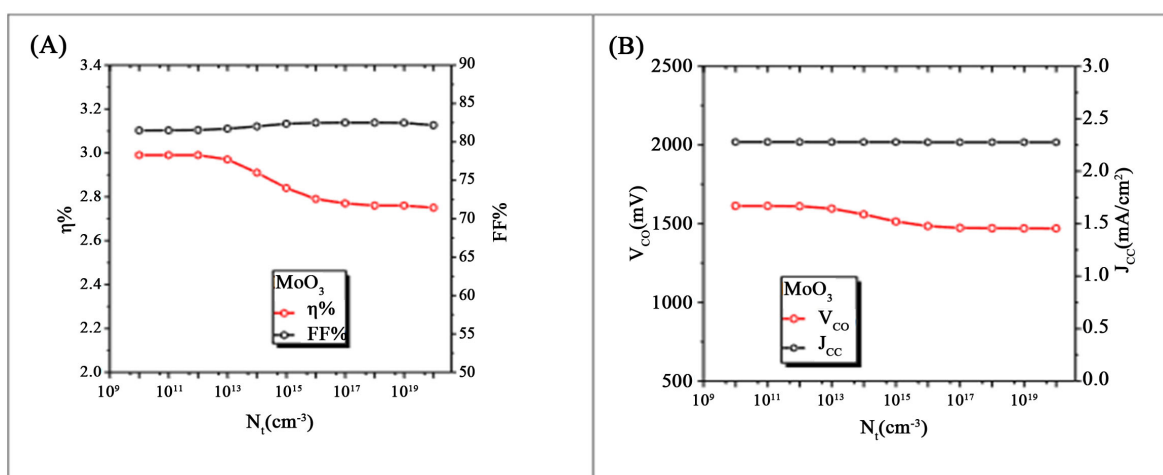


Figure 8. J-V characteristics of the MoO₃ layer as a function of recombination center concentration: Efficiency (η), Fill Factor (FF) (A), Voc, Jcc (B).

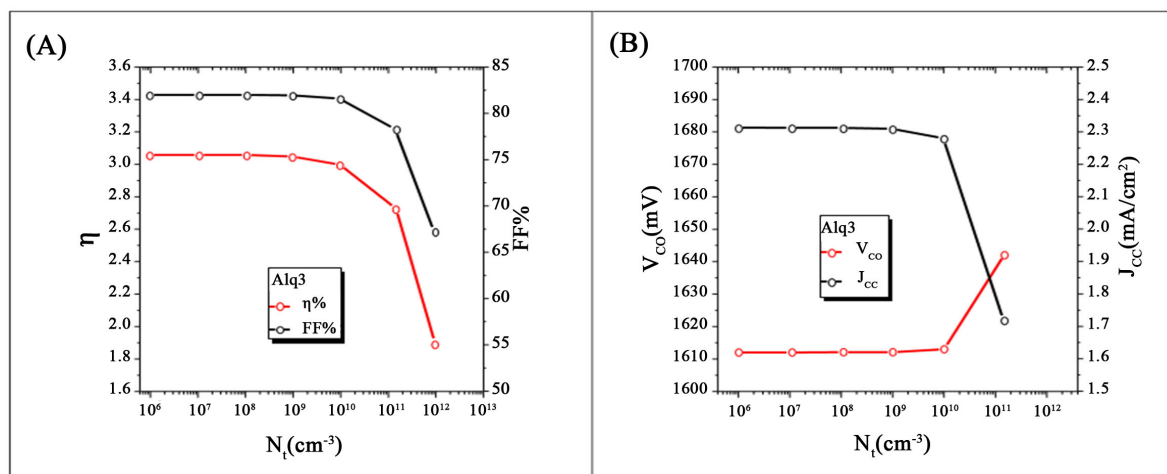


Figure 9. J-V characteristics of the Alq₃ layer as a Function of recombination center concentration: Efficiency (η), Fill Factor (FF) (A), Voc, Jcc (B).

4.8.4. Essential Characteristic Parameters of this Cell

We initiated our study by optimizing the performance of the organic photovoltaic cell. Detailed calculations allowed us to determine the essential characteristic parameters of this cell, namely: short-circuit current density (J_{cc}), fill factor (FF), open-circuit voltage (V_{oc}), and conversion efficiency (η). These parameters are crucial for evaluating the overall efficiency of the cell in converting light energy into electricity. The short-circuit current density (J_{cc}) measures the cell's ability to generate current under illumination, while the fill factor (FF) indicates the quality of the cell's current-voltage characteristic curve. The open-circuit voltage (V_{oc}) signifies the maximum potential the cell can reach in the absence of current, reflecting the efficiency of separating photo-generated charges. Finally, the conversion efficiency (η) expresses the percentage of light energy converted into electrical energy, providing a direct measure of the cell's effectiveness. These parameters are summarized in **Table 2**, illustrating the optimal performances achieved for this organic photovoltaic cell, thereby offering a comprehensive framework for the assessment and improvement of future solar devices.

Table 2. Characteristic parameters of optimized solar cell.

Cell Parameters	Simulation Results
Open-circuit voltage (V_{oc})	1,61 V
Short-circuit current density (J_{sc})	2,28 mA/Cm²
Fill factor (FF)	81,67%
Conversion efficiency (η)	3%

5. Conclusion

In this paper, we conducted a comprehensive optimization of an organic photovoltaic cell by analyzing various parameters to maximize their performance. The optimal parameters obtained are a efficiency of 3%, a fill factor of 81.67%, an open-circuit voltage of 1610 mV, and a short-circuit current of 2.28 mA/cm². The study revealed that doping of the PCBM layer significantly influences efficiency and short-circuit current, whereas high doping of the Alq₃ layer improves performance up to a threshold before causing degradation. In contrast, doping of the MoO₃ layer has no notable impact. The thickness of the CARAPA and PCBM active layers showed that non-optimal values degrade performance, whereas only the optimal thickness of the Alq₃ layer enhances efficiency. Finally, a high density of defects in the active layers and the MoO₃ layer leads to a decline in performance, while for the Alq₃ layer, a defect density exceeding 10⁹ cm⁻³ results in a rapid reduction in efficiency and other key parameters. This study underscores the importance of precise control over parameters to develop more efficient and durable solar cells.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this pa-

per.

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