



Article Performance Evaluation of Modified Zinc-Phthalocyanine Groups as an Active Material in Dye-Sensitized Solar Cells

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Abstract: The increasing demand for energy and electricity and the depletion of fossil fuels are global problems. In recent years, dye-sensitized solar cell (DSSC) technologies have gained notoriety for their application in solar energy. DSSCs are considered a promising alternative renewable energy source to both inorganic and organic photovoltaic (PV) cells. Many types of dyes are being investigated to enhance the light-harvesting properties of DSSCs, but the actual realization of these absorbers in cell structure requires optimum parameters. The main aim of this study was to simulate proposed zinc phthalocyanine (ZnPC)-based structures to validate their design, assess their performance for commercial implementation, and optimize the cell parameters for optimum efficiency. To that end, Scaps-1D was employed to evaluate the performance of DSSCs to determine their optimum parameters. We found that ZnPC and isopropoxy ZnPC molecules outperform others molecules because of better optoelectronic properties. Several other parametric effects, such as photoactive layer thicknesses, doping densities, trap densities, and charge carrier mobilities, were also evaluated to observe their impact on device performance. The results show that moderate thickness, low defect density, moderate doping, and charge carrier mobility are favorable for better device performance due to low recombination losses, electrical losses, and better transport of charge carriers. The utmost power conversion efficiency values found for ZnPC- and ZnPC: PC70BM-based DSSCs after optimization were 9.50% and 9.81%. This paper also suggests a practical method for efficiently using DSSC cells by modifying factors that are significantly reliant on DSSC performance and output.

Keywords: solar cell; dye-sensitized; electrical modeling; DSSC; PCE; zinc phthalocyanine

1. Introduction

Dye-sensitized solar cells (DSSCs) have emerged as the vanguard of the photovoltaic (PV) industry, heralding a new era of more efficient and cost-effective solar energy. Due to their impressive capacity for high efficiencies and use of readily available materials, DSSCs have gained widespread acknowledgment as a viable substitute for traditional silicon solar cells. They possess the inherent qualities necessary to supersede their first-generation counterparts [1–3]. Over the past decade, the allure of DSSCs has captivated the imagination of researchers and engineers alike, fueling an unprecedented surge of interest. The multifaceted applications that can be derived from this innovative energy source have been a driving force behind this fervor. DSSCs possess a unique adaptability that allows them to be seamlessly integrated into various contexts, enabling the realization of groundbreaking possibilities. The key benefits of these PV devices are their mechanical



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Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). flexibility, lightweight design, low cost, high productivity, and the capacity to be made at room temperature [4,5]. This type of solar cell has sparked considerable attention since the first DSSC was released by Grätzel et al. [3] in 1991. DSSCs are made of low-cost materials with high-efficiency potential and are abundant on the planet, making them a viable alternative to other generations of solar cells [6].

Optimizing and maintaining the layers of a DSSC can lead to enhanced system performance. In this type of solar cell, the dye undergoes oxidation, releasing electrons, and the electrolyte replenishes these lost electrons to prevent dye oxidation. The widely used liquid electrolyte in DSSCs is the iodide/triiodide (I/I₃) redox couple [7]. However, liquid electrolytes pose challenges such as solvent evaporation, low heat stability, and difficulty in sealing the cell. To address these issues, researchers are exploring the use of solid-state electrolytes in DSSCs [8], which offers advantages for future applications. A. Sevin et al. examined the electrochemical and photovoltaic properties of solar cells using cobalt/zinc phthalocyanine sensitizers. The study demonstrates that the cobalt(II) phthalocyanine (Co-PC) derivative exhibits a PCE of 4.18%, while the zinc(II) phthalocyanine (Zn-PC) derivatives yield a PCE of 2.99%. The use of sulfur atoms as linker atoms slightly improves solar cell efficiency. The results suggest that a low-cost sensitizer made up of symmetrically substituted phthalocyanine with an earth-abundant metal at the inner core can achieve high solar cell efficiency [9]. B. Kadem et al. investigated the effects of adding Zn-PC hybrids to a blend of P3HT: PCBM to improve the performance of organic solar cells [10]. The hybrids, which are covalently and non-covalently functionalized with single-walled carbon nanotubes and reduced graphene oxide, were found to enhance photon harvesting and charge carrier transport in solar cells. The addition of these hybrids resulted in a significant increase in electrical conductivity and improved charge collection efficiency, leading to higher power conversion efficiency (PCE) and fill factor (FF) in solar cell devices. Their best-performing device achieved a PCE of 5.3% and an FF of 68%. M. Stylianakis et al. demonstrated the potential of incorporating ZnPc into ternary organic solar cells to achieve PCEs [11]. They observed that the introduction of ZnPc into the active layer of the solar cells serves as an electron cascade material, improving charge transfer and reducing exciton recombination. This leads to enhanced energy level alignment between the polymeric donor and the fullerene acceptor, resulting in improved photovoltaic performance. Their fabricated ternary solar cells showed a PCE of 8.52%, which is a significant 15% increase compared to the reference binary cell. The addition of ZnPc into the active layer of the solar cells not only enhances the energy level alignment but also optimizes the morphology of the ternary active layer. Y. Zheng et al. discuss the use of a binary solvent additive to enhance the efficiency of PTB7:PCBM polymer solar cells [12]. The authors achieved a power conversion efficiency of over 9.5% by using a combination of diphenyl ether (DPE) and 1,8-diiodoctane (DIO) as the binary solvent additive. The addition of DPE improved the crystallinity of the PTB7 donor, while DIO enhanced the dispersion of the PCBM acceptor. This resulted in better donor/acceptor phase separation, increased light absorption, and improved charge transport efficiency. A DSSC incorporating TiO₂ as the electron extraction layer and N719 as the photo-harvesting layer achieved a power conversion efficiency (PCE) of 8.5% [13]. Y. Liu et al. employed a P3HT/ZnPc composite with tunable energy levels to serve as a hole transport material (HTM) to improve the stability and charge carrier transport at the interfaces [14]. This reduced the energy level difference and passivated surface defect states in CsPbBr₃, enhancing charge separation. Their solar cell configuration achieved a notable power conversion efficiency of 10.03%, displaying improved stability over 30 days in ambient conditions. The P3HT/ZnPc composite emerges as an effective HTM for high-efficiency and stable carbon-based CsPbBr₃ perovskite solar cells. Extensive research is being conducted to improve DSSCs' efficiency and make them viable for mass production [15,16]. Recent studies have shown promising results, with DSSCs achieving efficiency levels of around 11% or even higher [17,18].

In the realm of PV research, the SCAPS-1D software has emerged as a valuable tool for investigating and analyzing different generations of solar devices. Researchers have

utilized this simulation system to explore various aspects of thin-film solar cells, including layer thickness determination and the impact of material characteristics and device designs on PV performance. One noteworthy study by Farah J. and colleagues delved into the performance evaluation of DSSCs with different hole transport layers (HTLs) using SCAPS-1D. Among the HTLs tested, their optimized structure featuring CuI exhibited exceptional outcomes [19]. This finding highlights the significance of HTL selection in enhancing the efficiency of DSSCs. B.K. Korir et al. utilized SCAPS-1D to develop a solid-state dye-sensitized solar cell (SSDSSC). They focused on optimizing the output of the electron transport layer, resulting in a remarkable power conversion efficiency (PCE) of 5.38% [20]. This demonstrates the potential of simulation tools in optimizing material performance for improved solar cell efficiency. In another study, by K.A. Ojotu et al., SCAPS was employed to simulate solid-state DSSCs. Through meticulous device settings optimization, their solar cell achieved an impressive efficiency (PCE) of 4.90% and a fill factor (FF) of 56.45% [21]. This research emphasizes the significance of precise parameter adjustments for enhancing DSSC performance. Furthermore, N.S. Noorasid and collaborators explored SSDSSCs utilizing CuI as a hole transport material. Their numerical modeling and analysis using SCAPS-1D showcased the compelling nature of this combination. By adjusting various parameters, the researchers revealed that SSDSSCs with back contacts outperformed those without, mainly due to the benefits of reduced HTL thickness [22]. This study demonstrates the importance of device architecture and contact configurations in enhancing solar cell performance. A. Iqbal et al. aimed to improve the efficiency of a DSSC based on ZnPC: PC70BM by analyzing various parameters [23]. They used a solar cell capacitance simulator (SCAPS-1D) to estimate the performance of the DSSC with different photoactive layer thicknesses, series and shunt resistances, and back metal work functions. The findings of the study indicate that certain parameters significantly impact device performance, and they obtained a maximum PCE of 10.30%. By employing the SCAPS-1D software, K.S. Nithya produced an NFA-OSC, where CuI was utilized as an HTL, and the researchers believe their structure is more effective than more conventional ones. Their system reached a PCE of 15.68% while operating in ideal conditions [24]. In a notable study conducted by W. Abdel Aziz and colleagues, it was discovered that the graded bulk heterojunction (GBHJ) solar cell exhibited superior productivity compared to the bulk heterojunction (BHJ) solar cell. By employing non-fullerenes as acceptors, they achieved an impressive PCE of 12.39% [25]. This research demonstrated the potential of non-fullerene acceptors in enhancing the performance of organic solar cells (OSCs). Another group of researchers, led by B. Sharma, utilized the SCAPS-1D modeling tool to develop non-fullerene OSCs with CuSCN as the HTL. Through careful adjustments to the simulation settings, they achieved a remarkable PCE of 20.36% [26]. This achievement highlighted the efficacy of SCAPS-1D in designing and analyzing high-performance PV devices.

SCAPS-1D, an advanced modeling tool, has been extensively utilized in the design and study of various high-performance PV devices, including perovskite solar cells (PSCs) [27], copper indium gallium selenide solar cells (CIGS) [28], cadmium telluride-based solar cells (CdTe) [29], and OSCs [30]. This versatile tool has facilitated significant advancements in the understanding and optimization of these technologies. These research findings underscore the importance of exploring novel materials and employing sophisticated modeling tools like SCAPS-1D to push the boundaries of solar cell efficiency. By continuously improving our understanding and design capabilities, we can drive the development of high-performance PV devices, paving the way for a more sustainable and renewable energy future.

This study modeled suggested zinc phthalocyanine (ZnPC)-based structures to validate their design and assess their performance for commercial implementation, as well as optimize the cell parameters for optimum DSSC efficiency. It was found that these molecules can replace traditional dyes which are associated stability, volatility, and productivity concerns. In this study, we also investigated the behavior of devices with ZnPC and ZnPC: PC70BM absorber layers for DSSCs. In addition, we looked at several DSSC

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properties (photoactive layer thickness, doping density, carrier mobility, and ETMs) that contribute to device performance. Furthermore, our findings are compared to experimental data provided in other published literature.

2. Device Configuration and Modeling

2.1. Approach and Design

To design and analyze the simulated cell in various segments, the researchers relied on the powerful SCAPS software (version 3.3.07). This cutting-edge tool provided users with access to a range of panels within the application, granting them the ability to fine-tune settings and form insightful opinions on the outcomes. By harnessing the capabilities of SCAPS, the researchers gained valuable insights into the performance and characteristics of the simulated cell. This comprehensive software enabled them to explore various scenarios and evaluate the impact of different settings on the system's behavior. With its powerful simulation capabilities and robust mathematical foundation, SCAPS empowered the researchers to delve deeper into the intricacies of their designs, fostering a better understanding of the underlying physics and facilitating advancements in PV technology [31]. Figure 1a illustrates the working procedure of SCAPS-1D.



Figure 1. (a) Steps to initiate SCAPS-1D. (b) Diagrammatic representation of a ZnPC-based DSSC. (c) Schematic representation of a ZnPC:PC70BM-based DSSC.

In this study, a heterojunction structure was employed to investigate the performance of an SSDSSC. The cell structure comprised a single and bi-active layer, offering versatility in design and functionality. Various components were integrated into the device, including an absorber layer, an HTL consisting of PEDOT: PSS, an electron ETL comprised of PFN:Br, a transparent conducting oxide (FTO), and a metal contact (Au). These elements are visually depicted in Figure 1b,c, providing a clear representation of the cell's architecture.

To comprehend the energy behavior within the proposed structures, energy band diagrams were constructed. These diagrams, as shown in Figure 2a,b, illustrate the distribution of energy levels across the different layers. By examining the energy band alignment, the researchers gained insights into the charge transfer and transport processes occurring within the cell.



Figure 2. (a) Energy–band diagram of a ZnPC–based DSSC. (b) Energy–band diagram of a ZnPC:PC70BM–based DSSC.

The incorporation of a solid-state design and the utilization of a heterojunction structure offered a promising platform for enhancing the efficiency and performance of the DSSC. By carefully engineering the layers and optimizing the energy band alignment, the researchers aimed to maximize light absorption, charge separation, and collection, ultimately driving advancements in solar cell technology.

2.2. Device Simulation Parameters

The selection of simulation settings for the layers' structure drew upon the research presented in references [19,20,24–26,32–34]. The comprehensive list of parameters considered encompassed various material properties, such as donor and acceptor density, electron and hole mobility, and more. It was crucial to account for the distinct characteristics of each material in conjunction with the layout of the contact points. To facilitate a holistic understanding, Table 1 provides an extensive overview of the essential simulation parameters employed in this study. Furthermore, several other material properties, including the thermal velocity of electrons and holes, were adjusted to 10^7 cm/s to enhance realism within the simulations. The back metal electron work function of gold was kept at 5.1 eV, while the front TCO contact electron work function was defined as 4.4 eV [35,36]. Absorption profiles for all layers were obtained from relevant studies [33,34,37,38], facilitating the simplification of the device modeling process. Absorption profiles are typically added as layers in SCAPS-1D to incorporate the optical properties of the materials used in the device. To achieve a more realistic representation of the device, the model incorporated two interface defect layers denoted as IL1 (PFN:Br/photoactive layer) and IL2 (photoactive layer/PEDOT:PSS). These layers accounted for imperfections at the interfaces and their potential influence on device performance. In this study, IL1 and IL2 were assigned a value of 2×10^{10} cm⁻² [24].

The device modeling employed the AM1.5G spectrum and maintained an effective temperature of 300 K, ensuring compatibility with real-world operating conditions. All operating point settings and numerical factors were maintained at their actual values to preserve accuracy and consistency. The scanning voltage range was set from 0 to 1 volt, covering a broad spectrum of operating conditions. These parameters, meticulously chosen and implemented, formed the foundation of the simulations conducted within this program.

By utilizing these settings consistently throughout the simulations, the researchers could confidently analyze and compare the performance of the device under different conditions, driving advancements in DSSC technology.

Parameters	FTO [19,20,24]	PFN:Br [25,26]	PEDOT:PSS [25,32]	PC70BM [24,26,32]	ZnPC [26,33,34]
Thickness (nm)	100	100	150	50	200
Acceptor Density (cm^{-3})	0	0	10 ¹⁸	0	0
Donor Density (cm ⁻³)	10 ¹⁹	$9 imes 10^{18}$	0	0	0
Effective Density of states for valence band (cm ⁻³)	$9.2 imes10^{18}$	10 ¹⁹	$2.5 imes 10^{21}$	10 ¹⁹	10 ¹⁹
Effective Density of states for conduction band (cm ⁻³)	$1.8 imes10^{19}$	10 ¹⁹	$1.7 imes10^{19}$	10 ¹⁹	10 ¹⁹
Bandgap (eV)	3.5	2.8	1.5	2	1.86
Relative Dielectric Permittivity	9	5	3	3	5
Mobility of Electron (cm ² /Vs)	20	$2 imes 10^{-6}$	$1.69 imes 10^{-4}$	$2.2 imes 10^{-4}$	0.1963
Mobility of Hole (cm ² /Vs)	10	$1 imes 10^{-4}$	$1.69 imes 10^{-4}$	$2.5 imes 10^{-4}$	0.0627
Electron Affinity (eV)	4	4	3.4	3.9	3.7
Defect Density (cm ⁻³)	10 ¹⁵	10 ¹²	10 ¹⁵	10 ¹²	$5 imes 10^{13}$

Table 1. Parameters for different layers set in the simulation.

3. Analysis and Discussion

3.1. Evaluation of Different Photo-Harvesting Layers

In this study, a range of zinc-phthalocyanine (ZnPC) groups, including isopropoxy, cyano, fluoro, methoxycarbonyl, and dicyanomethyl, were investigated as potential absorber materials for DSSCs. These ZnPC groups exhibit distinct advantages over traditional materials, as they demonstrate lower reorganization energy, improved charge transfer characteristics, and higher optical conductivity. Consequently, their optoelectronic properties are more refined and promising for application in PV devices. The researchers found that these ZnPC groups hold great potential as viable replacements for existing absorber materials in DSSCs. Additionally, their noteworthy optoelectronic characteristics indicate their potential as pivotal components in the advancement of next-generation DSSCs. All of the simulations for the various groups of ZnPC were run at a thickness of 200 nm. The current density-voltage (J-V) curves and the quantum efficiency (QE) curves resulting from their differentiation are shown in Figure 3a,b, which make it clear that the Jsc and Voc values shift depending on the ZnPC group. Electrical losses in the photoactive and transport layers may be the origin of the small indentation shown in the J-V curve of ZnPC molecules above 0.75 V. In the context of this study, the presence of series resistance (Rs) was considered, representing the electrical resistance between the metal and the transparent electrode. This is an important factor that influences the overall performance of the solar cell. Among the various molecules investigated, ZnPC and isopropoxy ZnPC molecules emerged as particularly promising options, displaying superior outcomes in terms of PCE and short-circuit current density (Jsc). These molecules showcased exceptional optical and transport properties, contributing to their enhanced performance. ZnPC and isopropoxy ZnPC exhibited notable characteristics such as a high transport rate, a high absorption coefficient, and potential dielectric properties. These attributes played a significant role in achieving higher PCE values, with ZnPC demonstrating a PCE of 8.72% and isopropoxy ZnPC exhibiting a PCE of 7.65%.



Figure 3. (a) J–V comparison of different active layers. (b) QE comparison of different active layers.

Herein, a comprehensive numerical analysis was also conducted on DSSCs based on ZnPC and ZnPC:PC70BM. The focus of the investigation was on DSSCs with a photoactive layer thickness of 200 nm. The material parameters for all the designed layers are displayed in Table 1. The J-V and QE graphs of their comparison are shown in Figure 4a,b, which clearly illustrate that the outcomes of the ZnPC:PC70BM-based DSSC are significantly higher than those of the ZnPC-based DSSC. When the photons are incident on photoactive dye material, excitons are generated, which are bounded electron-hole pairs formed by Columb interaction. These excitons are separated by utilizing two different materials with correctly aligned band levels. These materials are called donors and acceptors. The junction between these two materials dissociates the bounded electron-hole pair and transports it toward the respective electrodes. Zn-PC is an efficient donor material despite having some acceptor parts. But we need a better acceptor material for exciton separation. As a result, we used PC70BM as an acceptor material in our simulation to enhance the device's performance and outcomes. The device output parameters Voc, Jsc, FF, and PCE for the ZnPC- and ZnPC:PC70BM-based DSSCs at a thickness of 200 nm were 0.83 V and 0.85 V, 16 mA/cm² and 18 mA/cm², 57.65% and 51.52%, and 7.65% and 8.36%. It was observed that ZnPC:PC70BM had a stronger interaction with the charge transporting layers than ZnPC. So, when light was applied to the dye material, it resulted in effective extraction, transport, and collection of charge carriers towards the relevant electrodes. Therefore, it vielded better outcomes.



Figure 4. (a) JV comparison of ZnPC- and ZnPC:PC70BM-based DSSCs. (b) Quantum efficiency comparison of ZnPC- and ZnPC:PC70BM-based DSSCs.

The numerical analysis of the SSDSSC was compared to actual published data, as shown in Table 2. It was observed that the simulation results are close to the experimental findings presented in previously published studies. By leveraging the advantageous optical and transport properties of these specific molecules, the researchers aimed to optimize the performance of the solar cell and unlock its maximum efficiency. These findings provide valuable insights into the potential of ZnPC and isopropoxy ZnPC as promising candidates for enhancing the overall performance of DSSCs.

Device Configuration	PCE (%)	Ref.				
Experimental Published Results						
FTO/dye & TiO ₂ (TNÅ)/Pt	8.34	[38]				
FTO/TiO ₂ /N719/modified CuSCN/carbon past/Pt-FTO	4.24	[39]				
4-HBa-ZnPc, 4-HBa-CoPc, 4-MKBa-CoPc	2.99, 3.70, 4.18	[9]				
P3HT:PCBM:ZnPc-SWCNTs	5.30	[10]				
ITO/PEDOT:PSS/PTB7:ZnPc:PC71BM/Ca	8.52	[11]				
FTO/TiO ₂ /CsPbBr3/P3HT:ZnPC/carbon	10.03	[14]				
Simulation Results						
FTO/PFN:Br/ZnPC/PEDOT:PSS/Au	7.65	This study				
FTO/PFN:Br/ZnPC:PC70BM/PEDOT:PSS/Au	8.36	This study				

Table 2. Comparison of the simulated results with published experimental results.

3.2. Effect of Active Layer Thickness and Defect Density on Cell Performance

The photoactive layer of any PV cell is essential to its device's operation and output. PV cells can be more or less productive depending on their photoactive layer thickness. This is because the thickness of the photoactive layer affects how well photons are absorbed and charge carriers are extracted. As the photoactive layer gets thicker, the dye can absorb more light, making the cell work better. Electron–hole pairs are generated when a dye absorbs photons, which are further dissociated and transported toward the respective electrodes. Meanwhile, DSSC performance suffered as a result of the thick photoactive layer. That is because increased thickness makes the film more resistant to electrical charge transfer, resulting in electron recombination and reducing solar cell performance. The thickness of the photoactive layer was altered in this study between 100 and 700 nm. The impact of this variation on device performance was studied by keeping all other parameters constant throughout the experiment.

The data presented in Figure 5a–d reveal a clear correlation between the variation in device performance and the depth of the active layer in the DSSCs. As the thickness of the absorber layer is increased from 100 nm to 500 nm, there is a noticeable improvement in the values of Jsc (short-circuit current), Voc (open-circuit voltage), and PCE. This enhancement can be attributed to the increased concentration of electron-hole pairs generated within the absorber layer due to the larger thickness [21,40–42]. However, when the photo-harvesting layer thickness is further increased from 500 nm to 700 nm, a different trend emerges. The longer distance for carriers to travel toward their respective electrodes leads to an increased recombination rate, causing a decline in Voc. Consequently, the PCE also decreases because the impact of the Voc reduction outweighs the negligible increase in Jsc. The highest achieved values for Voc and PCE were 0.8318 V and 8.71%, respectively. The decline in the fill factor from 63.65% to 42.43% with increasing layer thickness is an essential observation. The fill factor indicates the device's ability to deliver the full available power to the electrical load. The decrease in fill factor is attributed to the relatively thick active layer, which contributes to higher series resistance within the cell and a quicker depletion of the cell's internal power.



Figure 5. (**a**,**e**) Voc, (**b**,**f**) Jsc, (**c**,**g**) FF, and (**d**,**h**) PCE in relation to active layer thickness and defect density.

The significance of the photoactive layer's quality and structure in DSSCs' performance is highlighted. The photoactive layer has a pivotal function in light absorption, and for optimal efficiency, it necessitates a low defect density. Subpar film quality and unfavorable characteristics contribute to heightened defect states and increased recombination probability, detrimentally impacting the productivity of the device [26,43,44]. Energy defects are classified into two types: shallow and deep. Long electron–hole scattering and high Voc have resulted from the creation of shallow energy levels. However, the deeplevel defect is characterized by a high probability of creating energy defects, negatively impacting charge carriers' diffusion length. The increased efficiency of DSSCs at low defect density is attributed to low recombination at photoactive layer interfaces. To achieve higher performance in DSSCs, careful consideration and optimization of the photoactive layer's properties are essential. Ensuring a well-structured and defect-free photoactive layer is crucial for enhancing the overall efficiency and effectiveness of these solar cells.

Figure 5e–h present a detailed analysis of the output device's performance concerning defect density (Nt) in the dye-sensitized solar cells (DSSCs). The variation in Nt directly impacts the carrier lifetime, leading to changes in the recombination rate, which in turn influences the overall output performance of the device. The results demonstrate that a low defect density is beneficial for achieving improved device performance. A lower Nt value indicates fewer traps present in the absorber layer, allowing for a higher generation rate of electron–hole pairs. This translates to better carrier transport and reduced recombination, ultimately leading to enhanced output parameters.

On the other hand, an excessive concentration of defects introduces additional recombination centers and traps, leading to a degradation of the device's overall performance. Such high defect densities hinder efficient carrier movement and increase the chances of electron–hole pair recombination, negatively affecting the output characteristics of the DSSC. To optimize the device output, it is crucial to maintain a defect density below a certain threshold, specifically below 10¹⁵ cm⁻³. This threshold ensures a higher current density, which is a crucial factor for achieving improved solar cell efficiency. For instance,

the specific device output parameters for the ZnPC-based DSSC, with a photoactive layer thickness of 200 nm and a defect density of 5×10^{12} cm⁻³, exhibit promising results. The values include a Jsc of 16.02 mA/cm², Voc of 0.8364 V, FF of 60.75%, and PCE of 8.13%. By carefully controlling and reducing the defect density in the absorber layer, researchers can further enhance the performance of DSSCs. These findings offer valuable insights into the optimization of defect-related properties, paving the way for more efficient and high-performing solar cell devices. Such improvements are vital for advancing the practicality and widespread adoption of DSSCs as a viable renewable energy technology.

3.3. Effect of Active Layer Mobility and Doping Density on Cell Performance

Charge carrier mobility is a crucial factor in enhancing the efficiency and performance of DSSCs. It refers to the average ease with which charge carriers, namely electrons and holes, move from one location to another within the solar cell without being trapped. A specific relation describes this phenomenon. In the simulation conducted for DSSCs, two distinct categories of charge carriers were considered: free charge carriers and trapped charge carriers. Electrons and holes fall into these categories, each playing a vital role in the functioning of the solar cell. Free charge carriers are mobile and contribute to the generation of electric current, while trapped charge carriers are immobilized and unable to participate in the current flow. The ability of charge carriers to move freely without getting trapped directly influences the efficiency of charge transport within the DSSC. Higher charge carrier mobility translates to more effective and rapid movement of electrons and holes, leading to reduced recombination rates and increased overall device performance.

$$\mu_{e}(n) = \frac{\mu_{e}^{o} n_{free}}{n_{free} + n_{trap}}$$
(1)

In this study, the researchers explored the influence of charge carrier mobility on the performance of DSSCs. They systematically varied the charge carrier mobility within a range from 1×10^{-3} to 10 cm²/Vs to understand its impact on device efficiency. The findings revealed a critical mobility range that led to optimal device performance. Specifically, the saturation point for performance parameters was observed in the carrier mobility range of 1×10^{-1} to $1 \text{ cm}^2/\text{Vs}$. Within this range, the DSSC exhibited the best outcomes in terms of various performance parameters. Figure 6a-d present the results, demonstrating the relationship between charge carrier mobility and key performance metrics. As the carrier mobility decreases, the Jsc also reduces due to a decrease in the dissociation probability. This, in turn, negatively affects the overall efficiency and fill factor of the solar cell [29,44,45]. On the other hand, an increase in carrier mobility leads to higher short-circuit current density, potentially resulting in greater efficiency and fill factor. This indicates that efficient charge carrier transport is crucial for improving the performance of DSSCs. Upon careful evaluation, the researchers identified that the DSSC achieved the optimum values for Voc, Jsc, FF, and PCE at a carrier mobility of 10 cm^2/Vs . This suggests that at this specific mobility value, the charge carriers' movement is most favorable, resulting in improved device performance.

Another essential factor influencing cell performance is doping. The doping density must be appropriately set to produce good results. Doping affects the degree of semiconductor characteristics in two ways. The presence of doping atoms introduces motion impedance, impeding the free movement of charge carriers and consequently limiting their overall mobility within the material [18,46,47]. Dopants are classified into two types: donor and acceptor. Donor energy levels are usually below the conduction band, requiring very little energy to move from the donor level to the conduction band. In contrast, acceptor energy levels behave conversely to donor energy levels.

The photoactive layer doping in this study was changed from 10^{14} to 10^{17} cm⁻³ to observe how it affects cell output metrics. Figure 6e–h depict the performance metrics of the photoactive layer at various doping densities. According to Figure 6e–h, it was found that when doping density increases, the performance parameter swings because

doping lessens the influence of the built-in electric field of the photoactive layer. There is a considerable loss in performance characteristics as the PCE value drops from 7.36% to 7.18% and Jsc drops from 15.46 mA cm⁻² to 15.08 mA cm⁻², which might be attributed to unequal charge carrier mobilities. A slight decrease in Voc value may also be seen. Furthermore, carrier diffusion length and lifespan decrease when doping density increases, affecting the charge carrier conductivity and promoting the recombination of charge carriers. Ultimately, this phenomenon results in inadequate carrier transport at interfaces, which lowers the device's performance.



Figure 6. (a,e) Voc, (b,f) Jsc, (c,g) FF, and (d,h) PCE in relation to active layer mobility and doping density.

3.4. Influence of Different ETMs on Cell Performance

Electron transport materials (ETMs) play a pivotal role in facilitating the movement of electrons away from an interface while impeding the flow of holes. As a result, they have gained widespread adoption in DSSCs and PSCs due to their well-established development and effectiveness.

The integration of an ETM layer contributes significantly to achieving favorable outcomes in DSSCs. One essential property of an ETM is its lower electron affinity and lower unoccupied molecular orbital (LUMO) energy compared to the photoactive layer. This ensures proper band alignment and facilitates efficient electron extraction from the photoactive layer. Additionally, the ETM should exhibit a higher highest occupied molecular orbital (HOMO) energy level than the photoactive layer to prevent hole transport, enabling selective electron extraction. In addition to band alignment, an effective electron transport material (ETM) should possess qualities such as affordability, robust relative stability, and robust n-type conductivity. These attributes contribute to cost-effectiveness, long-term durability, and the facilitation of efficient electron transport within the solar cell structure [48–52].

Furthermore, an ideal ETM should possess a high bandgap and high transmittance in the ultraviolet–visible (UV–vis) range. This allows the absorber layer to pass through the ETM freely and ensures efficient light absorption by the photoactive layer. By enabling the unrestricted flow of light while promoting electron transport, the ETM maximizes the overall performance and efficiency of the solar cell. So, there must be strong communication between the ETM and the photoactive layer to improve performance. In this simulation, we studied the influence of different ETM layers on double PSCs. All the main parameters for the ETM layers were carefully selected from the published data [21,22,24,25,40,53–55] listed in Table 3.

Parameters	PFN:Br [22,24,54]	TiO ₂ [22,24,25,53,54]	ZnO [21,22,24,40,55]	SnO ₂ [21,22,24,40,55]
Thickness (nm)	100	100	100	100
Acceptor Density (cm^{-3})	0	0	0	0
Donor Density (cm^{-3})	$9 imes 10^{18}$	$9 imes 10^{18}$	$9 imes 10^{18}$	$9 imes 10^{18}$
Effective Density of states for valence band (cm^{-3})	10^{19}	10^{19}	10^{19}	10^{19}
Effective Density of states for conduction band (cm^{-3})	10^{19}	10^{19}	10^{19}	10^{19}
Bandgap (eV)	2.8	3.2	3.4	3.6
Relative Dielectric Permittivity	5	9	10	9
Mobility of Electron (cm ² /Vs)	$2 imes 10^{-6}$	20	20	100
Mobility of Hole (cm ² /Vs)	$1 imes 10^{-4}$	10	10	25
Electron Affinity (eV)	4	3.9	4.3	4
Defect Density (cm ⁻³)	10^{15}	10^{15}	10^{15}	10^{15}

Table 3. Material parameters for different ETM layers set in the simulation.

Figures 7 and 8 show J-V curves and a comparison of performance parameters for the realized DSSC with PFN:Br, TiO₂, ZnO, and SnO₂ as the ETM. The DSSC with the ETM PFN:Br yields a power conversion efficiency of up to 7.65%. Moreover, ZnO and SnO₂ exhibit a higher PCE than PFN:Br. We also considered the performance of devices without ETM. It was observed that ETM significantly impacts cell output parameters comparatively to HTM because carrier transport is mainly due to electrons. TiO₂ gives the best performance with a PCE of 8.57%. That is because of its high n-type conductivity, high transport properties, better band alignment, and better communication with the photo-harvesting layer.



Figure 7. J-V curve of different ETM layers.



Figure 8. Photovoltaic performance parameters (**a**) Voc, (**b**) Jsc, (**c**) FF, and (**d**) PCE comparison of different ETMs.

3.5. Optimization of Parameters

Table 4 provides an overview of the adjusted device settings and additional information on the optimized outcomes, and Figure 9 shows J-V curves for DSSC after optimizing the parameters. After optimization, the performance of both the ZnPC- and ZnPC:PC70BMbased DSSCs saw a substantial improvement; consequently, we produced a favorable result with PCEs of 9.5% and 9.81%, respectively. It was clear from this that the output of the DSSC may be improved by altering the parameters appropriately.

Table 4. Optimized numerical parameters and results.

Parameters	ETL	Absorber Layer	Н	TL
Thickness (nm)	_	300	-	_
Material	TiO ₂	_	-	_
Electron Mobility (cm ² /Vs)	_	$1 imes 10^{0}$	-	_
Hole Mobility (cm ² /Vs)	—	$1 imes 10^0$	-	_
Defect Density (cm^{-3})	—	$1 imes 10^{13}$	$1 \times$	10 ¹⁶
Device Configuration	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
PFN:Br/ZnPC/PEDOT:PSS	0.9151	18.57	55.63	9.50
PFN:Br/ZnPC:PC70BM/PEDOT:PSS	0.9184	22.50	47.48	9.81

It is not surprising that the simulated efficiency of the DSSC after the final optimization is significantly higher than the experimental efficiency of the device. The dye material's inherent instability may be the root cause of this disparity. It has been suggested that several factors, including moisture, humidity, and the presence of water or solvents in a DSSC can account for this behavior [56,57]. This seems even more likely, considering that our lab has an unusually high humidity level (54%). For example, excessive humidity may cause film pinholes to grow, which would eventually deteriorate the characteristics of the

photoactive layer and result in low productivity. The experimental study that proved a non-ideal shape makes this relatively evident. Fabricated PV cells suffer from numerous power losses, including recombination and absorption loss, due to the device's significant degradation and instability. However, optical effects like reflection and recombination losses were ignored during the simulation when analyzed with SCAPS-1D.



Figure 9. J-V curve of the initial and optimized structures.

The findings from our simulations indicate the following: (a) the optimal photoactive layer thickness should be 300 nm; (b) the photoactive layer defects should be as low as possible; (c) the mobility of the charge carrier should be moderate, around 1–10 cm²/Vs, and (d) the amount of doping should be controlled to yield high productivity alongside TiO₂ as an electron transport medium. It is necessary to conduct more studies to examine the effects of the oxygen level, which might lead to more efficient carrier transportation and improve the performance of DSSCs. However, the final optimized simulation might be employed to exemplify the prospective cell outcome and indicate the manufacturing circumstances that need to be tuned to successfully increase the solar cell properties.

4. Conclusions

Different dyes are being researched to enhance the performance of DSSCs; however, the actual implementation of these photoactive absorbers in the device structure needs suitable parameters to obtain high productivity. In this work, several ZnPC-based dyes were used as viable alternatives to traditional dyes for DSSC in a simulation-based study. In light of our findings, ZnPC and Isopropoxy ZnPC stand out as outstanding compounds with remarkable optoelectronic capabilities. This study also examined ZnPC and ZnPC:PC70BM-based DSSCs; however, the ZnPC:PC70BM-based DSSC yielded the best results, with a PCE of 9.81%. The effects of the absorber layer thickness on the device and its mobility, carrier doping, and defect density were also examined. As revealed in this study, it is feasible to increase the photovoltaic characteristics of a material by decreasing the defect density, keeping a medium absorber layer thickness and carrier doping, and enhancing the charge carrier mobility. Furthermore, the influence of several ETMs on the performance of the DSSC was investigated, and the findings revealed that TiO₂ outperformed the other ETMs due to its appropriate optoelectronic characteristics. The discovery and development of

superior absorber materials for high efficiency, greater stability, and low-cost manufacture is the central issue for DSSC technology. This study proposes a framework for efficiently using various absorbers, particularly ZnPC, in DSSC device designs. The possibility of optimizing parameters is necessary to understand the physics of this technology.

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