

$\begin{array}{l} \hline Enhancing \, MAPBI_3 \, Perovskite \, Solar \, Cell \, Performance \\ Using \, WS_2 \, \text{as an Electron Transport Layer} \end{array}$

M. MOUSTAFA ^{1,*}, A. ABD EL-SAMAD ¹, H. H. ZEENELABDEN ¹, Z. ABU WAAR ², AND M. SWILLAM ¹

¹Department of Physics, School of Sciences and Engineering, The American University in Cairo, New Cairo 11835, Egypt

²Department of Physics, College of Science, The University of Jordan, Amman, 11942, Jordan

* Corresponding Author: mohamed.orabi@aucegypt.edu

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Abstract. Planar perovskite solar cells (PSCs) have surfaced as a promising photovoltaic technology due to their potential for low-temperature processing and streamlined fabrication. A key factor in enhancing the performance of planar PSCs is the electron transport layer (ETL). This study explores the use of WS₂, a transition metal dichalcogenide (TMDC), as an alternative ETL in the methylammonium lead iodide (MAPbI₃) active layer planner *n-i-p* structured perovskite solar cells. Numerical investigation using wxAMPS software evaluates the feasibility of WS₂ as a replacement for conventional ETLs, addressing challenges related to toxicity and stability. To optimize device performance, comprehensive simulations analyze the effects of various parameters, including ETL thickness, hole transport layer, absorber layer, doping concentration, defect density, and bandgap. The optimize the band gap value of the WS₂ ETL layer have been reported to be 150 nm and 1.8 eV, respectively. The optimized configuration achieves performance metrics as follows: a power conversion efficiency of 26.34%, a fill factor of 82.84%, a short-circuit current density of 22.7 mA/cm² and an open-circuit voltage of 1.41 V. These results underscore the potential of WS₂ TMDC- ETLs for high-efficiency PSCs, paving the way for practical applications following experimental validation.

Keywords: transition metal dichalcogenides, wxAMPS simulation, perovskite solar cells, electron transport layer

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1. Introduction

Organic-inorganic perovskite-based solar cells (PSCs) have gained immense attention in the photovoltaic field, attributable to their exceptional and tunable electro-optical properties. These include but are not limited to, wide optical absorption throughout the visible and near-infrared spectra, extended carrier diffusion lengths, low exciton binding energy $(\sim 2 \text{ meV})$, direct band gap, and remarkable power conversion efficiencies (PCEs), positioning them as a leading contender for next-generation solar energy applications [1–4]. Over the past decade, advancements in perovskite composition, optimization of transport layers, and interface passivation have driven an impressive increase in PCE, rising from 3.8% to 25.2% [5–10]. Planar heterojunction architectures, specifically regular *n-i-p* and inverted *p-i-n* configurations, have emerged as dominant designs for high-performance PSCs. In these structures, the perovskite absorber layer is positioned between an electron transport layer (ETL) and a hole transport layer (HTL). This arrangement enables efficient charge transport, extraction, and collection, significantly boosting the solar cell's overall efficiency. Perovskites are represented by the general formula ABX_3 , where A is an organic cation such as methylammonium (CH₃NH₃⁺) or formamidinium (NH=CHNH₃⁺), B is an inorganic cation like Pb²⁺ or Sn²⁺, and X is a halide ion (I⁻, Br⁻, or Cl⁻).

Optimizing the charge mobility and the electron energy level of the transport layer is essential for enhancing the PCE of planar heterojunction PSCs [11,12]. These factors are critical for improving charge extraction efficiency and reducing charge recombination at the transport layer/perovskite interfaces, including the ETL/perovskite and HTL/perovskite junctions [13,14]. In conventional *n-i-p* planar PSCs, a compact titanium dioxide (TiO₂) thin film is widely used as the ETL. This is primarily due to its well-aligned conduction band (CB) energy level with perovskite materials and its excellent transmittance across the visible spectrum [12,15–17]. However, TiO₂ suffers from low electron mobility and instability under UV irradiation. The trap states in TiO₂, caused by oxygen vacancies (or Ti³⁺ sites), slow down electron transport. At the same time, forming a Schottky contact with the perovskite due to surface defects hinders charge extraction and reduces the open-circuit voltage (Voc), limiting further improvements in PCE [18–20]. Furthermore, hydroxyl groups on the TiO₂ surface can degrade the perovskite layer, adversely impacting the device's stability [20–22]. Additionally, TiO₂ requires annealing at high temperatures (~500 °C) to achieve the crystalline rutile phase, which restricts using PSCs in flexible devices.

To achieve robust performance and enhance the reproducibility and stability of PSCs, various alternative ETL materials are being explored to address the limitations of TiO₂. Materials such as IGZO, SnO₂, C₆₀, and ZnO are being studied as potential substitutes. This revision refines the structure, clarifies key points, and improves the technical flow while keeping the content intact. Among these, n-type SnO_2 is frequently chosen to replace TiO_2 as the ETL in *n-i-p* PSCs due to its superior electrical conductivity and lower density of defect states. The electrical conductivity of SnO_2 (~4×10⁻⁵ S×cm⁻¹) is notably higher than that of TiO_2 (around 1×10^{-5} S×cm⁻¹), attributed to the reduced concentration of oxygen vacancies in SnO₂ [23, 24]. Moreover, the conduction band (CB) energy level of SnO₂ aligns more closely with that of the perovskite at the ETL/perovskite interface, enhancing charge transport and extraction [8, 22, 25-27]. Consequently, n-i-p PSCs utilizing SnO₂ ETLs have demonstrated higher power conversion efficiencies (PCEs) than those based on TiO₂ ETLs [8, 22]. However, despite these advantages, hysteresis is frequently observed in n-i-p planar PSCs employing pristine SnO₂ ETLs without additional interfacial treatments [28–30]. This phenomenon is primarily caused by defect states at the SnO2/perovskite interface [27, 31]. As a result, significant research efforts have focused on mitigating hysteresis and enhancing device performance by passivating interface defects at the SnO₂/perovskite junction [27, 29, 32-34]. Recent advancements include doping the SnO₂ layer to improve its conductivity and further eliminate hysteresis, thereby boosting device performance [35]. These findings suggest that PSC performance can be further optimized by employing ETLs with higher conductivity, fewer defect states, and effective interface passivation techniques [36].

Transition metal dichalcogenides (TMDCs) have emerged as promising alternatives for electron transport layers (ETLs), gaining increasing interest due to their exceptional chemical, physical, and optoelectronic properties. Their strong light absorption capability enhances photon interaction, making them highly suitable for efficient light energy harvesting applications [37]. TMDCs are layered materials with the general formula MX_2 , where M is a transition metal, and X is a group VI chalcogen. These two-dimensional structures consist of covalently bonded MX_2 sheets held together by weak van der Waals (vdW) forces. Depending on their crystalline phase, they can exhibit a wide range of electronic behaviors, from semiconducting to quasi-metallic or metallic. Additionally, the chemically inert nature of TMDCs contributes to their excellent environmental stability and slow degradation rates [38], offering long-term durability for energy-harvesting devices. One of the most attractive features of TMDCs is their tunable bandgap (E_g), typically ranging from 1 to 2.5 eV [39, 40], making them ideal candidates for diverse optoelectronic applications [41, 42]. Furthermore, vdW heterostructures formed by incorporating TMDC nanomaterials introduce beneficial lattice mismatches that further enhance charge transport properties [43]. The advent of layered TMDCs has opened new frontiers in materials science, driving extensive research into their potential for next-generation photovoltaic and optoelectronic applications.

In this study, we explore tungsten disulfide (WS_2), a group VI TMDC, as an ETL material due to its outstanding electrical, optical, and electrochemical properties, making it a strong contender for high-performance visible-light optical devices [44, 45]. WS₂ has already demonstrated remarkable success in enhancing the efficiency of Cu(In, Ga)Se₂ (CIGS) and CdTe solar cells [46-48], attributed to its high carrier mobility, superior electron conductivity (~10⁻³ Ω^{-1} cm⁻¹), and intrinsic n-type semiconducting behavior [49]. Notably, Li et al. [48] reported WS_2 's exceptional electron conduction properties in dye-sensitized solar cells (DSSCs), highlighting its capability as a charge transport material. Additionally, WS_2 is compatible with scalable, low-temperature deposition techniques such as solution processing and sputtering, making it a cost-effective and practical choice for photovoltaic applications [50, 51]. Recently, TMDCs have been successfully integrated into various organic solar cells, including bulk-heterojunction, organic-inorganic quantum dot, and perovskite solar cells (PSCs), reinforcing their versatility. WS₂ offers outstanding electron transport characteristics, which enhance charge carrier extraction and overall device efficiency in DSSCs and PSCs. Its ability to be synthesized via low-temperature sputtering further strengthens its viability for large-scale production [52]. Sobayel et al. [53] conducted numerical simulations of planar PSCs utilizing WS₂ as an ETL, demonstrating significant improvements in device performance. Additionally, first-principles studies have predicted that WS_2 -based ETLs can achieve power conversion efficiencies (PCEs) of up to 25.70% [53]. With its high electron mobility [54, 55], tunable bandgap [56], and exceptional charge transport properties, WS₂ stands out as a next-generation ETL material poised to drive substantial advancements in high-efficiency PSCs [57].

In this study, we present the simulation of a perovskite solar cell incorporating WS_2 -TMDC as ETL, employing the wxAMPS software. The research optimizes key parameters, including band gap values, layer thickness, and defect density, to enhance overall device performance. Furthermore, we explore the impact of varying the thicknesses of the spiro-OMeTAD hole transport layer and the methylammonium lead iodide (MAPbI₃) active perovskite layer on the overall performance of the solar cell. The ultimate goal is to fine-tune these parameters to achieve a high power conversion efficiency (PCE) in MAPbI₃-based PSCs, paving the way for improved device stability and performance.

2. Device structure and methodology

Numerical modeling enhances understanding of the fundamental principles of solar cells and aids in identifying key factors affecting their performance. This study conducted simulations using the Analysis of Microelectronic and Photonic Structures (wxAMPS) software. Based on the foundation of the original AMPS code, wxAMPS improves data input efficiency and result visualization, facilitating comprehensive analysis and comparison. Unlike the drift-diffusion model, wxAMPS integrates two distinct intra-band tunneling models, allowing for more accurate simulations of heterojunction solar cell properties. In the numerical simulations performed with wxAMPS, Poisson's field in one-dimensional (1D) space is represented by Eq. (1). The delocalized conduction band states containing unpaired electrons are depicted by Eq. (2) [58–62]. Eq. (3) outlines the continuity equation for delocalized free holes in the valence band, while Eq. (4) describes the net direct recombination rate [58–62].

$$\frac{dy}{dx}\left(-\varepsilon(x)\frac{d\Psi}{dx}\right) = q\left[p(x) - n(x) + N_d^+(x) - N_a^-(x) + p_t(x) - n_t(x)\right],$$
(1)

where *n* and *p* represent the concentrations of free electrons and holes, respectively; n_t and p_t represent the densities of trapped electrons and holes, respectively; and N_{d^+} and N_a^- represent the proportions of ionized donors and acceptors, *q* is the electron charge, Ψ is the electrostatic potential, and ε is the interfacial permittivity of the semiconductor. The charge transport features, recombination rates, and generation rates are *all included* in the continuity equation, as shown by Eqs. (2) and (3):

$$\frac{1}{a}dJ_n / dx = R_n(X) - G(X), \qquad (2)$$

$$\frac{1}{a}dJ_p / dx = G(X) - R_p(X), \qquad (3)$$

$$R_D(x) = \beta \left(n_p - n_i^2 \right). \tag{4}$$

When R_n and R_p are the steady-state recombination velocities of electrons and holes, these forms describe the continuity equations. *G* denotes the optical generation rate, while J_n and J_p denote the electron and hole current densities. G(x) refers to the carrier generation rate as a function of *x* due to the external light supply in the continuous equation.

In conventional solar cell structures, PSCs consist of a light-absorbing intrinsic (i) semiconductor layer of perovskite, which is positioned between charge-selective electrodes to facilitate charge separation. These electrodes include an ETL (*n*-type), an HTL (*p*-type), an optically transparent conducting oxide (TCO), and a back electrode contact. The architectures are classified based on the polarity of the charge-selective layer, with the regular *n-i-p* configuration (ITO/WS₂/Perovskite/Spiro-OMeTAD/Ag) illustrated in Fig. 1a. In this configuration, the MAPbI₃ perovskite material is sandwiched between WS₂ as the ETL and Spiro-OMeTAD as the HTL, with indium tin oxide (ITO) and silver (Ag) serving as the front and back contacts, respectively. The parameters of each layer are detailed in Table 1. In this Table, N_c and N_v are the effective density of states of the conduction and valence bands, respectively, while N_d and N_a refer to the donor and acceptor densities, both set at 1×10^9 cm⁻³. The simulated parameters were selected based on previously published studies [63–68]. The band diagram of the *n-i-p* PSC at equilibrium is depicted in Fig. 1b. An energy barrier of 0.9 eV exists between the conduction band minimum (E_c) of the WS₂ and the lowest unoccupied molecular orbital (LUMO) of the MAPbI₃ absorber material, along with an offset of approximately 0.35 eV between the highest occupied molecular orbitals (HOMO) of both the absorber material and the HTL. The simulation was performed in 300 K.



Fig. 1. (a) The structure of the simulated perovskite solar cell, (b) The band diagram of the *n-i-p* PSC at equilibrium (E_c and E_v are the conduction and valence energy, respectively. E_{fn} and the E_{fp} represent the Fermi level for electrons and holes respectively).

Parameters	WS ₂	CH ₃ NH ₃ PbI ₃	Spiro-MeOTAD
Thickness, nm	50-400	100-800	300
Permittivity	5.1	10	3
E_g , eV	1.3-2.4	1.54	2.91
Electron affinity (χ), eV	4.7	3.93	2.05
N_{c} , cm ⁻³	9.7×10^{18}	2.8×10^{18}	2.2×10 ¹⁸
N_{ν} , cm ⁻³	1.34×10^{19}	3.9×10^{18}	1.8×10 ¹⁹
Electron mobility,	100	15	1×10-4
cm ² /v/s			
Hole mobility, cm ² /v/s	25	15	1×10-4
N_d	1018	1×10 ⁹	0
Na	1×10^{14}	1×10^{9}	4.1×10 ¹⁷
Energy level	1.1	1.2	1.1
Capture <i>n</i>	1×10^{19}	1×10 ⁻²⁰	1×10 ⁻¹⁹
Capture <i>p</i>	10-18	1×10 ⁻¹⁹	1×10 ⁻¹⁸
Defect density	1014	1×10 ¹⁵	1×1017

Table 1. The parameters of the simulated perovskite solar cell device [63-68].

3. Results overview and discussion

As previously mentioned, electron transport materials (ETMs) are vital in determining solar cell performance, so careful selection is essential. Due to its advantageous properties, WS_2 emerges as a suitable and promising material for use as an ETL in solar cells. Various factors related to the ETL, including band gap, layer thickness, and defect density, significantly influence the overall performance of the solar cell. Therefore, this section will focus on optimizing these different ETL parameters to enhance the efficiency and stability of the device. The optimized energy bandgap for the ETL was investigated, revealing that the bandgap of WS_2 can vary from 1.3 eV to 2.4 eV. This energy bandgap is crucial as it determines the HOMO levels for both the ETL and HTL. For the HTL, a higher HOMO level relative to the perovskite absorber promotes efficient hole extraction. In contrast, a lower LUMO level helps block electrons from the absorber in perovskite solar cells. Conversely, this relationship reverses for the ETL. The solar cell performance results with different bandgaps are shown in Fig. 2. As indicated, increasing the bandgap of the ETL

enhances cell performance, leading to improved photoconversion efficiency. A larger bandgap allows the ETL to act as a more transparent window, facilitating the transmission of a wider light spectrum. Fig. 2a and Fig. 2d indicate that the efficiency and V_{oc} increase significantly up to a bandgap of 2.1 eV; beyond this point, no substantial changes are observed as the bandgap rises from 2.1 eV to 2.4 eV. The optimal PCE and V_{oc} of 23.50% and 1.422 V are attained at a bandgap of 2.1 eV. In contrast, the short-circuit current density (J_{sc}) remains steady at 25.41 mA/cm² across varying ETL bandgaps, as demonstrated in Fig. 2b. The fill factor (FF) is also affected by the bandgap, with the highest value reached at 1.7 eV, after which it declines as the bandgap increases (Fig. 2c). These results suggest that the appropriate band alignment with the absorber layer is essential for enhancing overall performance.



Further analysis can be conducted by considering the conduction band offset (CBO) at the perovskite/ETL interface, which is influenced by bandgap alignment and the activation energy (EA) of the ETLs. The CBO is defined as the difference in electron affinity between the ETL (χ ETL) and the perovskite absorber ($\chi_{Perovskite}$), while the activation energy is calculated as $E_A = E_g$ -|CBO|. A high CBO value and increased carrier mobilities contribute to a higher V_{oc} . Furthermore, the EA significantly impacts the performance of PSCs. Low CBO values result in lower EA, which increases interface recombination and limits electron flow at the perovskite/ETL interface, consequently reducing V_{oc} . Conversely, a positive CBO enhances EA, resulting in decreased interface recombination, increased V_{oc} , and thus improved PCE.

At a bandgap of 2.1 eV, the influence of the ETL layer thickness was investigated, as this parameter is crucial for optimizing the efficiency of $MAPbI_3$ -based perovskite solar cells. Fig. 3

illustrates the optimization results, demonstrating how varying the thickness of the WS₂ ETL affects the performance of the solar cell. All photovoltaic parameters exhibit similar trends in response to changes in ETL thickness. The PCE, the J_{sc} , and FF achieve their peak values of 23.5013%, 22.1565 mA/cm², and 74.5833%, respectively, at an ETL thickness of 150 nm, as shown in Figs. 3a, b, c. Beyond this optimal thickness, cell performance declines significantly. The decrease in PCE occurs when the ETL thickness exceeds 150 nm, primarily due to the limitations on electron transport to the transparent conducting oxide (TCO) layer and increased charge carrier recombination. Additionally, the thicker ETL contributes to a rise in series resistance within the device, which subsequently reduces the FF [69-71]. Notably, the V_{oc} remains unchanged as the thickness varies, as shown in Fig. 3d. The findings highlight the significance of optimizing the ETL thickness to maximize the performance of MAPbI₃-based perovskite solar cells.



Fig. 3. The obtained solar cell performance versus the WS₂-ETL thickness: (a) PCE, (b) J_{sc}, (c) FF, and (d) V_{oc}.

In the next phase of the study, we optimized the ETL's donor doping density (N_d) by incorporating the previously determined optimal energy bandgap and thickness. Doping in the ETL significantly influences energy levels, conductivity, and material properties. Specifically, a doped ETL can reduce electronic trap states, facilitating faster electron transport and enhancing electronic performance [72]. In this study, we varied the doping density of the WS₂ layer from 10^{10} cm⁻³ to 10^{18} cm⁻³. The results are illustrated in Fig. 4. The data indicates that doping densities below 10^{17} cm⁻³ have a negligible effect on device performance. However, beyond this threshold, a noticeable performance improvement is observed. The increased ETL doping concentration leads to higher electron conductivity due to forming a strong built-in potential (V_{bi}) at the perovskite/ETL interface. The strong V_{bi} effectively collects more electrons while repelling



minority charge carriers (holes), thereby minimizing interface recombination and enhancing device performance [73].

Fig. 4. The obtained solar cell performance versus donor concentrations of the ETL: (a) efficiency, (b) short-circuit current (Jsc), (c) fill factor (FF), (d) open-circuit voltage (Voc).

Fig. 5 presents the impact of ETL donor concentration on the current-voltage (*J-V*) characteristics and quantum efficiency (QE) results. The maximum photocurrent is achieved at the highest donor concentrations of 10^{17} cm⁻³ and 10^{18} cm⁻³, as shown in Fig. 5a. Furthermore, the quantum efficiency exceeds 86% at these higher donor concentrations, as illustrated in Fig. 5b. These findings underscore the importance of optimizing donor doping density in the ETL to enhance the overall performance of perovskite solar cells.



Fig. 5. (a) The *J*-*V* curve and (b) the wavelength dependence of quantum efficiency of the cell with different donor concentrations of the ETL.

Most studies on perovskite solar cells concentrate on methylammonium lead triiodide (MAPbI₃) as the active material. In our investigation, we begin by examining how varying the thickness of the MAPbI₃ absorber layer affects the performance of the solar cells. In the perovskite absorber layer, free charge carriers are produced by the absorption of incoming photons. The efficiency of this process is significantly influenced by factors such as layer thickness, defect density, and other intrinsic properties of the absorber material. Consequently, the solar cell's performance is closely tied to these parameters. The relationship between the thickness of the absorber layer and the diffusion length of charge carriers is crucial; both aspects affect the rate of recombination and the extraction of charge carriers. To investigate this, we maintained the thickness of the ETL at 150 nm while varying the thickness of the MAPbI₃ active layer from 100 nm to 1 μ m. The variations in J_{sc}, V_{oc}, FF, and PCE with changes in active layer thickness are depicted in Fig. 6a-d. Fig. 6a illustrates that as the thickness of the absorber layer increases, I_{sc} tends to rise while V_{oc} decreases. The increase in I_{sc} can be attributed to a higher generation rate of charge carriers due to enhanced absorption of photons. In thinner layers, particularly those below 500 nm, the absorption of long-wavelength photons is less effective, resulting in lower charge carrier generation and, consequently, reduced J_{sc} . Conversely, a thinner absorber layer exhibits lower recombination rates, contributing to a higher V_{oc} . As the absorber layer thickness increases, the absorption of long-wavelength photons improves, leading to greater charge carrier generation and increased J_{sc} . However, this also leads to a higher recombination rate as the carriers traverse longer distances to reach the respective electrodes, ultimately reducing V_{oc} as shown in the simulation results in Fig. 6.



Fig. 6. The simulated results of the change of short-circuit current (J_{sc}) (a), open-circuit voltage (V_{oc}) (b), fill factor (FF) (c), and efficiency (d) versus the active layer thickness of MAPbI₃.

Furthermore, increased absorber thickness leads to higher series resistance, negatively impacting the FF. Despite these drawbacks, the rise in J_{sc} contributes to increased PCE. Our simulation results suggest an optimal absorber thickness of around 500 nm yields the best device performance. When analyzing the overall device structure, we observed that increasing the perovskite layer thickness from 100 nm to 800 nm gradually decreases V_{oc} across all device configurations. J_{sc} initially increases Fig. 6a, and PCE rises correspondingly before plateauing, indicating that excessively thick active layers enhance recombination opportunities for the charge carriers. In contrast, a very thin active layer proves inefficient at blocking holes, causing V_{oc} to drop from 1.4873 V to 1.3723 V, as depicted in Fig. 6b. The impact on FF is minimal, as shown in Fig. 6c. Notably, PCE increases from 19.5% to 23.64% with an increase in active layer thickness up to 600 nm, after which a slight decline in efficiency is observed with further increases in MAPbI₃ thickness, as illustrated in Fig. 6 d.

The performance of PSCs is not solely determined by the thickness of the active layer but is also significantly influenced by other critical parameters. Among these, the generation and recombination of charge carriers play pivotal roles in determining device efficiency. When photons are absorbed by the perovskite material, free charge carriers - electrons and holes are generated. These carriers migrate to their respective electrodes, forming an electric current. However, the efficiency of this process can be compromised by the quality of the perovskite absorber film. Photo-generated charge carriers are often lost due to the presence of a substantial number of defects within the perovskite material. These defects act as recombination centers, increasing charge carrier recombination and significantly impairing device performance. The impact of defect density on PSC performance can be effectively described using recombination mechanisms. A key model for analyzing these processes is Shockley-Read-Hall (SRH) recombination. SRH recombination accounts for charge carrier losses caused by trap states within the bandgap of the absorber material. The recombination rate in the SRH model is defined as [74, 75]:

$$R^{SRH} = \frac{v_{TH}N_t\sigma_n\sigma_p[np-n_t^2]}{\sigma_p[p+p_1] + \sigma_n[n+n_1]}.$$
(5)

Here, v_{TH} represents the thermal velocity of electrons, N_t is the number of defects per unit volume, σ_n and σ_p are the capture cross-sections of electrons and holes, respectively, and nand p are the concentrations of electrons and holes at equilibrium. Additionally, n_i is the intrinsic carrier density, while p_1 and n_1 denote the concentrations of holes and electrons in the valence band and trap defects, respectively [75]. The equation above highlights that the defect density N_t is directly proportional to the recombination rate R^{SRH} . This study analyzed the impact of varying defect density in the MAPbI₃ absorber layer on device performance with a fixed absorber thickness of 600 nm. The defect density N_t was varied from 1×10^{17} to 1×10^{18} cm⁻³ and its influence on the simulated photovoltaic performance is summarized in Fig. 7. As depicted in Fig. 7a-d, all electrical characteristics exhibit a negative trend with increasing defect density in the active layer. Specifically, increasing N_t from 1×10^{17} to 1×10^{18} cm⁻³ results in a notable decrease in J_{sc} from 23.3636 mA/cm² to 20.8386 mA/cm² and V_{oc} from 1.37 V to 1.27 V). Since the FF is strongly dependent on V_{ocr} a significant drop in FF is also observed, from 74.9771% to 72.11%. Consequently, the PCE plummets from 23.3636% to 20.83%. These results underscore the detrimental impact of higher defect density on device performance. As N_t increases, the number of defect states rises, leading to enhanced recombination rates. This directly reduces the charge carrier lifetime, affecting J_{sc} , V_{oc} , FF, and the PCE. While thicker absorber layers can absorb more light, potentially increasing J_{sc} , the negative impact of higher recombination from increased N_t outweighs the benefits of enhanced photon absorption. In this case, the rise in recombination due to defects dominates, resulting in a consistent decline in all electrical parameters. These findings reaffirm the critical importance of minimizing defect density in the perovskite absorber layer to optimize the performance of perovskite solar cells.



Now, we focus on the effect of the HTL thickness on the performance of MAPbI₃-based perovskite solar cells. The thickness of the HTL is a critical parameter that must be optimized to achieve efficient device operation. Fig. 8 illustrates the simulation results, highlighting the influence of HTL thickness on key photovoltaic parameters. As shown in Fig. 8a, the device's efficiency exhibits a significant decline as the HTL thickness increases from 25 nm to 350 nm. This reduction in efficiency can be attributed to the fact that beyond the optimal HTL thickness, the recombination of charge carriers surpasses the rate of charge extraction. Specifically, the PCE drops from 26.3431% to 23.0568% at the corresponding thickness from 25 nm to 350 nm. A similar trend is observed for the J_{sc} and FF, which achieve their maximum values at an HTL thickness of 25 nm, as shown in Figs. 8b, c. This optimal thickness allows for efficient charge transport and minimal recombination. However, as the HTL thickness increases, the reduced mobility of charge carriers and longer transport paths lead to higher recombination rates, thereby lowering J_{sc} and FF. In contrast, the V_{oc} remains constant across the studied thickness range, as seen in Fig. 8d. This indicates that V_{oc} is predominantly determined by factors such as energy band alignment and interface quality,

which are not significantly affected by variations in HTL thickness within this range. In conclusion, our findings underscore the importance of optimizing the HTL thickness to achieve the best device performance. The results demonstrate that a thickness of 25 nm is optimal for maximizing J_{sc} , FF, and PCE while maintaining a stable V_{oc} . Increasing the HTL thickness beyond this value reduces efficiency due to enhanced recombination and reduced charge extraction.



Fig. 8. The change of efficiency (a), short-circuit current (J_{sc}) (b), FF (c), and (V_{oc}) (d) with HTL thickness.

4. Conclusions

In conclusion, a PSC with an *n-i-p* configuration was optimized using the wxAMPS software. A theoretical model was developed based on MAPbI₃ as the absorber layer and WS₂-TMDC as an ETL. The study investigated the impact of ETL, absorber, and HTL thickness on device performance, identifying optimal thicknesses of 150 nm, 600 nm, and 25 nm for the ETL, absorber, and HTL, respectively. Additionally, a WS₂ bandgap of 2.1 eV yielded the highest performance. of 26.34%, FF of 82.84%, J_{sc} of 22.7 mA/cm², and V_{oc} of 1.41 V. The optimization results also revealed that reducing the defect density in the active layer significantly improves cell performance, as fewer defects lower recombination losses. Furthermore, higher donor concentrations in the ETL enhance device efficiency by improving electron conductivity and reducing interface recombination. These findings emphasize the critical role of structural and material parameter optimization in achieving high-performance PSCs.

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Анотація. Планарні перовскітні сонячні елементи (PSC) стали перспективною фотоелектричною технологією завдяки можливості їхньої низькотемпературної обробки та спрощеного виготовлення. Ключовим фактором підвищення ефективності планарних PSC є шар транспортування електронів (ETL). У цьому дослідженні розглядається використання WS₂, дихалькогеніду перехідного металу (ТМDС), як альтернативного ETL у планарній структурі n-i-р перовскітних сонячних елементів на основі активного шару метиламоній свинцевого йодиду (МАРЫ₃). Доцільність застосування WS₂ як заміни традиційних ETL, вирішуючи проблеми, пов'язані з токсичністю та стабільністю, оцінено чисельним моделюванням за допомогою програмного забезпечення wxAMPS. Для оптимізації продуктивності пристрою, на основі комплексного моделювання проаналовано вплив різних параметрів, включаючи товщину ETL, шар транспортування дірок, шар поглинача, концентрацію легування, щільність дефектів і заборонену зону.Оптимальна товщина шару WS₂ ETL встановлена на рівні 150 нм, а ширина його забороненої зони – 1,8 еВ. Оптимізована конфігурація досягає таких показників ефективності: коефіцієнт перетворення енергії 26,34%, фактор заповнення 82,84%, густина струму короткого замикання 22,7 мА/см² і напруга холостого ходу 1,41 В. Отримані результати підкреслюють потенціал WS₂ ТМDС-ЕТL для високоефективних PSC, відкриваючи можливості для практичного застосування після експериментальної перевірки.

Ключові слова: дихалькогеніди перехідних металів, моделювання wxAMPS, перовскітні сонячні елементи, шар транспортування електронів