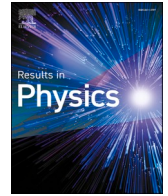


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Optimizing hole transport materials and electrodes for enhanced performance in RbGeBr₃-based on perovskite solar cells utilizing fullerene as an electron transport material

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ABSTRACT

In this work, the behavior of the electron transport material C60 and various organic and inorganic hole transfer materials, along with an inorganic perovskite material RbGeBr₃, has studied in different perovskite solar cells. The finite element method is utilized to compute solutions to the Poisson, continuity, and electrical transport equations. To obtain the highest efficiency among these cells, the thickness of the electron-transporting and light-absorbing layers has been changed. Additionally, how the various electron-collecting metal electrodes affect each structure's optimum efficiency has been investigated. Among all these designed structures, the architecture FTO/C60/RbGeBr₃/NiO/Au has presented the highest efficiency of 16.48 %, along with an open circuit voltage of 0.92 V and a short circuit current of 22.25 mA/cm². Moreover, by changing the gold contact instead of the nickel contact, the efficiency obtained was approximately the same value. The results of this research could assist with creating improved and more efficient mineral perovskite-based solar cells.

Introduction

Continuing our current path of burning fossil fuels and producing large quantities of greenhouse gases will lead to a catastrophic future, threatening the lives of billions. The primary driver of global warming is carbon dioxide, a chemical that humanity has been releasing into the atmosphere unchecked since the Industrial Revolution. Since then, the atmospheric concentration of carbon dioxide has increased by more than 40 %, with a record level reached in 2015. To address this crisis, prioritizing clean energy sources such as water, wind, and solar energy has become essential. One promising approach is harnessing the abundant thermal energy and the light energy produced by the sun. This green resource, freely available and renewable, holds immense potential, generating approximately 1.5×10^{18} kWh/year radiation annually-over 100 times more energy than all fossil fuel reserves combined [1]. The journey of solar energy utilization began in 1883 when Charles Edgar Fritts created a selenium solar cell with less than 1 % efficiency. Since then, solar cell research has made significant advancements. By the mid-1950 s, the first silicon solar cell with a 5.4 % efficiency had been developed using direct sunlight [2]. However, the high cost of pure silicon in manufacturing has posed a challenge. To address this

limitation, scientists have focused on reducing the production and manufacturing costs of solar cells through advancements in photovoltaic technology. As a result, the scientific community has explored various types of solar cells, each with unique advantages and limitations [3–6].

The perovskite solar cells (PSCs) are among the new-generation solar cell technologies that have garnered significant attention since 2014, primarily due to their remarkable efficiency improvements compared to earlier generations. Between 2014 and now, the PSC efficiency has increased from 3.8 % to an impressive 25.5 % [5–7]. The PSCs utilize perovskite materials as absorber layers, which offer exceptional physical properties, including a direct band gap, minimal crystal defects, low exciton binding energy, high charge mobility, balanced electron-hole transfer, high efficiency, and low production costs [7–11]. Several perovskite compositions, such as MAPbI₃, FAPbBr₃, and CsSnCl₃, share similar structural characteristics based on a cubic perovskite unit cell, which exhibits an ABX₃ configuration [12,13].

Since 2014, scientists have focused on utilizing organic-mineral perovskite materials as light-absorbing layers in PSCs. The exploration of these materials aligns with broader efforts in the development of clean energy technologies, including hydrogen energy systems. These materials consist of compounds where cation sites (A) are substituted by

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MA, FA[14,15], and elements such as lead, germanium, and tin at site B [16–18], while halides such as iodide, bromide, and chloride replace the X sites [19–21]. Various designs and methodologies have been implemented to optimize PSC efficiency. Examples include the use of different electron electrical transport materials (ETM) and hole electrical transport materials (HTM) [22–24], combinations of diverse perovskite materials [25–27], multiple contacts, innovative structural designs [28,29], and investigated the heat generation and thermal stability of perovskite tandem solar cells[30,31].

However, PSCs face challenges such as inherent instability, photochemical degradation of organic components, and susceptibility to temperature[32–34]. These limitations have expanded research into mineral perovskite materials, including cesium (Cs), potassium (K), and rubidium (Rb) [35–37]. Significantly, replacing organic cations with minerals like cesium has enhanced the efficiency of perovskite solar cells, boosting it from 2.9 % to 20.8 % over the last six years [38–40]. Moreover, compared to organic–inorganic perovskite materials, most mineral perovskites exhibit superior resistance to humidity and enhanced stability under high-temperature and high-light conditions [36,41–43]. Despite these improvements, there remains significant potential for further advancements by exploring diverse perovskite structures to achieve optimized solar cell performance.

In a previous study [44], this research team investigated the mineral perovskite RbGeBr_3 for the first time in two distinct structural configurations. The primary objective was to examine the behavior of RbGeBr_3 as a light-absorbing layer in the PSCs. This inorganic perovskite material demonstrated promising performance in PSCs, achieving a maximum efficiency of 11.89 %. Additionally, the impact of temperature variations on the performance of the PSC was analyzed.

This study presents the first comprehensive investigation of RbGeBr_3 inorganic perovskite as a light-absorbing material integrated with a stable fullerene (C_{60}) as an electron transport layer (ETL). It examines six primary perovskite solar cell (PSC) architectures, each featuring a distinct hole transport layer (HTL) and employing gold (Au) as the electron-collecting electrode (ECE). To further optimize device performance and cost-effectiveness, the research also explores alternative ECE materials—silver (Ag), nickel (Ni), and chromium (Cr)—by substituting gold and conducting parallel performance evaluations across these configurations.

The focus of this work is on the behavior of the mineral perovskite RbGeBr_3 as a light-absorbing layer combined with C_{60} in the ETL and different materials in the HTL alongside varying metal contacts. The current continuity equations and the charge density, commonly used in research based on semiconductor materials, are solved for these architectures. The key performance parameters—including the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and maximum efficiency (η_{max})—are calculated based on the optoelectronic properties of the materials. The power conversion efficiency (PCE) of all 24 architectures is systematically compared and evaluated. The results of this research offer valuable insights into developing perovskite solar cells based on mineral absorbers, paving the way for more complex structures and enhanced efficiency.

The paper is organized as follows: In Section 2, we provide an overview of the design and overall performance of the perovskite solar cell's electrostatic structure. Section 3 discusses four distinct architectures incorporating a mineral absorber layer, detailing the research methodologies and modeling techniques utilized. Additionally, this section presents the results and diagrams for all 24 architectures, analyzing the effects of temperature and thickness variations on performance metrics. Finally, Section 4 concludes the study, summarizing the key findings.

Design method for various PSCs with different HTLs

Based on the review of existing research and published results, studies on organic–inorganic perovskite materials in PSCs remain active

and ongoing [26,27,45]. Simultaneously, research on various inorganic perovskite materials is advancing rapidly due to their favorable physical properties, making them highly suitable for applications in electronic and photonic devices as well as PSCs. Examples of such materials include Cs_2TiBr_6 , $\text{Cs}_2\text{BiAgI}_6$, and TiGeX_3 , among others [46–49].

In 2015, Kolbak and her colleagues introduced the inorganic perovskite material CsPbX_3 as a light-absorbing layer in PSCs and analyzed its performance [43,50]. They compared the results with PSCs that utilized the organic–inorganic light-absorbing layer MAPbBr_3 under identical environmental conditions [43,51]. Their findings revealed that cesium-based solar cells exhibited superior stability at elevated temperatures, even after two weeks of exposure to dry air (15 %–20 % humidity), continuous intense light (at maximum power), and electron beam irradiation, outpacing the performance of methylammonium-based solar cells [7,36,52]. Subsequently, further research was conducted on cesium-based inorganic perovskite materials, including the work of Lin-Jer and colleagues on CsPbX_3 compounds [43].

Currently, the field of all-mineral solar cells offers significant potential for exploration due to the limited amount of existing research, particularly involving first-group elements such as Rb and K [44,53–55]. Considering this, the primary objective of this study is to investigate the light-absorbing properties of the mineral RbGeBr_3 in six distinct PSC configurations. The inorganic halide perovskite RbGeBr_3 exhibits semiconductor behavior with a direct band gap of 1.49 eV in its cubic phase[48,53]. Additionally, using density functional theory (DFT) calculations, the primary electronic and optical characteristics of perovskites have been determined [53,55,56].

In the design of photovoltaic architectures, common electron transport materials (ETM) such as TiO_2 , ZnO , and SnO_2 are widely utilized due to their proven ability to enhance the overall efficiency of perovskite solar cells. Alongside these established materials, emerging alternatives like C_{60} (fullerene) have demonstrated noticeable performance, either as standalone ETLs or in hybrid configurations when integrated with conventional ETM, offering a variety of pathways for optimizing device functionality [57–59].

Furthermore, fullerene or buckyball (C_{60}) has been widely employed in perovskite solar cell (PSC) technology owing to its remarkable capabilities as an electron transport layer (ETL) [60–62]. The fullerene, as an ETL material, plays a crucial role in facilitating the efficient movement of electrons within the photovoltaic devices. Its distinctive spherical, cage-like structure, composed of 60 carbon atoms with a conjugated π -electron system, enables high electron mobility, thereby reducing charge recombination losses and improving overall device efficiency [62–64]. Mehrabian et al. demonstrated the numerical optimization of cesium tin-germanium triiodide/antimony selenide perovskite solar cell with fullerene nanolayer, which achieved to a power conversion of 11.42 % in 2025 [65]. Beyond its superior charge transport properties, C_{60} acts as an effective interfacial layer between the photoactive perovskite layer and the electrode, ensuring efficient electron extraction and transfer to the external circuit [66]. Its compatibility with diverse organic and inorganic materials enhances its versatility as an ETL in PSC architectures [67–69]. For instance, the effect of electron transporting layer (ETL) material on the performance of the perovskite solar cell has been studied through substituting the ETL with TiO_2 and C_{60} nanolayers in 2021 [70]. C_{60} and its derivatives also contribute to the long-term stability of PSCs by suppressing degradation pathways within the perovskite layer, extending operational lifetime [71–73]. For example, in 2021, Youners et al, was studied the unencapsulated C_{60} -doped solar cell exhibited superior ambient stability compared to the pristine device, owing to the enhanced hydrophobic nature and reinforced morphology of the doped PC_{61}BM electron transport layer and demonstrated power conversion efficiency of 17.46 % [66]. Another key advantage lies in their ability to passivate structural defects in perovskite crystals, which are known to impair solar cell performance [74,75]. Fullerenes effectively reduce trap states, minimize non-radiative recombination, and enhance charge carrier collection,

leading to higher power conversion efficiencies (PCEs) [76–78].

Despite these benefits, the molecular-level interactions between C60 and perovskite, particularly concerning adsorption energetics, binding sites, charge transfer dynamics, and the role of perovskite defects in modulating surface energetics, remain insufficiently explored. Further investigation into these aspects is crucial for optimizing fullerene-based electron transport layers (ETLs) in high-performance perovskite solar cells (PSCs). This study is significant as it illustrates the first investigation of inorganic perovskite RbGeBr₃ as a light-absorbing layer, paired with C₆₀ as the fixed electron transport layer (ETL), in six main PSCs configurations incorporating various hole transport layers (HTLs) and gold (Au) as the electron-collecting electrode (ECE). Subsequently, the Au contact is substituted with alternative ECEs—namely Nickel (Ni), Silver (Ag), and Chromium (Cr)—and eighteen distinct architectures are examined to determine the optimal configuration for investigating photovoltaic efficiency.

Fig. 1 presents an overview of the electrostatic structure of a PSC, comprising multiple layers of different materials [44], and it depicts the energy level of materials in the PSC structures. In this study, six basic planar structures were investigated as inorganic perovskite solar cells. The selection of materials for the different layers and their placement order was based on a thorough review of reliable sources, including studies on their counterparts and organic-mineral solar cells in this field [37,40]. The goal of this study was to investigate the behavior of RbGeBr₃ mineral perovskite in a solar cell and compare its performance to that of cesium-based mineral perovskite solar cells, which have been explored both experimentally and theoretically [37,38]. In this investigation, all the structures share the same general configuration, as depicted in Fig. 1a. Each of the six inorganic PSCs begins with FTO as the initial transparent electrode layer [79], which allows light to pass through while conducting current, forming an ohmic contact with the C60 electron transport layer. The photovoltaic (PV) efficiency of perovskite solar cells (PSCs) is strongly influenced by the alignment of energy levels. Generally, for effective electron extraction at the ETL/absorber interface, the electron transport layer (ETL) must possess a higher electron affinity compared to the absorber layer. Conversely, the hole transport layer (HTL) should have a lower ionization energy than the absorber layer to enable efficient hole extraction at the absorber layer/HTL interface. Additionally, mismatches in energy bands at these interfaces significantly affect important PSC parameters.

As shown in Fig. 1b, C60 demonstrates excellent alignment with the absorber material RbGeBr₃ [80], which promotes efficient electron extraction and transport. RbGeBr₃, possessing a bandgap of 1.49 eV, absorbs light to generate charge carriers. These carriers are effectively separated and moved through the system due to optimal energy band alignment [79]. The hole transport layers (HTLs); Cu₂O[81], Spiro-OMeTAD[82], CuSCN[81], NiO[83], P3HT[82], and PEDOT: PSS[79], are designed to extract and transport holes while blocking electrons, thereby reducing recombination losses. Back Metal Contacts[82,84], collect holes and enable efficient charge transfer to the external circuit. Energy level disparities between these layers produce a built-in electric

field that drives charge carrier movement, while the well-matched band alignment ensures electrons and holes are efficiently separated and transported to their respective electrodes. This coordinated mechanism reduces recombination losses, leading to a high power conversion efficiency.

The electron transport layer (ETL) is composed of the semiconductor material C₆₀ [85–87], with RbGeBr₃ acting as the light-absorbing layer [53,54]. The hole transport layers (HTLs) include both organic materials such as P3HT [51,88], PEDOT: PSS [51,89], and Spiro-MeOTAD [90–92], as well as inorganic materials like CuSCN [51,93], Cu₂O [94,95], and NiO [51,96,97]. In all structures, the electron-conducting electrode is initially replaced with gold (Au) [98]. For further investigation, Ag [98], Ni [97], and Cr [99] are substituted in the remaining architectures.

The multilayer sequence for the structures in this study is listed below, from the first desired configuration to the last structure:

- FTO/C60/RbGeBr₃/P₃HT/Au
- FTO/C60/RbGeBr₃/CuSCN/Au
- FTO/C60/RbGeBr₃/NiO/Au
- FTO/C60/RbGeBr₃/Spiro-OMeTAD/Au
- FTO/C60/RbGeBr₃/Cu₂O/Au
- FTO/C60/RbGeBr₃/PEDOT: PSS/Au

Table 1 illustrates the numerical parameters utilized in the electrical part. Here, N_c and N_v are the effective density of states of the conduction and valence bands, respectively. μ_e and μ_h are electron and hole mobility, respectively, χ is electron affinity, E_g is the material band gap, N_a and N_d are acceptor and donor densities, respectively.

Theory and general equations

The study employs the semiconductor module within a two-dimensional COMSOL simulator [100]. For the simulation to operate efficiently, optical characteristics are required. The material's complex refractive index is given by [101]

$$N(\omega) = n(\omega) + ik(\omega). \quad (1)$$

Here, $n(\omega)$ represents the real part of the refractive index, which influences light reflection, while $k(\omega)$ is the imaginary part, which plays a key role in stimulating the material's absorption of the solar spectrum. The absorption coefficient, which is critical for understanding the material's response to incident light, is given by the equation $\alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda}$ [101]. To determine how the material interacts with incident light, particularly within the solar spectrum at 1.5 AM, it is essential to understand the absorption coefficient. The carrier generation rate [101] is given by

$$G(x, \lambda) = \frac{4\pi}{hc} \int_{\lambda_1}^{\lambda_2} k(\lambda) \Phi(\lambda) \exp(-\alpha(\lambda)x) d\lambda. \quad (2)$$

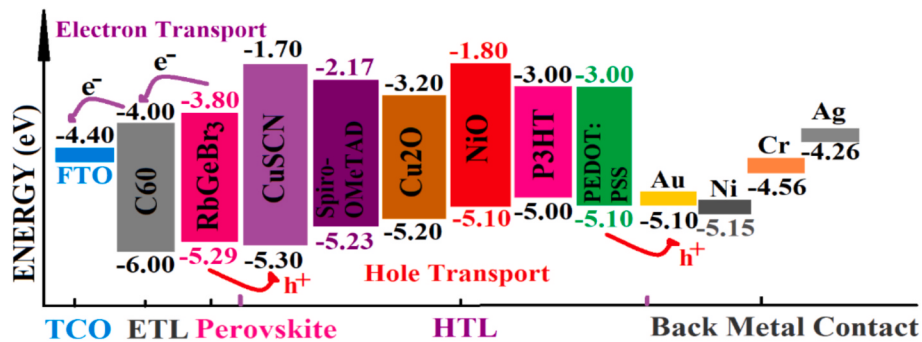


Fig. 1. The Energy alignment of all materials.

Table 1

The electrical parameters of PSC.

	ETL	Absorbing layer	HTL					
Parameter	C ₆₀	RbGeBr ₃	P ₃ HT300 nm	PEDOT:PSS	Spiro-MeOTAD	Cu ₂ O	NiO	CuSCN300 nm
Thickness	60 nm-90 nm	100 nm-300 nm		300 nm	300 nm	300 nm	300 nm	
The size of thickness								
χ (eV)	3.90	3.80	3.50	3.40	2.20	3.40	1.46	1.90
E_g (eV)	1.70	1.49	1.70	1.60	3.00	2.20	3.80	3.60
ϵ_r	4.20	7.00	3.00	3.00	3.00	7.50	10.7	10.0
N_c (cm ⁻³)	8×10^{19}	3.76×10^{19}	2×10^{21}	2.2×10^{15}	2.2×10^{18}	2×10^{19}	2.8×10^{19}	2.2×10^{19}
N_v (cm ⁻³)	8×10^{19}	2.08×10^{18}	2×10^{21}	1.8×10^{18}	1.8×10^{19}	1×10^{19}	1×10^{19}	1.8×10^{18}
N_a (cm ⁻³)	0	2×10^{13}	3.7×10^{18}	3.7×10^{18}	5×10^{18}	5×10^{18}	1×10^{18}	5×10^{18}
N_d (cm ⁻³)	1×10^{17}	0	0	0	0	0	0	0
μ_e (cm ² /V.s)	8×10^{-2}	8.5×10^2	1.8×10^{-3}	4.5×10^{-2}	2.1×10^{-3}	2×10^2	12.0	100
μ_h (cm ² /V.s)	3.5×10^{-3}	8.5×10^2	1.86×10^{-2}	4.5×10^{-2}	2.16×10^{-3}	8.6×10^3	2.80	2.50

The solar spectrum is represented by $\Phi(\lambda)$, with the range of incident wavelengths defined by λ_1 at 300 nm and λ_2 at 800 nm. This wavelength range is selected based on the fact that the investigated perovskite material (RbGeBr₃) has a band gap of 1.49 eV, and its extinction coefficient approaches zero at a wavelength of 800 nm. Fig. 2 illustrates the absorption coefficient of the RbGeBr₃ material [53,102].

In addition, the equations shown below can be used to calculate the cell's [103]. The difference between the photon current, I_{ph} , and the dark saturation current, I_0 , that is highly dependent on temperature, and V_a is the external voltage applied to the generated current. So, it is the net current I in the following equation as

$$I = I_{ph} - I_0 \left[\exp \left(\frac{eV_a}{K_B T} \right) - 1 \right] \quad (3)$$

The open-circuit voltage V_{oc} is written in Eq. (4). The quantity of I_0 represents the difference between the current density influenced by the applied voltage in the system and the current density in the absence of voltage, is given by

$$V_{oc} = \left(\frac{K_B T}{q} \right) \ln \left(\frac{J_{sc}}{J_0} \right). \quad (4)$$

The final efficiency is obtained as [103]

$$\eta = \frac{P_{max}}{P_{in}} = \frac{I_{max} V_{max}}{P_{in}} \quad (5)$$

In this context, P_{max} is the output power of the solar cell and P_{in} is the light input power, which in each PSC is equivalent to 100 mW/cm².

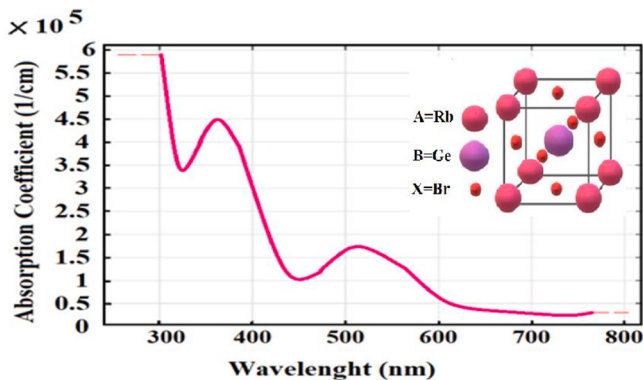


Fig. 2. The absorption coefficient of RbGeBr₃ material, and the cubic structure of RbGeBr₃ with the composition ABX₃.

Simulation results

The main purpose of this article is to design and study inorganic PSCs, where the inorganic perovskite material RbGeBr₃ is used as the light-absorbing layer, along with C₆₀ as the constant electron transport layer (ETL) in all architectures. However, the hole transport layer (HTL) materials vary between different configurations at a temperature of 300 Kelvin. Initially, six main structures, all with Au contacts, were investigated, and results for these PSCs were obtained. To further optimize performance, two steps were explored: In the first stage, the ETL thickness was increased from 60 nm to 90 nm, and the thickness of the light-absorbing layer (TAL) was increased from 100 nm to 300 nm.

The thickness of the HTL layer and the electron-collecting metal electrode (ECE) were maintained at 300 nm and 100 nm, respectively, as discussed in Section 4.1. In the second stage (Section 4.2), gold (Au) was replaced by nickel (Ni), chromium (Cr), and silver (Ag) as the ECEs, and the results were recalculated. Additionally, the effect of temperature on these PSCs was analyzed to identify the configuration with the highest efficiency. The four key solar cell parameters—short circuit current density (J_{sc}), open circuit voltage (V_{oc}), fill factor (FF), and power conversion efficiency (PCE)—were evaluated to compare the performance and efficiency of the most optimal structure.

The first step: The effect of increasing thickness

The thickness of the ETL and TALs was varied to determine the optimal values that maximize efficiency across different configurations. Specifically, the ETL thickness was increased from 60 nm to 90 nm, while the TAL thickness was varied from 100 nm to 300 nm. This analysis examined the impact of these changes on the four key performance metrics of the PSCs, highlighting the critical role that the relationship between these thicknesses plays in influencing overall efficiency.

I. FTO/C60/RbGeBr3/P3HT/Au

In the first architecture, where C₆₀ is the ETL, RbGeBr₃ is the light-absorbing layer, and Au is the electron-collecting metal electrode (ECE), and all of them are constant in all various structures, the HTL layer is P₃HT as an organic material. Fig. 3 shows the average terminal current density–voltage (J–V) and the output power–voltage (P–V) curve.

In the above situations, the J_{sc} is calculated at 19.86 mA/cm², the V_{oc} is approximately 0.94 V, as shown by the blue line. The red line illustrates that the P_{max} of the cell is 14.5 mW/cm². Fig. 4 illustrates the impact of increasing the ETL thickness from 60 nm to 90 nm and the TAL thickness from 100 nm to 300 nm on the four key performance metrics of PSCs.

Fig. 4a shows that as the thickness of the ETL layer increases from 60 nm to 90 nm, the J_{sc} generally decreases. The plot illustrates the strong impact of the thicknesses of ETL and TAL on PSC performance. The

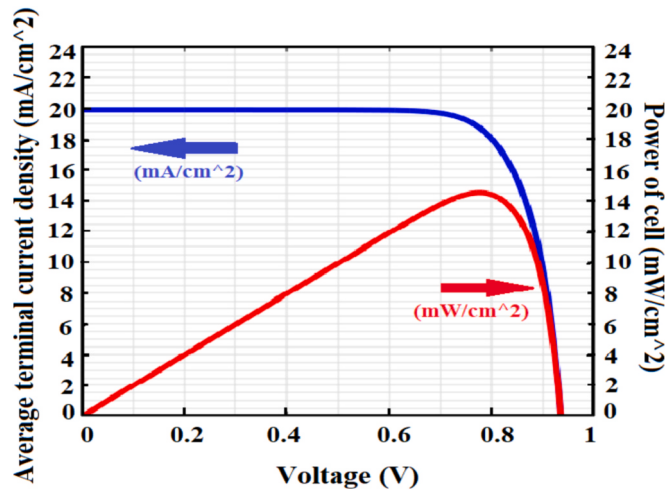


Fig. 3. The blue line represents the current–voltage (J–V) characteristics, while the red line illustrates the power–voltage (P–V) performance of the FTO/C60/RbGeBr₃/P₃HT/Au cell at 300 K.

highest J_{sc} , 22.47 mA/cm², occurs when the ETL is 60 nm and the TAL is 300 nm. It then steadily decreases to 11.79 mA/cm², as shown by the green line. The yellow and red lines follow a similar decreasing pattern as ETL thickness increases. With an increase in TAL thickness from 100 nm to 300 nm, there is a rise of about 2.61 mA/cm² in J_{sc} . Fig. 4b shows the relationship between ETL and TAL thickness and the open-circuit voltage V_{oc} . The maximum V_{oc} of 0.94 V is shown by the green line, but it decreases to about 0.91 V as the ETL thickness increases. Additionally, as the TAL increases from 100 nm to 300 nm, V_{oc} decreases, with the lowest V_{oc} of 0.84 V occurring when the ETL is 90 nm and TAL

is 300 nm. The increase in ETL thickness may raise the resistance to electron transport, leading to a decrease in voltage. Thicker TALs absorb more light and potentially generate more charge carriers, but require effective charge transport, which could be hindered by the increased resistance in the thicker ETL. Fig. 4c illustrates how efficiency is affected by the thickness of the ETL and TAL. When the TAL is 100 nm (green line), the efficiency starts at approximately 14.53 % and decreases to about 7.33 % as the ETL thickness increases. This decreasing pattern is similar to that seen in the other lines, with the lowest efficiency observed for the highest ETL thickness (90 nm). The TAL is responsible for light absorption and charge carrier generation; thicker TALs absorb more light, which can generate more charge carriers. The highest efficiency of 15.71 % is calculated when the TAL is 200 nm and the ETL thickness is 60 nm. However, even though increasing TAL thickness, from 200 nm to 300 nm, results in slightly lower efficiency (15.53 %), this could be due to increased recombination and challenges in transporting charge carriers through the thicker layers. Fig. 4d compares the fill factor (FF) of a solar cell relative to the ETL and TAL thicknesses. The green line (TAL = 100 nm) shows that as the ETL increases, the FF decreases from approximately 0.785 to around 0.775. The red line (TAL = 200 nm) demonstrates that FF is less sensitive to changes in ETL thickness. The yellow line indicates an optimal ETL thickness of around 80 nm for obtaining the maximum FF when the TAL is 300 nm, which is 0.793, with a slight decrease beyond this point. The sensitivity of the fill factor to ETL thickness varies with TAL, suggesting that the interaction between these layers needs to be carefully optimized for the best solar cell performance.

II. FTO/C60/RbGeBr₃/CuSCN/Au

In the second architecture, similar to the first structure, the ETL is C60, RbGeBr₃ as, the light-absorbing layer, and Au is the electrode; all of them are constant. However, the HTL layer is CuSCN an inorganic material. Fig. 5 illustrates the average terminal current density–voltage (J–

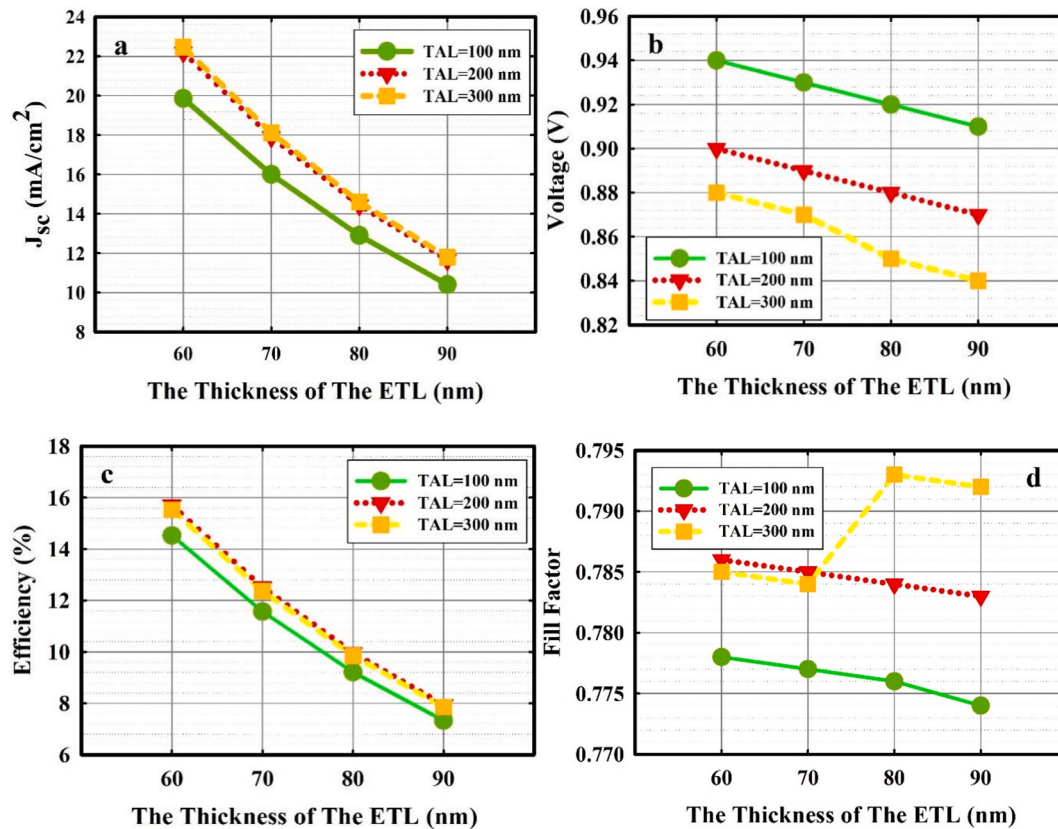


Fig. 4. The effect of increasing the thicknesses of the ETL, and TAL in the cell of FTO/C60/RbGeBr₃/P₃HT/Au on the four outputs, (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, (d) the results of the FF.

V) by the blue line and the output power voltage (P-V) by the red line.

The blue line shows the J_{sc} is calculated at 19.90 mA/cm^2 , the V_{oc} is approximately 0.95 V . The red line represents the P_{max} of the cell achieves 15.11 mW/cm^2 . Fig. 6 shows the effect of increasing the thickness of the ETL from 60 nm to 90 nm and the TAL from 100 nm to 300 nm on the four important factors of conclusion in PSCs, respectively. The yellow dashed line in Fig. 6a, where the TAL is 300 nm , shows the highest J_{sc} of 22.50 mA/cm^2 , which decreases significantly to 11.82 mA/cm^2 as the thickness of the ETL increases from 60 nm to 90 nm . However, by increasing the TAL from 100 nm to 300 nm , the J_{sc} has the usual increase from 19.90 mA/cm^2 to 22.50 mA/cm^2 . The highest J_{sc} for all lines is obtained in the lowest thickness of the ETL at 60 nm . Despite increasing the thickness of the ETL, the J_{sc} generally decreases across all lines in this figure. This decrease is due to the thicker ETL layer increasing the resistance to electron flow, thereby reducing the efficiency of charge collection. Fig. 6b shows the relationship between ETL thickness and voltage. The graph displays three lines representing various TALs. The maximum V_{oc} is calculated for the lowest thickness of the ETL at 60 nm in all lines.

The highest V_{oc} starts at approximately 0.95 V , which is decreased to about 0.91 V where the ETL is 60 nm and the TAL is 100 nm at the green line. For all three TAL values (100 nm , 200 nm , and 300 nm), the V_{oc} decreases steadily as the ETL thickness increases. The results indicate that thinner TALs (100 nm) maintain a higher voltage compared to the thicker TALs (300 nm). Fig. 6c illustrates that as the thickness of the ETL increases, the efficiency of the PSCs decreases steadily. Also, the efficiency depends on the TAL simultaneously. The highest efficiency, which is 16.29% , is observed at the thinnest of the ETL (60 nm), along with the TAL being 200 nm . TAL of 200 nm consistently shows the highest efficiency across all the ETL thicknesses, followed by 300 nm and then 100 nm . This conclusion depicts that an intermediate TAL yields better performance. Moreover, the green line in Fig. 6d represents where the thickness of the ETL varied from 60 nm to 70 nm , the FF increased sharply from approximately 0.801 to around 0.810 . Then it starts to decrease gradually from 0.81 to around 0.804 . Additionally, beyond 70 nm , the resistance starts to increase, so it can impede the movement of electrons, leading to increased recombination losses. Concerning the TAL, where the TAL is 100 nm , the optimal ETL thickness is around 70 nm , where the FF reaches its peak. As a result, the FF decreases gradually in the two remaining TALs. However, the FF shows less sensitivity when TAL is at 200 nm . This highlights how both the ETL and TAL thicknesses influence the four key performance factors of PSCs.

III. FTO/C60/RbGeBr₃/NiO/Au

In the third structure, the difference is in the change of the HTL to

NiO, an inorganic material, while all other conditions for investigation remain the same as in the two previous architectures. Fig. 7 depicts the J_{sc} is 19.92 mA/cm^2 , along with the V_{oc} of 0.95 V , at the blue line. Moreover, the P_{max} attains 15.27 mW/cm^2 as shown in the red line.

Fig. 8a shows how the J_{sc} is impacted by increasing the thickness of the ETL and the TAL in PSCs. In all three lines observed in this figure, by increasing the thickness of the ETL, the J_{sc} decreases steadily. The highest J_{sc} is 19.92 mA/cm^2 , where the thickness of the ETL is 60 nm and the TAL is 100 , then decreases sharply to 10.47 mA/cm^2 when the thickness of the ETL increases to 90 nm . This pattern is followed by the red line and the yellow line in this graph. By increasing the thickness of the ETL, the J_{sc} generally decreases due to the resistance to electron flow increasing, so it reduces the efficiency of charge collection. Simultaneously, when the TAL varies from 100 nm to 300 nm , the J_{sc} increases. The yellow line, where the TAL is 300 nm compared to the TAL is 100 nm , has the highest J_{sc} equal to 22.53 mA/cm^2 , where the ETL is 60 nm , then it decreases gradually to 11.83 mA/cm^2 , where the thickness of the ETL is 90 nm . In Fig. 8b, the green lines, where the TAL is 100 nm , by increasing the thickness of the ETL from 60 nm to 90 nm ; the maximum V_{oc} equals to 0.95 V decreases to approximately 0.92 V . Both remaining lines (the red line and the yellow line), also shows a decreasing trend in voltage with increasing ETL thickness and the TAL. There is an optimal ETL thickness for each TAL that maximizes the V_{oc} . Beyond this optimal thickness, the increasing resistance causes a decline in voltage. Additionally, Fig. 8c illustrates that as the TAL increases from 100 nm to 200 nm , the efficiency rises from 15.27% to about 16.48% . However, the efficiency decreases slightly to 16.27% when the TAL reaches 300 nm . These findings indicate that the highest efficiency across different TAL values occurs when the ETL thickness is at its lowest, around 60 nm . All three lines demonstrate that for all TAL values, the efficiency decreases sharply as the ETL thickness increases due to the rising resistance and potential recombination losses. For example, the highest efficiency of 16.48% occurs when the ETL is 60 nm and the TAL is 200 nm , while in the red line, the efficiency drops to 8.33% . Therefore, optimizing both the ETL and TAL is crucial for achieving maximum efficiency in PSCs. Fig. 8d shows a graph comparing the fill factor (FF) of the PSCs as a function of ETL and TAL thickness. In the green line, where the TAL is 100 nm , the FF decreases gradually from 0.806 to 0.802 as the ETL thickness increases from 60 nm to 90 nm . This decreasing trend is observed in the red and yellow lines as well.

As the ETL thickness increases, the resistance or energy mismatching at high thicknesses may increase, leading to higher recombination losses and a reduction in FF. Moreover, as the TAL increases, FF steadily decreases. While thicker TALs can enhance light absorption, they may also increase recombination, which negatively affects the FF.

IV. FTO/C60/RbGeBr₃/Spiro-MeOTAD/Au

In the fourth design, the HTL is Spiro-MeOTAD as an organic material. Fig. 9 illustrates the average terminal circuit density with the blue line, and the red line shows the output power as a function of applied voltage. The J_{sc} is at 19.88 mA/cm^2 , the V_{oc} is at 0.92 V , and the output power is at 14.85 mW/cm^2 .

Fig. 10a illustrates that when the thickness of the ETL increases from 60 nm to 90 nm , the J_{sc} initially reaches its highest value and then steadily decreases from 22.49 mA/cm^2 to around 11.81 mA/cm^2 . This decrease corresponds to the yellow line, where the ETL thickness is 60 nm and the TAL is 300 nm . The red line, where the TAL is 200 nm , shows that the J_{sc} started slightly lower than the yellow line, reaching about 22.22 mA/cm^2 before decreasing. The green line follows this J_{sc} 's pattern as mentioned above. The graph indicates how the ETL and TAL play crucial roles in the final J_{sc} results. Fig. 10b specifies the impact of the ETL thickness and the TAL on the voltage. The V_{oc} experiences decrease by increasing the thicknesses of the ETL and the TAL, as shown in Fig. 10b. In the green line, where the TAL is 100 nm and the thickness of the ETL varies from 60 nm to 70 nm , the maximum V_{oc} is 0.92 V , then it slowly decreases to 0.90 V . Similarly, as both TAL and ETL thickness increase, the V_{oc} decreases in both remain lines. The red line with the

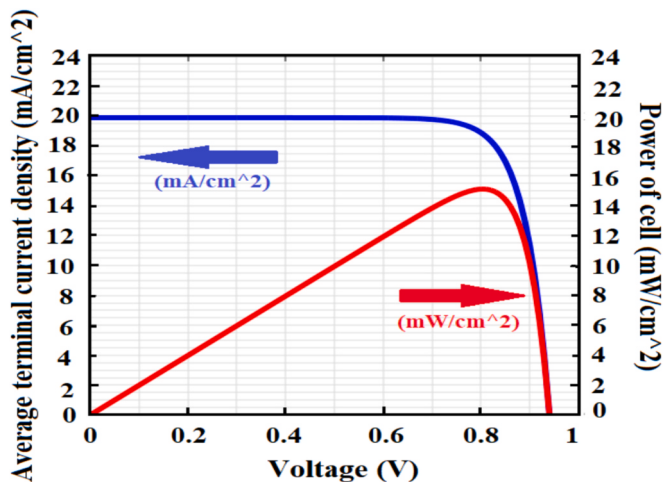


Fig. 5. The blue line represents the current–voltage (J-V) characteristics, while the red line illustrates the power–voltage (P-V) performance of the FTO/C60/RbGeBr₃/CuSCN/Au cell at 300 K .

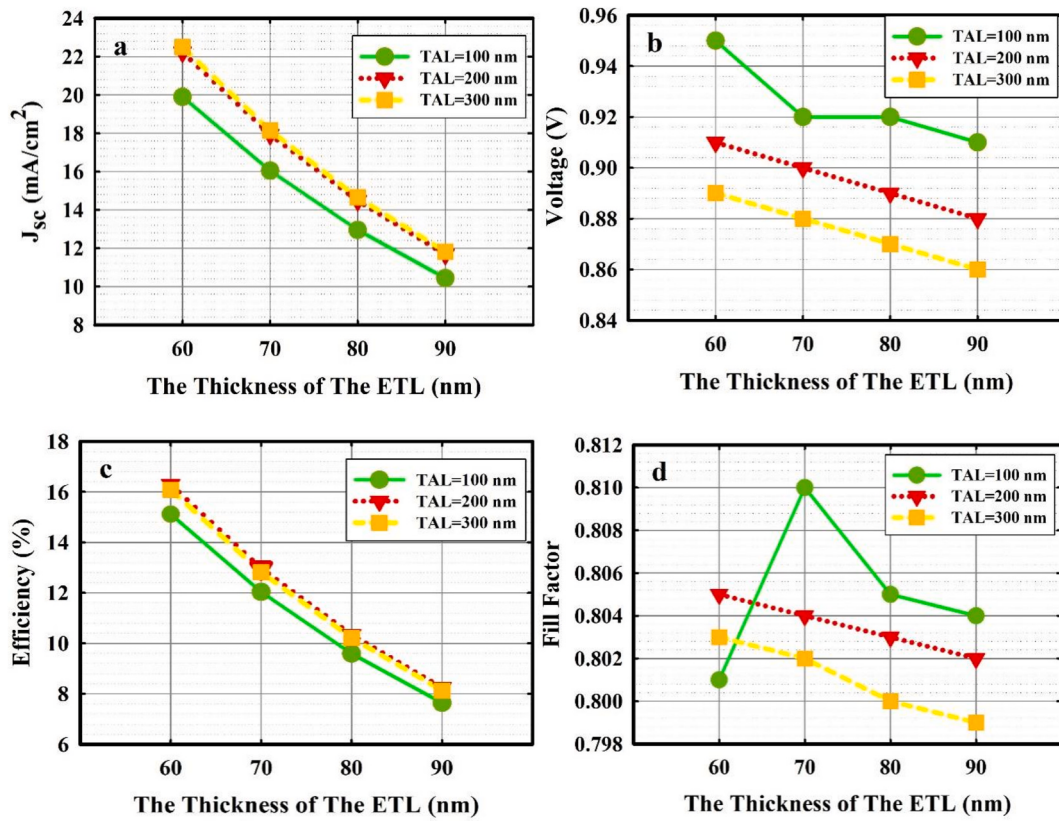


Fig. 6. The effect of increasing the thicknesses of the ETL and TAL in the cell of FTO/C60/RbGeBr₃/CuSCN/Au on the four outputs, (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, (d) the results of the FF.

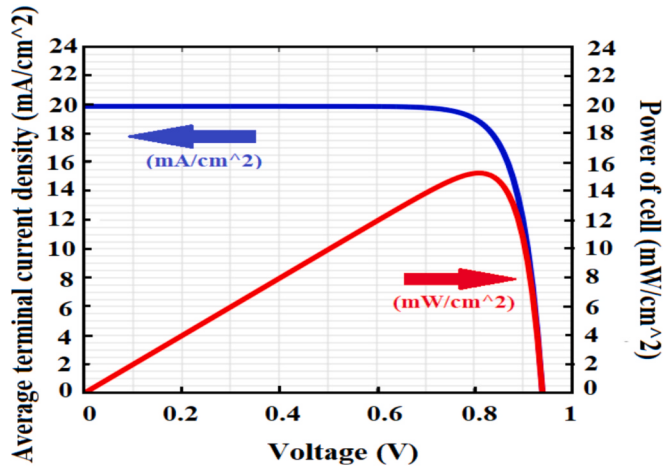


Fig. 7. The blue line represents the current-voltage characteristics, while the red line illustrates the power-voltage performance of the FTO/C60/RbGeBr₃/NiO/Au cell at 300 K.

TAL equals 200 nm and the yellow line with the TAL equals 300 nm, showing the V_{oc} starts at 0.90 V and 0.88 V, respectively. However, both decrease by about 0.03 V when the ETL thickness reaches its maximum of 90 nm. As the ETL thickness increases, the resistance to electron transport can rise, leading to a reduction in voltage. Thicker TALs generally absorb more light, potentially generating more charge carriers. However, thicker layers also require effective charge transport, which may be hindered by the increased resistance in a thicker ETL. Fig. 10c shows the efficiency, which varies with increasing ETL and TAL thicknesses. The lowest ETL thickness for all TALs corresponds to the

highest efficiencies. Among these, the maximum efficiency of 16.13 % is observed when the TAL is 200 nm, as shown by the red line. As the ETL thickness increases, the efficiency decreases by approximately 7.97 percentage points when the ETL reaches 90 nm. The yellow line shows a minimal decrease of about 0.27 percentage points when the TAL thickness increases to 300 nm. This slight reduction may be attributed to decreased recombination losses and the impact of thicker TALs on charge carrier transport. Moreover, the green line in Fig. 10d shows that when the ETL thickness increases from 60 nm to 70 nm, the fill factor (FF) decreases from approximately 0.810 to around 0.803. It continues to decrease gradually, reaching 0.801. This trend can be explained by the increasing resistance with thicker ETLs, which impedes electron movement and leads to higher recombination losses. For a TAL of 100 nm, the optimal ETL thickness is around 60 nm, where the FF reaches its peak. The red and yellow lines show that the FF stabilizes at around 0.806 when the ETL thickness is 60 nm and 70 nm. However, the FF is less sensitive to changes in ETL thickness when the TAL is 200 nm. These findings demonstrate the influence of both ETL and TAL on the four key performance factors of PSCs.

V. FTO/C60/RbGeBr₃/PEDOT: PSS/Au

In the fifth structure, the HTL is PEDOT: PSS as an organic material. The other layers are the same as the four configurations mentioned above. The average terminal circuit density (J-V), the output power are illustrated in Fig. 11. The blue line in Fig. 11 shows that the highest J_{sc} is 19.78 mA/cm² and the maximum V_{oc} is 0.92 V, where the thickness of the ETL is 60 nm and the TAL is 100 nm. The red line represents the power of the cell equal to 14.60 mW/cm². Fig. 12 illustrates the effect of the increasing thicknesses of the ETL and the TAL on the output results in PSCs. Plot 12a shows the lowest thickness of the ETL for all TALs, resulting in the highest J_{sc} . Among the highest values of J_{sc} for different TALs, the maximum J_{sc} is 22.48 mA/cm², which belongs to the TAL equal to 300 nm. The red line, where the TAL is 200 nm, has slightly

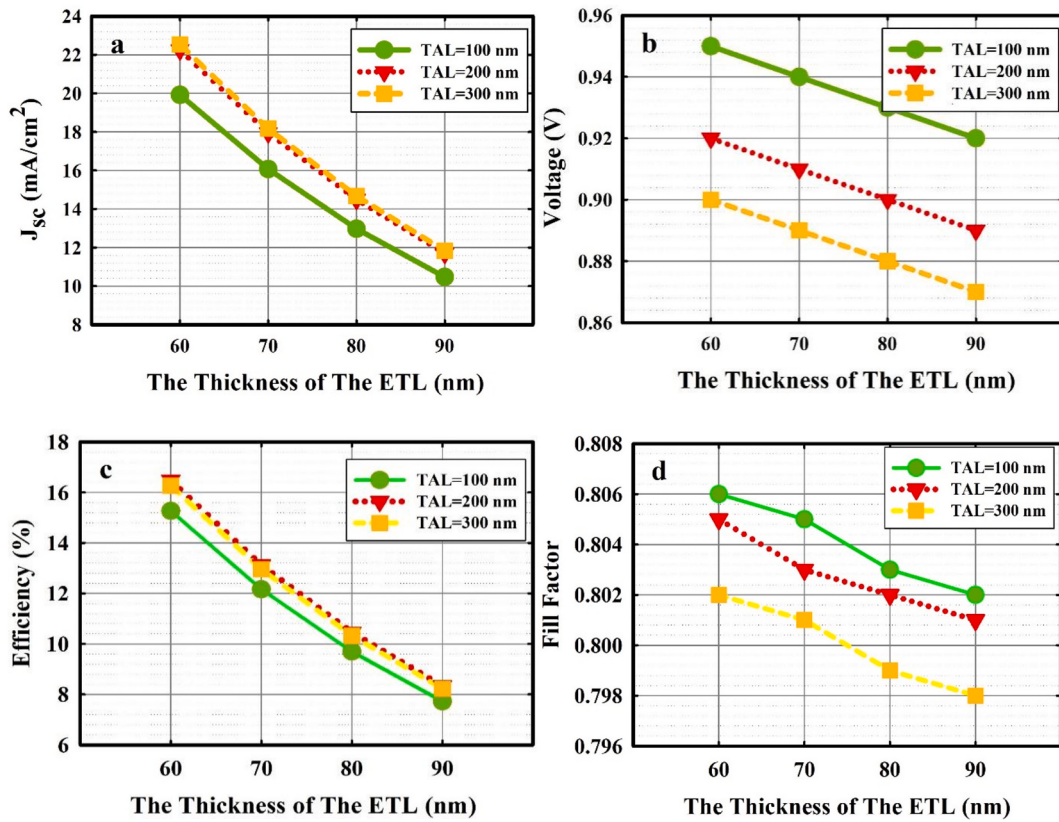


Fig. 8. The effect of increasing the thicknesses of the ETL, and TAL in the cell of FTO/C60/RbGeBr₃/NiO/Au on the four outputs, (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, (d) the results of the FF.

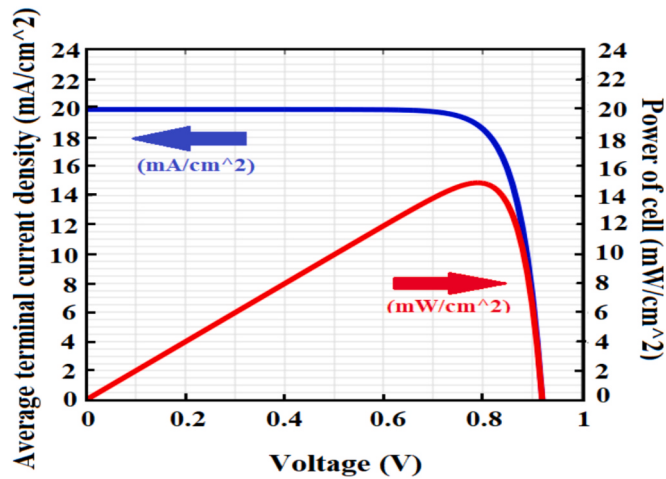


Fig. 9. The blue line represents the current-voltage characteristics, while the red line illustrates the power-voltage performance of the FTO/C60/RbGeBr₃/Spiro-MeOTAD/Au cell at 300 K.

different values in all the thicknesses of the ETL by about 0.20 mA/cm² in comparison to the yellow line.

However, where the ETL increases from 60 nm to 90 nm, in all three lines indicates that the J_{sc} decreases gradually. For instance, in the green line, the J_{sc} starts from 19.87 mA/cm² and then decreases significantly to 10.42 mA/cm², which is the lowest value in all thicknesses. Fig. 12b shows the impact of increasing the ETL and TAL thicknesses on voltage. All three lines illustrate that as the ETL thickness increases, the V_{oc} steadily decreases.

This is due to the increased resistance caused by a thicker ETL, which

negatively affects the voltage. The highest V_{oc} of 0.92 V is observed when the TAL is 100 nm, but it decreases to 0.89 V as the ETL thickness increases. Similarly, as the TAL increases, the V_{oc} generally decreases. The yellow line, where the TAL is 300 nm, starts with the lowest initial V_{oc} of 0.88 V, suggesting that thicker TALs are more prone to voltage drops due to increased recombination and resistance. Fig. 12c illustrates the efficiency trend concerning ETL and TAL thicknesses. As the TAL increases from 100 nm to 200 nm, the efficiency increases, reaching a maximum value of 15.92 %. The yellow line, where the TAL is 300 nm, follows a similar trend to the red line, with only a slight difference in values. Fig. 12d shows the relationship between the fill factor (FF) and the thicknesses of the ETL and TAL. It demonstrates an inverse behavior for FF as the ETL thickness increases for all TAL values. The FF starts at 0.803 when the ETL is 60 nm and increases slowly to a peak value of 0.805. However, when the TAL increases to 300 nm, the FF gradually decreases to 0.796, a 0.07 difference compared to the TAL of 100 nm. These results represent the need for careful optimization of the interplay between these layers to achieve the best PSC performance.

VI. FTO/C60/RbGeBr₃/Cu₂O/Au

In the sixth structure, the HTL is Cu₂O as an inorganic material. The other layers are the same as the five structures mentioned above. Fig. 13 represents the average terminal circuit density (J -V) equal to 19.89 mA/cm², and the output power is 14.9 mW/cm² in the blue line and the red line, respectively. Additionally, the V_{oc} is 0.92 V, which is the highest voltage.

Fig. 14a shows the impact of the ETL and TAL thicknesses on J_{sc} in this configuration. As the ETL thickness increases, J_{sc} decreases significantly; however, increasing the TAL thickness results in a slight increase in J_{sc} . The highest and lowest J_{sc} are observed under different conditions. When the ETL is 60 nm and the TAL is 300 nm, the highest J_{sc} is 22.49 mA/cm², while the lowest J_{sc} , 10.44 mA/cm², occurs when the ETL is 90 nm and the TAL is 100 nm. Fig. 14b illustrates that the

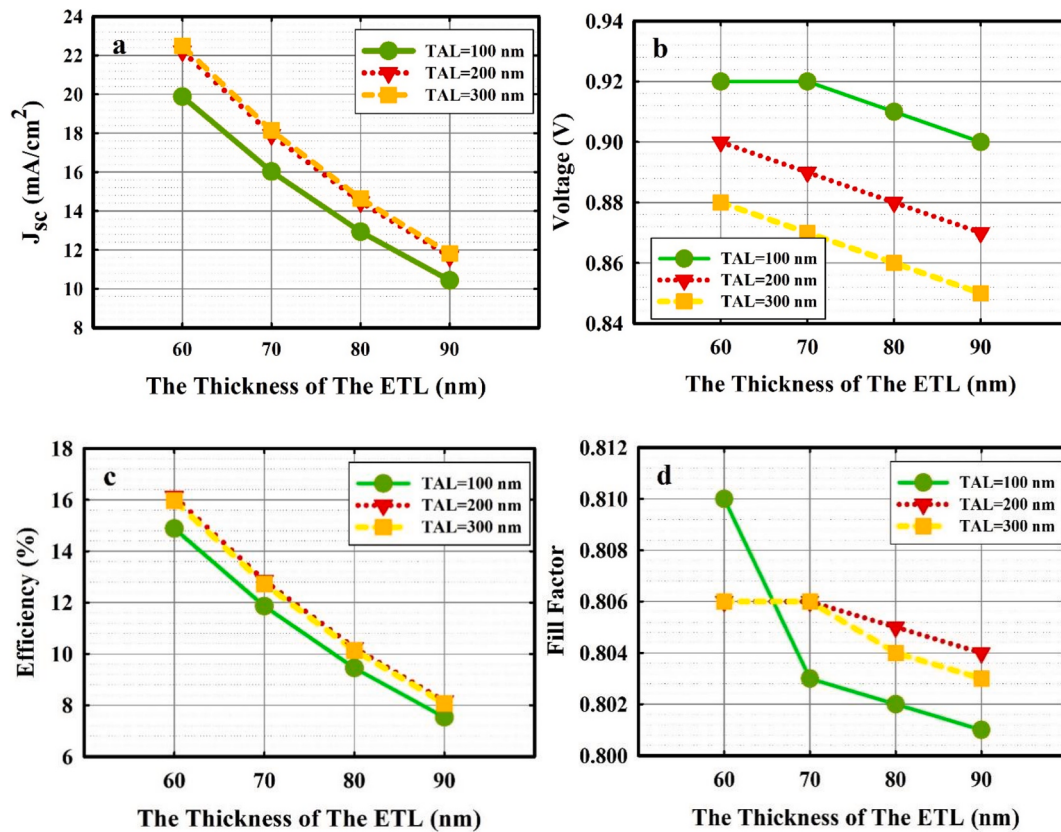


Fig. 10. illustrates the effect of increasing the thicknesses of the ETL and TAL in the cell of FTO/C60/RbGeBr3/Spiro-MeOTAD/Au on the four outputs: (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, and (d) the results of the FF.

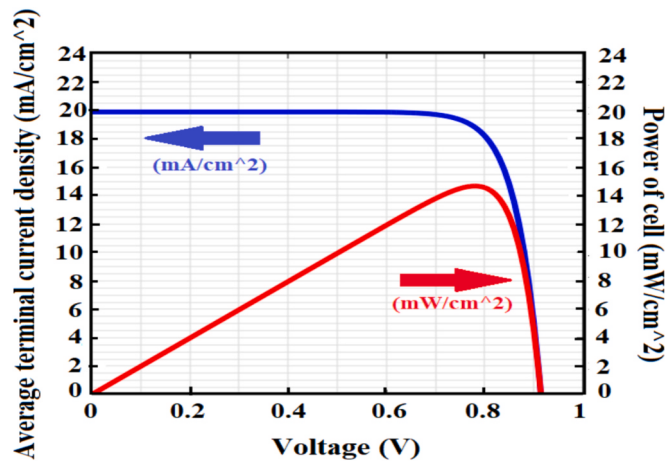


Fig. 11. The blue line represents the current-voltage characteristics, while the red line illustrates the power-voltage performance of the FTO/C60/RbGeBr3/PEDOT: PSS/Au cell at 300 K.

maximum V_{oc} is 0.94 V (green line), which then decreases slightly to 0.91 V on the same line. For the TAL of 200 nm and ETL thickness of 60 nm, V_{oc} is 0.90 V and decreases by about 0.03 V. The graph indicates that as the TAL thickness increases, V_{oc} becomes less sensitive to changes in the ETL thickness.

Moreover, when the TAL increases from 100 nm to 300 nm, the highest efficiencies exhibit minimal differences, with the lowest ETL thickness yielding the highest efficiencies across all TALs, as shown in Fig. 14c. The highest efficiency, 16.07 %, is seen in the red line. The yellow line, with a TAL of 300 nm, is very close to the red line, with

minimal differences in values at all points. Fig. 14d shows that when both the ETL and TAL thicknesses are thinner, the optimal FF is achieved. The highest FF, 0.813, decreases slightly to 0.810 in the green line. However, this is still the highest FF compared to the thicker TALs, as shown by the red and yellow lines. This suggests that the optimal ETL and TAL thicknesses, and their interplay in transporting or generating electrons, have a crucial effect on the key outputs of the solar cells.

The second step: The influence of different electrodes

In the first step, as discussed above, and in the analysis of the results from the figures and plots, further investigation was conducted by replacing the usual electron-collecting metal electrode (ECE) of Au with other metals such as Ni, Ag, and Cr. The work function of Au, commonly used in PSCs, is $\varphi_m = 5.1\text{eV}$. Additionally, all of these metals can be employed as ECEs in PSCs. These materials have specific advantages: Ni offers good mechanical and thermal properties, enhancing electron transport; Ag, known for its high electrical conductivity, is widely used in solar cell junctions and electrodes; and Cr, with its good mechanical properties and corrosion resistance, can improve the long-term stability of the solar cell. In this study, a Schottky diode was employed due to its lower voltage drop compared to conventional diodes, which helps minimize energy losses. The general trend observed indicates that as the contact metal's work function decreases, the devices' shunt resistance and open-circuit voltage decrease, resulting in sloped current density (J - V) curves at the short-circuit point [104]. Incorporating these metals with the Schottky diode can enhance the stability and extend the lifespan of the solar cells. The work functions of Ag, Ni, and Cr, used in this investigation, are $\varphi_m = 4.26\text{eV}$, $\varphi_m = 5.15\text{eV}$, and $\varphi_m = 4.5\text{eV}$ respectively [84,105]. The highest efficiencies were measured for all six basic Au configurations, which were studied with the different ECEs. In the new structures, the ETL layer is C₆₀ with a thickness of 60 nm, the HTL

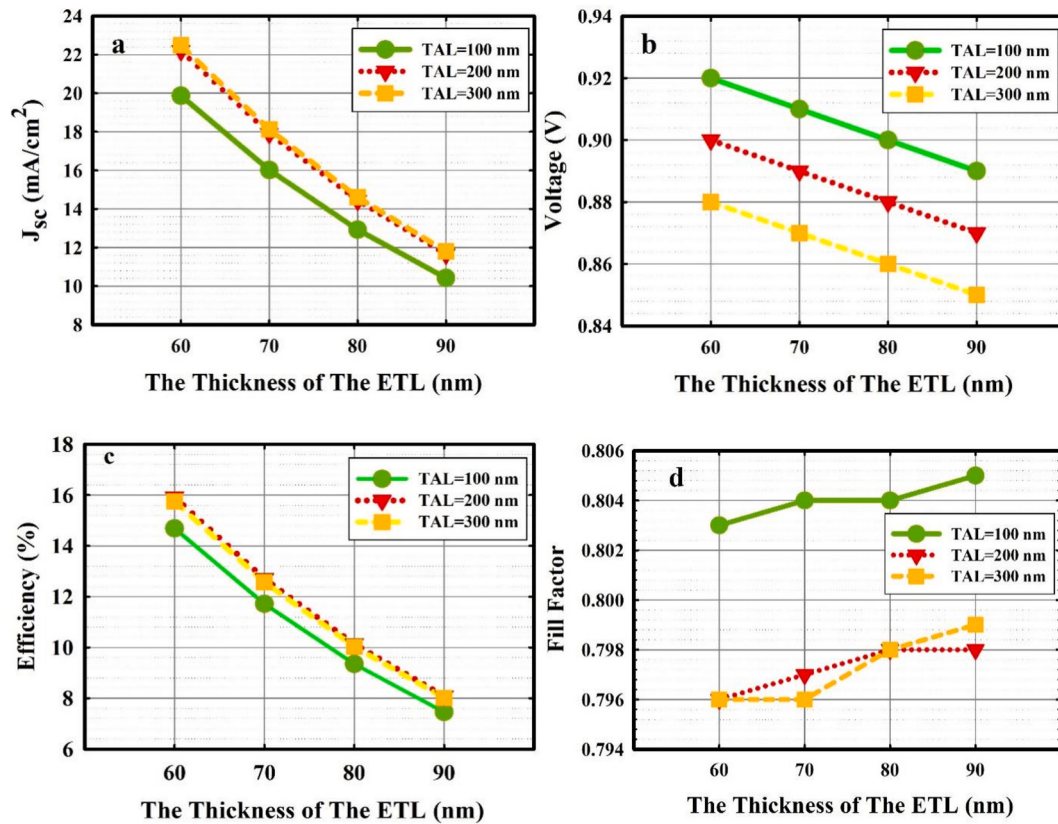


Fig. 12. Illustrates the effect of increasing the thicknesses of the etl, and tal in the cell of FTO/C60/RbGeBr₃/PEDOT: PSS/Au on the four outputs, (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, (d) the results of the FF.

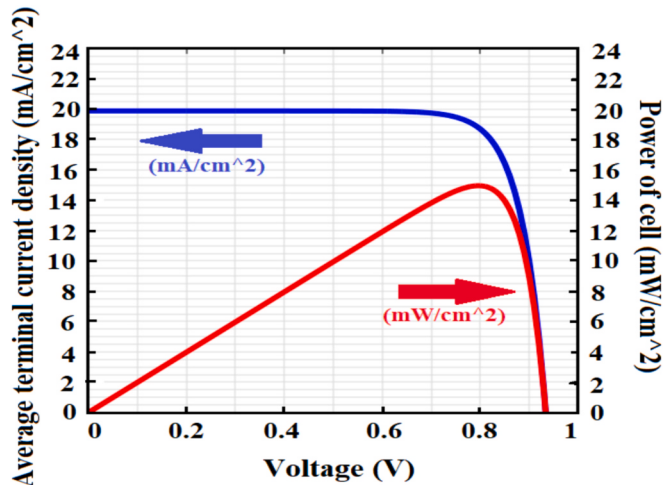


Fig. 13. The blue line represents the current-voltage (J-V) characteristics, while the red line illustrates the power-voltage (P-V) performance of the FTO/C60/RbGeBr₃/Cu₂O/Au cell at 300 K.

layer has a constant thickness of 300 nm, the light-absorbing layer is RbGeBr₃, which varies in thickness from 100 nm to 300 nm, and the ECEs are maintained at a constant thickness of 100 nm.

I. FTO/C60/RbGeBr₃/P₃HT/Au, Ag, Ni, and Cr

In the first structure, FTO/C₆₀/RbGeBr₃/P₃HT/Au, the ECEs (Ag, Ni, and Cr) replace Au. Fig. 15a illustrates the impact of these changes on the output results of the PSCs. It shows that as the TAL increases from 100 nm to 300 nm, J_{sc} increases gradually for all ECEs in Fig. 15a. This suggests that the TAL plays a crucial role in light absorption and charge

carrier generation, as thicker TALs can absorb more light and potentially generate a greater number of charge carriers. The highest J_{sc} of 22.47 mA/cm² is observed for both Ni and Au, followed by Ag at 22.45 mA/cm² and Cr at 22.43 mA/cm², showing a very small reduction. The maximum V_{oc} remains the same at 0.94 V but decreases to 0.88 V across all ECEs, as shown in Fig. 15b. Fig. 15c reveals that the highest efficiency of 15.72 % is achieved with the Au contact when the TAL is 200 nm. In the same configuration, replacing Au with Ni results in an efficiency of 15.7 %. Ag gives an efficiency of 13.68 %, and Cr results in the lowest efficiency of 10.77 %. The best FF value, shown in Fig. 15d, occurs when the TAL thickness is 200 nm. Both Au and Ni have an approximate FF of 0.785, making them the top performers for FF.

II. FTO/C60/RbGeBr₃/CuSCN/Au, Ag, Ni, and Cr

In the second structure, FTO/C₆₀/RbGeBr₃/CuSCN/Au, the contacts Au are replaced by Ni, Ag, and Cr. Fig. 16 illustrates the impact of these changes on the output results of PSCs. Additionally, Fig. 16a shows that the J_{sc} for all the ECEs increases softly when the TAL varies from 100 nm to 300 nm. The highest J_{sc} is 22.50 mA/cm², related to Au, where the TAL is 300 nm. It can be compared to the remaining ECEs, which depict the highest value of approximately 14.65 mA/cm². Fig. 16b, where the TAL is 100 nm, shows that the maximum V_{oc} equals 0.95 V, with an ECE of Au, then decreases to 0.92 V, the highest V_{oc} for the remaining ECEs. Where the TAL is 200 nm, the maximum efficiency is obtained for all ECEs as shown in Fig. 16c. Refers to Au contact, the highest efficiency is 16.29 %, and the second place is Ni contact with 10.34 %. Fig. 16d depicts where the TAL rises from 100 nm to 300 nm, the FF decreases for all ECEs, except Au contact, which indicates different behavior between ECEs.

III. FTO/C60/RbGeBr₃/NiO/Au, Ag, Ni, and Cr

The third configuration with different ECEs and their effect on the final results of PSCs is investigated. In these structures, where the TAL increases from 100 nm to 300 nm, the J_{sc} increases gradually in all ECEs.

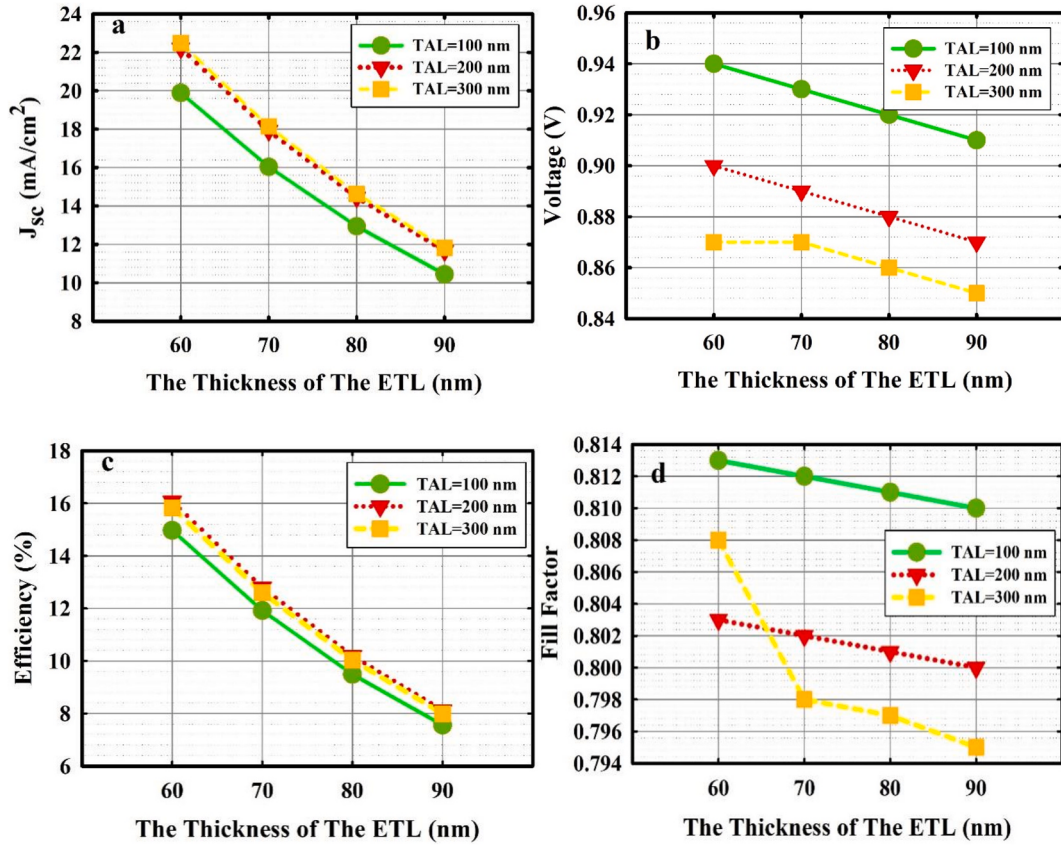


Fig. 14. Illustrates the effect of increasing the thicknesses of the etl, and tal in the cell of FTO/C60/RbGeBr₃/Cu₂O/Au on the four outputs, (a) the results of the J_{sc} , (b) the results of the V_{oc} , (c) the results of the efficiency, (d) the results of the FF.

The maximum J_{sc} is 22.53 mA/cm², which belongs to Au, then decreases very slightly by about 0.03 mA/cm² with Cr contact when the TAL is thicker, as illustrated in Fig. 17a. Fig. 17b depicts the highest V_{oc} is 0.95 V, the same for all ECEs, except Ni, which has a minimal difference of about 0.01 V with them. These values of the V_{oc} are obtained when the TAL has the thinnest thickness. Where the TAL is 300 nm, the V_{oc} decreases gradually to approximately 0.9 V for all ECEs in this design. Fig. 17c indicates that the highest efficiency is calculated at 16.48 %, the same for the Au and Ni contacts. In this situation, with the TAL is 200 nm, the lowest efficiency refers to the Cr contact with the 10.46 % efficiency. Where the TAL is 300 nm, the efficiencies for all ECEs show very small differences, with the TAL being 200 nm. For all ECEs, where the TAL rises, the FF decreases slightly, except for the Cr contact, which has the lowest FF in all the TALs. The highest FF is 0.816, which belongs to the Ni contact as depicted in the bar chart of the FF as shown in Fig. 17d.

IV. FTO/C60/RbGeBr₃/Spiro_OMeTAD/Au, Ag, Ni, and Cr

In the fourth configuration, by replacing the different ECEs, where the TAL changes from 100 nm to 300 nm, the J_{sc} increases softly in all ECEs; for instance, for Ni contact, the J_{sc} starts from 19.87 mA/cm² to 22.48 mA/cm², as shown in Fig. 18a. The highest J_{sc} is 22.49 mA/cm² with Au contact, and the lowest J_{sc} refers to Cr contact with 21.98 mA/cm², where the TAL is 300 nm. Fig. 18b shows that all the ECEs have approximately the same V_{oc} approximately in all TALs. The maximum V_{oc} is 0.92 V, then decreases to 0.88 V where the TAL is thicker. Fig. 18c depicts that when the TAL is 100 nm, the efficiency starts from 14.88 % for the Au contact, then it decreases sharply to 7.61 % for the Cr contact. TAL is 200 nm, indicating that all the ECEs have the highest efficiency related to themselves. In this circumstance, the efficiency of the Ni contact is 16.10 %, in comparison to Au, which has the highest efficiency equal to 16.13 %. The FF is decreased slightly by increasing the TAL in

all ECEs, as illustrated in Fig. 18d. The highest FF is equal to 0.813, which belongs to the Au contact, then the second place belongs to the Ni contact with the 0.811 value. The Cr contact shows the lowest FF in all TALs.

V. FTO/C60/RbGeBr₃/PEDOT:PSS/Au, Ag, Ni, and Cr

Fig. 19 shows that the fifth structure's conclusions are influenced when the ECEs vary and the TAL increases. Fig. 19a indicates that by increasing the TAL from 100 nm to 300 nm, the J_{sc} rises generally; for example, it starts from 19.85 mA/cm² to 22.44 mA/cm², which is the same value for Ag and Cr contacts. The highest J_{sc} is 22.48 mA/cm², which is for Au contact, then the J_{sc} of Ni is 22.47 mA/cm², where the TAL is 300 nm. As a result, the thicker TAL determines the highest J_{sc} in all ECEs. Fig. 19b illustrates that the highest V_{oc} is 0.92 V and the lowest V_{oc} is 0.88 V, which are the same values for all the ECEs in all TALs. Fig. 19c shows Au has the maximum efficiency of about 15.92 %, and the second place for efficiency belongs to the Ni contact, which is 15.89 %. Moreover, Ag and Cr have the same value of efficiency, which has the lowest efficiency at around 13.88 %. These efficiencies are calculated when the TAL is 200 nm, and it is observed that is the optimal thickness. When the TAL is increased and the ECEs are changed, the FF values indicate various behaviors as illustrated in Fig. 19d. For instance, the FF values related to Ag and Cr contacts represent the slow decrease from 0.705 to 0.691, where the TAL is 100 nm and the TAL is 300 nm, respectively. The optimal FF is approximately 0.802, which is related to Au contact.

VI. FTO/C60/RbGeBr₃/Cu₂O/Au, Ag, Ni, and Cr

Fig. 20 in the last configuration illustrates the impact of the various ECEs and TALs on the output results. Fig. 20a shows very small differences between values of the J_{sc} around 0.01 mA/cm² for all ECEs in every TAL. Au and Ni indicate the highest J_{sc} at 22.49 mA/cm² in the thicker TAL, which starts from 19.89 mA/cm² in the thinner TAL.

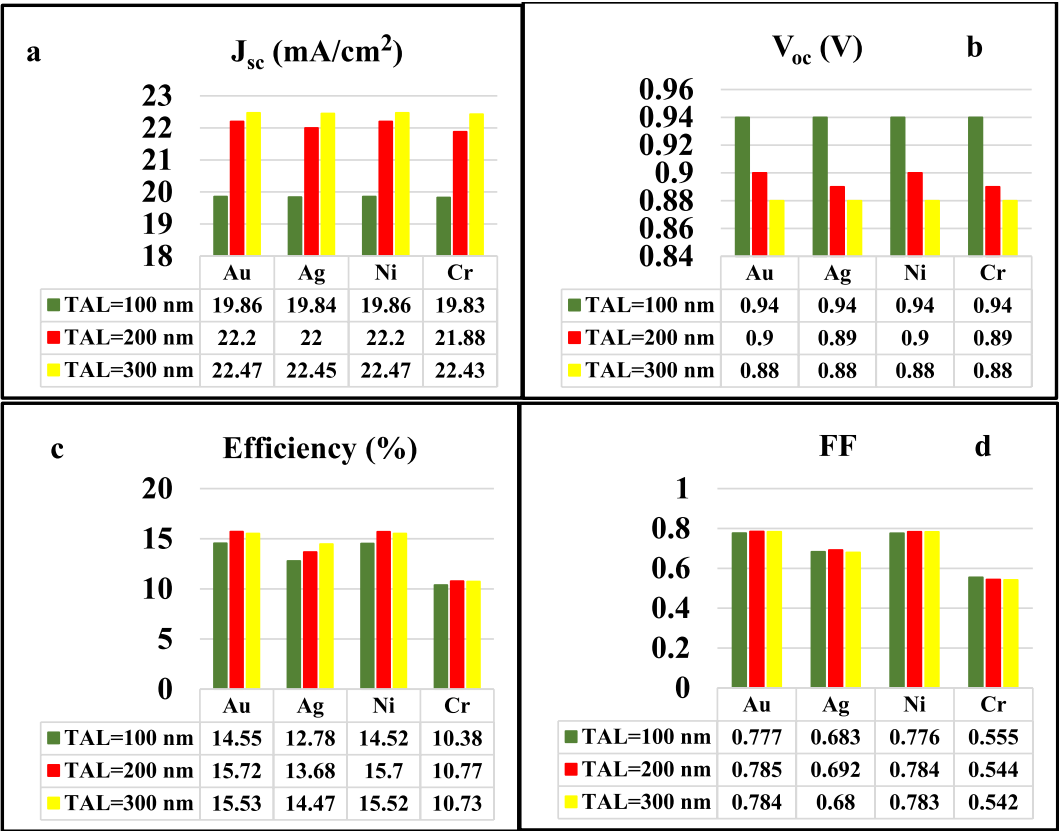


Fig. 15. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC containing FTO/C60/RbGeBr₃/P₃HT/contact.

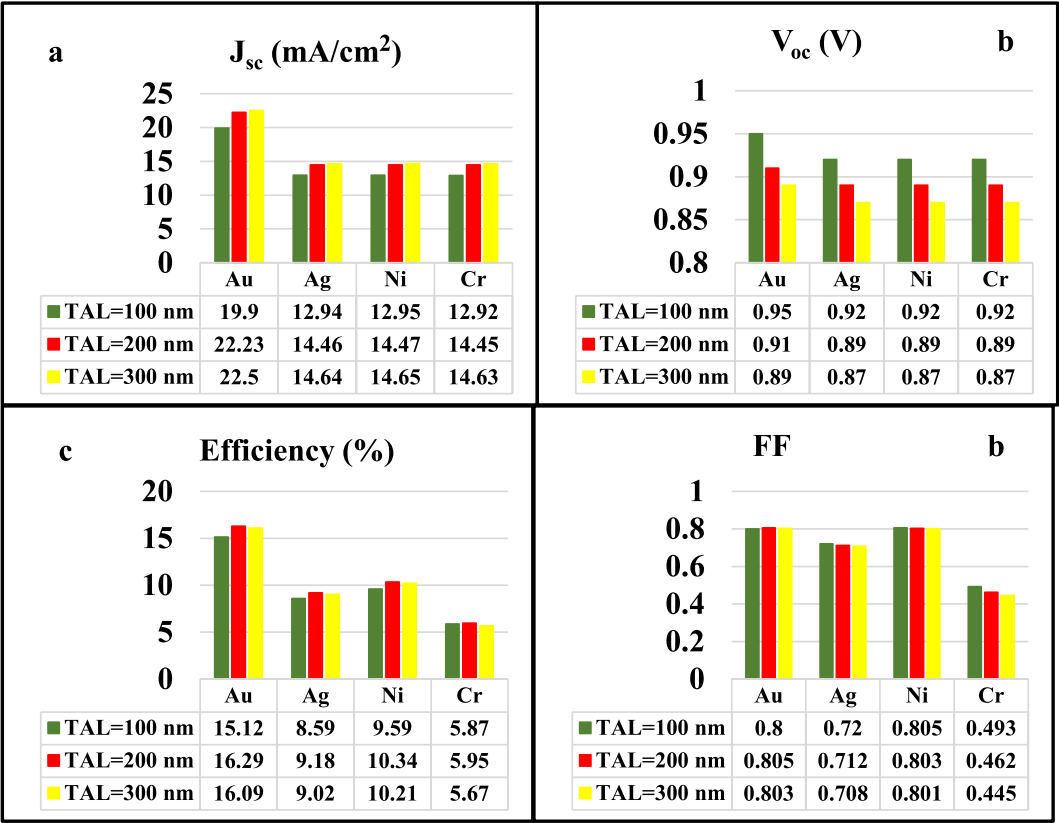


Fig. 16. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC containing FTO/C60/RbGeBr₃/CuSCN/contact.

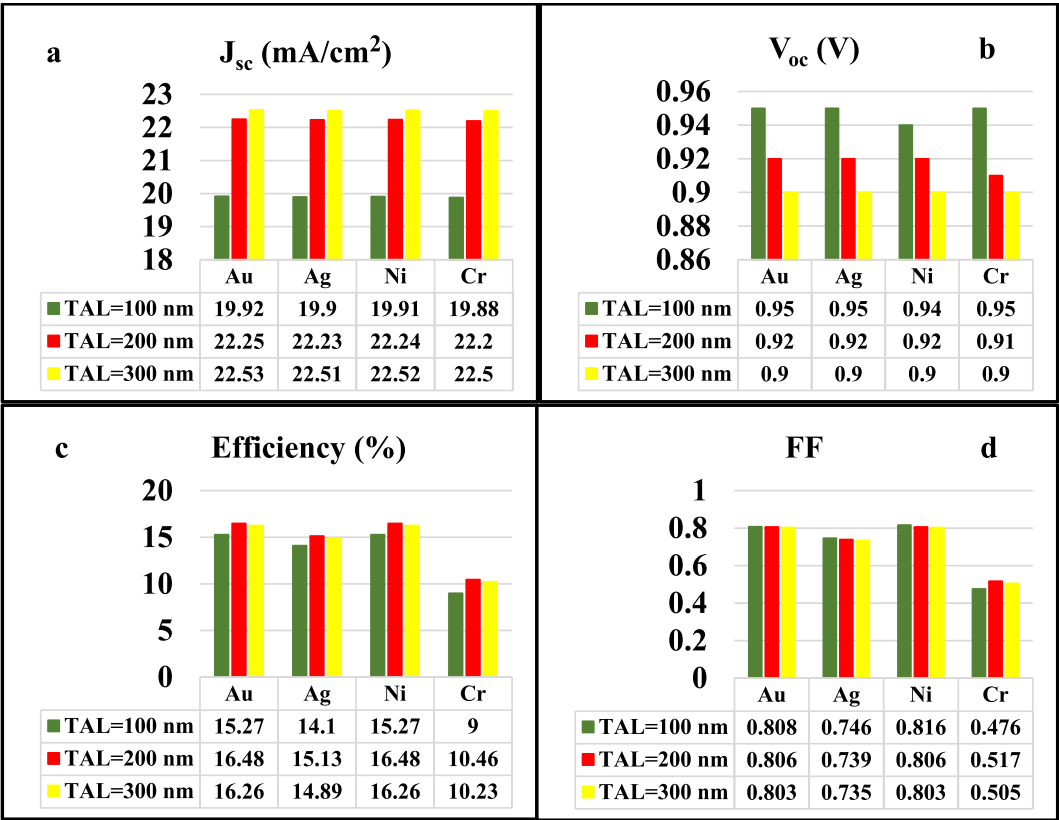


Fig. 17. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC containing FTO/C60/RbGeBr₃/NiO/contact.

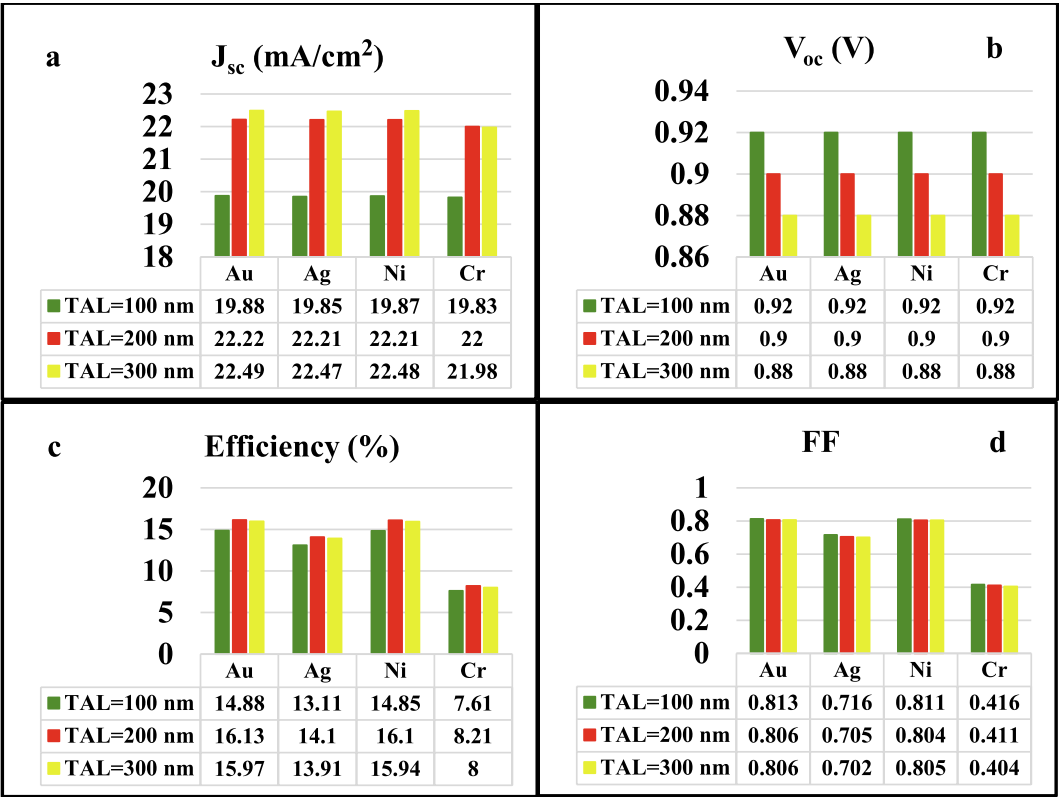


Fig. 18. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC containing FTO/C60/RbGeBr₃/Spiro-MeO-TAD/contact.

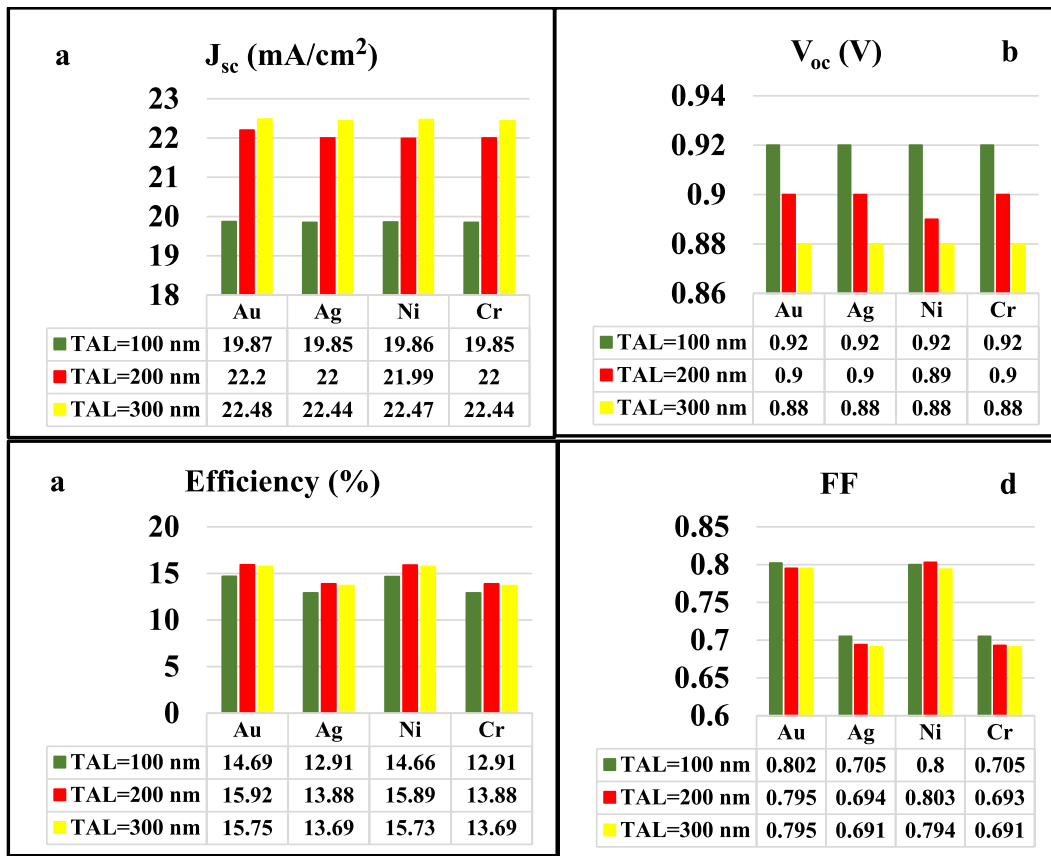


Fig. 19. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC containing FTO/C60/RbGeBr₃/PEDOT:PSS/contact.

Fig. 20b represents where the TAL is 100 nm, the maximum V_{oc} is 0.94 V, and it is the same for all ECEs, then it decreases to 0.87 V by increasing the TAL, except for Cr. The Au contact has the highest efficiency, equal to 16.07 %, where the TAL is 200 nm. Then, the second place is for Ni, which is 14.03 % in this condition, as illustrated in Fig. 20c. In this structure, where the TALs increase, all ECEs experience different behaviors related to the trend of the FF, as shown in Fig. 20d. For instance, the highest FF is 0.830 related to Au contact, where the TAL is 100 nm. However, the highest FF for Ni contact is calculated at 0.793, where the TAL is thicker.

Physical interpretation of key trends

As mentioned in the second part, “Design method for various PSCs with different HTLs”, the energy band diagram illustrates the arrangement of energy bands across the materials within a solar cell, demonstrating how their alignment facilitates the efficient flow of electrons and holes, which is essential for the device’s electrical conductivity. Proper energy band positioning is critical for optimal solar cell operation, as achieving high efficiency depends on careful material selection and precise tuning of energy levels. Materials used for the electron transport layer (ETL) and hole transport layer (HTL) typically possess higher electron affinities and ionization potentials compared to those of the perovskite layer, enabling effective charge separation and transport. Moreover, the thickness of the electron-transporting layer (ETL) and the thickness of the light-absorbing layer (TAL) have a crucial effect on the performance of PSCs. For the efficient performance of the PSCs, the TAL and ETL have to be varied from 100 nm to 300 nm and 60 nm to 90 nm, respectively. Also, the thickness of the hole-transporting layer (HTL) and the electron-collecting electrode (ECE) are constant at 300 nm and 100 nm, respectively.

The data about short-circuit current indicate that increasing the thickness of the absorber layer (TAL) led to a significant rise in the J_{sc} . This enhancement can be attributed to the increase in the probability of the electron-hole pair creation within the absorber layer, which directly augments charge carrier generation. On the other hand, increasing the TAL resulted in a higher chance for electron-hole recombination, which hindered efficient charge separation at the interfaces. This reduction in charge separation efficiency ultimately led to a decline in the V_{oc} [69,106]. Additionally, in most of the obtained data related to FF graphs, it has been represented that as the TAL increases, the slope of the FF graph declines slightly. This reduction is due to an enhanced chance for recombination or increased electrical resistance. It has also been reported that increasing the perovskite thickness leads to a decline in the FF due to an increase in electric resistance [107].

Moreover, the thickness of the ETL is enhanced from 60 nm to 90 nm, and the benefit thickness is found to be 60 nm. When the thickness of the ETL is increased above 60 nm, all data obtained from the graphs J_{sc} , V_{oc} , FF, and the power conversion efficiency of the device begin to decrease. This is due to the restriction of the transport of electrons to the FTO layer of the PSCs and due to an increase in the recombination of charge carriers, which reduces V_{oc} of the device, also the J_{sc} generally decreases due to the resistance to electron flow increase, so it is reducing the efficiency of charge collection. An increase in the thickness of ETL also causes a corresponding increase in the series resistance of the device, which in turn reduces the FF of the device [108].

To enhance the power conversion efficiency of PSCs, choosing the light-absorbing layer and the HTL combination is a crucial step. For optimal light harvesting and carrier transport from the perovskite absorb layer, the efficient absorb thickness with HTL is equally important [51]. In this paper, the thickness of the hole transport layer (HTL) is constant at 300 nm. The hole transporting material (HTM) is responsible

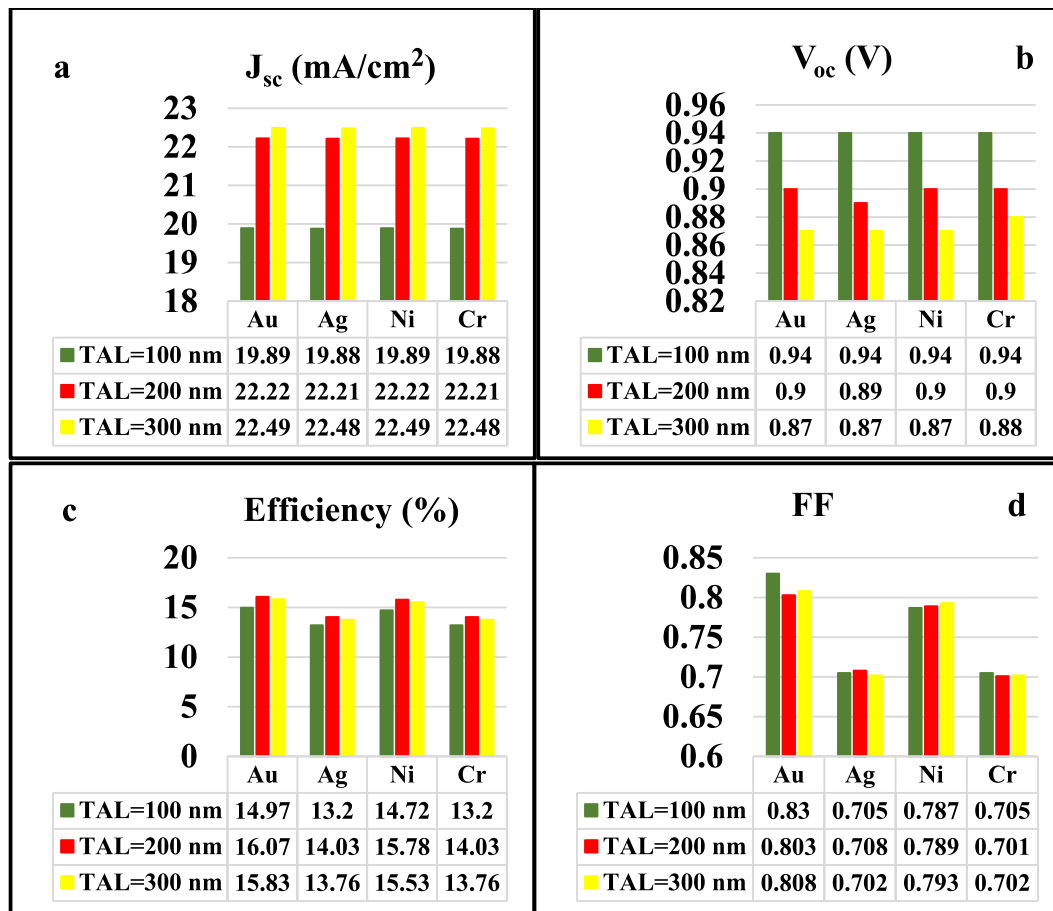


Fig. 20. The effect of various electron collectors (contact) of Au, Ag, Ni, and Cr on the four output results in a PSC contains of FTO/C60/RbGeBr₃/Cu₂O/contact.

for extracting holes from the light-absorbing layer (Perovskite) and transporting them to the back metal contact. For this purpose, the HTM's highest occupied molecular orbital (HOMO) must align with the perovskite's valence band (VB) to minimize energy barriers for hole extraction. Mismatching energy levels creates resistance, increasing recombination losses and reducing the open-circuit voltage (V_{oc}). Therefore, the efficiency of the device decreases when the thickness of the HTL is increased beyond 300 nm, as the recombination of charge carriers exceeds the charge extraction when the optimum thickness is exceeded [109,110].

Finally, we discuss the effect of defect densities at the interfaces of the layers on the charge-transport layer. Several studies have demonstrated the influence of defect density on device efficiency, indicating that as defect density at the interface between the light-absorbing layer and the charge-transport layer (electron- or hole-transporting layer) increases, the resulting device efficiency experiences a notable decline [111,112]. For this purpose, we treated the bulk defect densities for proposed RbGeBr₃-based PSCs, utilizing the trap-assisted recombination and selected the explicit trap distribution. The consequences depict the role of absorber defect density and thickness on power conversion efficiency at 100 to 300 nm and 1×10^{12} to 1×10^{18} cm⁻³ N_t . When the N_t is considered at one of the values mentioned above, and the absorber layer thickness increases, the open-circuit voltage (V_{oc}) experiences a slight decrease at each given defect density. On the other hand, for every thickness, a significant reduction in V_{oc} was calculated as the defect density increased. For instance, in the structure with the highest calculated efficiency, the maximum open-circuit voltage was 1.35 V at a defect density of 1×10^{12} cm⁻³. However, when the N_t increased to 1×10^{18} cm⁻³, the voltage sharply dropped, reaching 0.85 V. Moreover, with increasing absorber layer thickness at any defect density, an

acceptable increase in short-circuit current was achieved. However, at any given thickness, as the defect density increased, the short-circuit current exhibited a very slight reduction, on the order of hundredth of a decimal. Numerical results showed that increasing N_t reduces charge transfer and also increases recombination rates, and hence, the power conversion efficiency decreases significantly. These findings emphasize the necessity of employing high-quality absorber films with minimal defect concentrations to reduce recombination rates induced by trap defects. Such mitigation is critical for optimizing the performance of perovskite-based systems, as defect-mediated recombination pathways are known to impose deleterious effects on photovoltaic efficiency.

Furthermore, in general, comparing which material performs better among those used as electron transport layers (ETLs) in perovskite solar cells requires careful consideration of the material type, its application method, compatibility with adjacent layers in the cell, and experimental/environmental conditions. For instance, Xu, C. et al. conducted a comparative study on TiO₂ and C₆₀ electron transport layers (ETLs) to investigate their effects on the power conversion efficiency (PCE) of perovskite solar cells. The reported results demonstrated that a single layer, such as c-TiO₂ and C₆₀, shows a uniform, dense, and well-defined morphology with minimum roughness, and its film quality is much better than that of c-TiO₂/m-TiO₂ and c-TiO₂/C₆₀ composite layers [59]. In 2023, Mehrabian M. and colleagues conducted a study on perovskite solar cells based on several ETLs. Their results demonstrated that the perovskite solar cell incorporating the ZnO electron transport layer achieved a power conversion efficiency (PCE) of 20.08 %, higher than that of the TiO₂ and C₆₀-based ETLs, which yielded 18.83 % and 17.63 %, respectively [57].

Consequently, this study identified an optimal layer configuration for maximizing device efficiency, with thicknesses of 60 nm for the ETL,

200 nm for the TAL, and 300 nm for the HTL. The maximum power conversion efficiency is achieved by 16.48 % for the architecture, FTO/C60/RbGeBr₃/NiO/Au, along with the J_{sc} equal to 22.25 mA/cm², and the V_{oc} is 0.92 V. Xiangyue M. et al., were reported the power conversion efficiency of 15.38 % by studying a PSC structure, FTO/C60/MAPbI₃/caron [58]. Compared to the mentioned paper, the maximum efficiency of the result obtained from this paper is 1.1 % higher.

Conclusions

In this work, the six main configurations of PSCs are studied, with C60 as the electron transporter layer (ETL), RbGeBr₃ as a potential light-absorbing mineral active layer, and Au as the electron-collecting electrode constant (ECEs). The main purpose of this paper is to investigate the behavior of the inorganic perovskite material along with the C60 and the various hole transporter materials (HTL). C60 demonstrates excellent alignment with the absorber material RbGeBr₃, which promotes efficient electron extraction and transport. Additionally, for all structures, we obtained four important output factors for all perovskite solar cells. Moreover, the results illustrate that the relationship between the ETL thickness and the TALs is crucial to finding the optimal thickness for PSCs to achieve the highest efficiency, similar to its effect on organic-inorganic solar cells. Among these designs of the perovskite solar cells, the third structure utilizing selected layers of FTO/C60/RbGeBr₃/NiO/Au has presented the highest efficiency of 16.48 % along with the J_{sc} equal to 22.25 mA/cm², and the V_{oc} is 0.92 V, where the thickness of the ETL is 60 nm, the TAL is 200 nm, and the HTL is 300 nm constant. The second arrangement, FTO/C60/RbGeBr₃/CuSCN/Au represents an efficiency is 16.29 %, the J_{sc} is 22.23 mA/cm², and the V_{oc} is 0.91 V. Notably, this structure with the Au electrode provided the best efficiency and J_{sc} when compared to the other electrodes.

In the next step, further investigation was conducted by replacing the Au electrode with various electron-collecting electrodes (ECEs), such as silver (Ag), chromium (Cr), and nickel (Ni), to explore which configuration achieves the highest J_{sc} , V_{oc} , and efficiency for the six basic configurations. All eighteen structures with the different ECEs were studied, and the four important factors were calculated for each structure. Among the investigated structures, FTO/C₆₀/RbGeBr₃/NiO/Ni achieved the highest efficiency of approximately 16.48 %, with a J_{sc} of 22.24 mA/cm² and a V_{oc} of 0.92 V at the optimal ETL and TAL thicknesses. When Ag replaced Ni, the highest efficiency dropped to 15.31 %, with a J_{sc} of 22.23 mA/cm² and a V_{oc} of 0.92 V, still at the optimal ETL and TAL thicknesses. The Cr electrode showed the lowest efficiency of 0.47 % under similar conditions. The next structure investigated, FTO/C₆₀/RbGeBr₃/Spiro-MeOTAD/Ni, achieved a maximum efficiency of 16.10 %, with a J_{sc} of 22.21 mA/cm² and a V_{oc} of 0.90 V. Overall, all the configurations studied in this paper indicate that the Ni electrode achieves the highest efficiency after Au, compared to the other electrodes in all structures. These results reinforce the idea that the efficiency of perovskite solar cells is significantly influenced by various factors. The choice of semiconductor material for different layers, the optimal thickness of these layers, and the electron-collecting electrodes are some of the key factors that play a crucial role in determining the overall efficiency of the solar cell.

Practical viability of the work

The primary aim of this study was to evaluate the viability of employing the perovskite material RbGeBr₃ as a light-absorbing layer in combination with fullerene (C60) and diverse hole-transporting materials (HTMs) while accurately investigating their resulting photovoltaic performance across distinct device architectures. Considering the significant material expenses associated with solar cell fabrication, coupled with the economic demands of manufacturing and production processes, employing computational modeling tools—such as COMSOL Multiphysics, SCAP-1D, or similar numerical simulation platforms—to derive

scientifically trustful and rational conclusions in perovskite solar cell research represents a strategically prudent and methodologically rigorous approach. This methodology not only prevents the prohibitive costs of iterative experimental prototyping but also ensures theoretical validation and optimization before physical implementation, thereby aligning with the principles of cost-efficiency and scalable innovation in photovoltaic technology development. The outcomes of this research revealed the material's potential suitability for use as a light-absorbing layer in solar cells. Moreover, it is essential to acknowledge that the synthesis techniques of these devices, ambient conditions during the production phase, the accuracy and the precision, and methodology of layering these materials atop one another, and even the inherent morphological characteristics of the materials substantially impact the operational efficiency observed in empirical investigations and experimental evaluations. These parameters collectively constitute critical determinants of the functional efficacy and practical viability of photovoltaic systems.

CRedit authorship contribution statement

Shima Valizadeh: Writing – original draft, Visualization, Validation, Project administration, Methodology, Investigation, Data curation, Conceptualization. **Aliasghar Shokri:** Writing – review & editing, Visualization, Validation, Project administration, Methodology, Investigation, Data curation, Conceptualization. **Sani M. Lawal:** Writing – review & editing, Validation. **Nazila Fough:** Writing – review & editing, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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