Impact of Cu-based Hole Transport Layer in CIGS Solar Cells using SCAPS-1D Simulation Program

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Abstract: In this work, we applied the SCAPS-1D simulation tool to optimize and explore the potential of Cu-based materials ashole transport layer (HTL) including copper sulfide (CuS), copper oxide (Cu_2O), and copper thiocyanate (CuSCN) in CIGS solar cell. The effects of changing the bandgap, thickness, acceptor density, and operating temperature on the power conversion efficiency (PCE) of CIGS solar cells with these HTLs were examined.Our results showed that the solar cell's efficiency is significantly impacted by the bandgap of the HTL, with Cu_2O achieving the highest PCE of 39.83% at an optimal bandgap of 2.2 eV. Moreover, the study also demonstrated that variations in thickness had minimal impact on efficiency, highlighting the effective charge transport capabilities of these materials. The acceptor density variation showed that efficiency remains constant at lower densities but increases significantly beyond a certain threshold due to enhanced charge carrier collection. On the other hand, the PCE was decreased with temperature increment as a result of decreasing open-circuit voltage and increasing recombination. Among the studied Cu-based HTLs, Cu_2O emerged as the most promising candidate, offering superior performance and stability. This study suggests that these materials, which are readily available, inexpensive, and non-toxic, hold great potential as HTLs and can be integrated into advanced solar cell fabrication to achieve further efficiency improvements.

Keywords: Thin-film, CIGS solar cells, Hole transport layer, Bandgap, Thickness, SCAPS 1-D simulation tool.

Introduction: The global demand for renewable energy sources has prompted considerable developments in photovoltaic technology with the aim of obtaining high efficiency, low-cost solar energy conversion. The CIGSsolar cells have become the most desirable PVtechnologies available due to its outstanding optical and electrical characteristics[1]. In comparison to silicon solar cells, CIGS solar cells are very tempting due to their flexibility and straight bandgap, which enable significant absorption of sunlight over a wide spectrum[2], [3]. These qualities make them perfect for several kinds of applications, including portable and building-integrated photovoltaics. Despite these benefits, CIGS solar cell performance and scalability may be constrained by a number of variables, the most important of which is the effectiveness of charge carrier extraction and transport inside the device. A hole transport layer is an interlayer placed between CIGS and back contact to enhance the functionality of CIGS devices[4]. The HTL has significantrole to the operation of a conventional CIGS solar cell because it extracts and transports photogenerated holes from the absorber layer to the external circuit while also obstructing electrons from preventing recombination.

Therefore, the entire performance of the solar cell depends on the selection of HTL material. In CIGS and other types of solar cells, traditional HTL materials like PEDOT and Spiro-OMeTAD have been widely employed[5], [6]. However, these materials can have problems such high cost, instability under operating circumstances, and inadequate energy level alignment with the CIGS absorber. To address these challenges, there is growing interest in exploring alternative HTL materials that can offer better performance, stability, and cost-effectiveness. The favorable electronic features of copper (Cu)-based HTLs, such as their high conductivity, acceptable energy level alignment with CIGS, and potential for lower material prices, have drawn attention among the numerous contenders. Cu-based materials also provide compatibility with current CIGS fabrication techniques, which may make it easier to integrate them into the manufacturing of solar cells for commercial use. The SCAPS-1D simulation tool enables precise modelling of thecharacteristics of thin-film solar cells. By leveraging this tool, we aim to conduct a comprehensive analysis of how Cu-based HTLs influence key performance metrics of CIGS solar cells, including power conversion efficiency (PCE), open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF).

Thus, the influence of variations in the bandgap (Eg), thickness, acceptor density and operating temperature of Cu-based HTLs on the device's overall performanceis a particular focus in this study. The crucial factor that influences the alignment of energy levels at interfaces, the effectiveness of charge carrier extraction, and the reduction of recombination losses is the bandgap of the HTL. The aim of our simulations is to identify the most suitable material parameters and to optimizethe Cu-based HTLs by varying the bandgap, thickness, acceptor density and operating temperature. The outcomes of this study are expected to be useful in the design and refining of HTLs for CIGS solar cells, which will aid in the development of photovoltaic systems that are more reliable and efficient. Furthermore, this study may have wider ramifications for the use of HTL materials inseveral types of thin-film solar cells, which might result in improvements in various photovoltaic technologies.

Materials and Methods: SCAPS-1D simulation program is applied for simulating the electrical behavior of thin-film solar cells which was developed by the University of Gent, Belgium[7]. It enables in-depth examination of a number of device characteristics, such as carrier transport, recombination processes, and energy band alignment. One-dimensional solar cell modelling software, known as SCAPS, initially emerged for cell designs belonging to the $CuInSe_2$ and CdTe families[8]. However, a number of modifications have improved its capabilities, allowing it to be used with both crystalline and amorphous solar cells [7]. The three nonlinear differential equations that resolves for functioning are Poisson's equations, which are the continuity equations for free electrons and holes.

The Poisson’s equation is written as following [9]

$$\frac{d^2\psi(\mathrm{x})}{dx^2} = q/\varepsilon_0\varepsilon_r\left[p(x) - n(x) + N_D - N_A + \rho_p - \rho_n\right] \quad (1)$$

Here q is the charge of electrons, ρ_p and ρ_n represent holes and electrons distribution, N_D and N_A indicate donor and acceptor density accordingly.

The continuity equations for electrons and holes are written as [7]

$$-\frac{1}{q}\frac{dJ_n}{dx} + R_n(x) - G(x) = 0 \quad (2)$$

$$\frac{1}{q}\frac{dJ_p}{dx} + R_p(x) - G(x) = 0 \quad (3)$$

Here, J_n and J_p represent electron and hole current density respectively, $R_n(x)$ and $R_p(x)$ are recombination rate of holes and electrons, $G(x)$ is the rate of carrier generation.

In this work, we modelled and analyzed the functionality of Copper Indium Gallium Selenide (CIGS) solar cells with different copper-based hole transport layers (HTLs) using the SCAPS-1Dsimulation program. We insert hole transport layer (HTL) between CIGS absorber and back contact layer using the optimum value of CIGS solar cell [10].Copper Sulphide (CuS), Copper Oxide (Cu_2O), and Copper Thiocyanate (CuSCN) are the copper-based materials that were chosen for the HTL in this investigation. These materials were selected because they had promising electrical characteristics, including excellent hole mobility, appropriate work function alignment with the absorber layer, and the possibility of being fabricated at a reasonable cost.

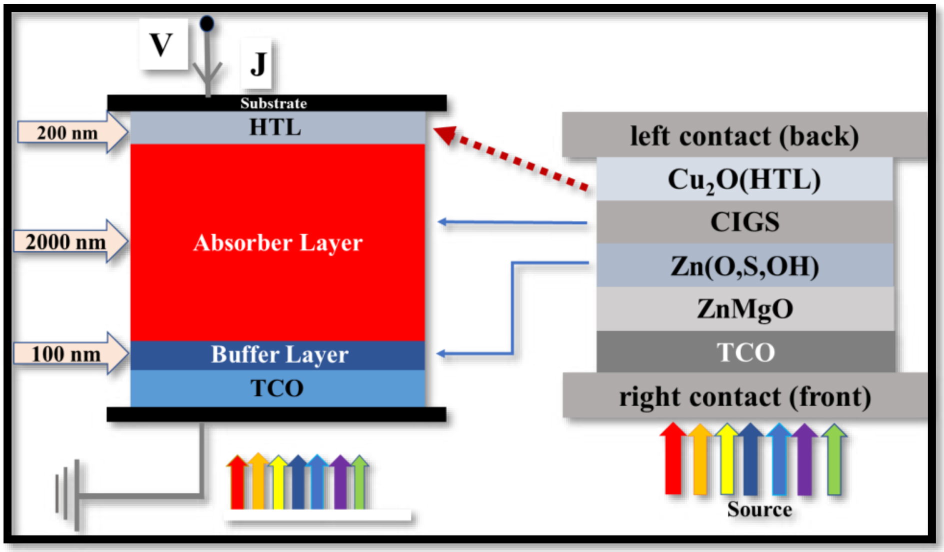

Fig 1.Configuration of the CIGS solar cell device.

Figure1 illustrates the design that is utilized to produce the solar cell.The light source is emanating from the right contact direction.Thissimulation work has taken into account an operating temperature of 300 K and a solar spectrum AM1.5. The HTLs were inserted with an initial thickness of 0.2 µm in between the Mo back contact and the CIGS absorber layer.This simulation tool is used to investigate how the effects of varying bandgap, thickness, acceptor density, and operating temperature on the CIGS solar cellperformance.In this investigation, Table 1 summarizes the optical and electrical input values for the CIGS absorber layer and a number of HTL layers.

Table 1:Physical parameters for CIGS layer and different HTLs used in device simulation[10], [11], [12], [13]

Parameters	CIGS	Cu_2O	CuS	CuSCN
Thickness (nm)	2000	200	200	200
Bandgap (eV)	1.08	2	2.2	3.5
Electron affinity, χ_e (eV)	4.25	3.4	2.9	1.4
Dielectric constant, ε_r	13.6	7.1	9	10
Density of states at conduction band, $N_C(cm^3)$	1.2E+18	2E+17	2.2E+18	2.2E+19
Density of states at valence band, $N_V(1/cm^3)$	1.7E+19	1.1E+19	1.8+19	1.8+18
Electron thermal velocity, $\upsilon_{th,e}$ (cm/s)	1E+7	1E+7	1E+7	1E+7
Hole thermal velocity, $\upsilon_{th,h}$ (cm/s)	1E+7	1E+7	1E+7	1E+7
Electron mobility, μ_e $(cm^2(Vs)^{-1})$	100	200	100	100
Hole mobility, μ_h $(cm^2(Vs)^{-1})$	25	80	25	25
Defect density(cm^{-3})	1.5×10^{13}	10^{14}	10^{14}	10^{14}

Results& Discussion

Effect of bandgap variation of Cu based HTLs

An optimal bandgap ensures that the valence band of the HTL aligns well with the valence band of the CIGS absorber, which facilitates efficient hole extraction while minimizing electron recombination at the interface[14], [15].

In this section, we discuss the impacts of varying the bandgap of Cu_2O, CuS, and CuSCN hole transport layers (HTLs) on the efficiency of CIGS solar cells. The findings indicate that, when the bandgap of the HTLs increases, the solar cells PCE rises, as seen in Figure 2. The bandgap of Cu_2O was varied from 1.4 to 2.2 eV and the highest efficiency of 39.83% was observed at a 2.2 eV bandgap.As the bandgap of Cu_2O increases, the alignment of energy levels between the CIGS absorber layer and the HTL improves. At lower bandgaps (1.4–1.6 eV), the alignment is less optimal, leading to higher recombination losses at the HTLabsorber interface. This results in lower efficiency. As the bandgap increases, the HTL becomes more selective for holes,limiting recombination and growing the extraction of charge carriers.Furthermore, the higher bandgap enhances the solar cell's overall electric field, resulting in more effective charge separation and collection.[10], [16]. This combination of reduced recombination and enhanced charge separation leads to the observed increase in efficiency[10].The 2.2 eV bandgap offers the best alignment, minimizing electron recombination and maximizing hole transport, thereby leading to the highest efficiency observed. Figure 3,4 and 5 represent that how PCE calculating parameters (Voc,Jsc,FF) vary with the bandgap variation of different Cu based HTL.

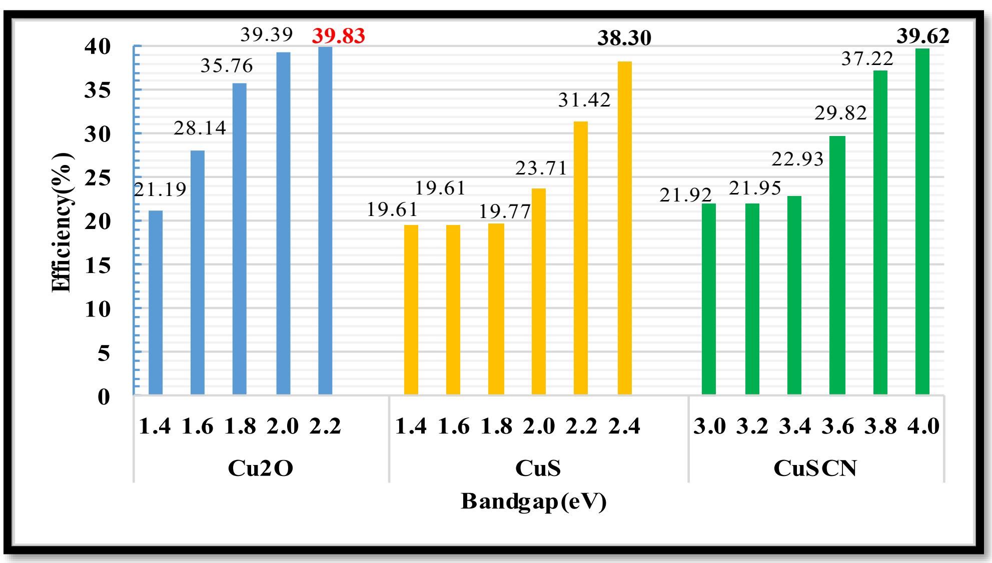

Fig 2. Effect of various Cu based HTLs on the solar cell efficiency with bandgap variation.

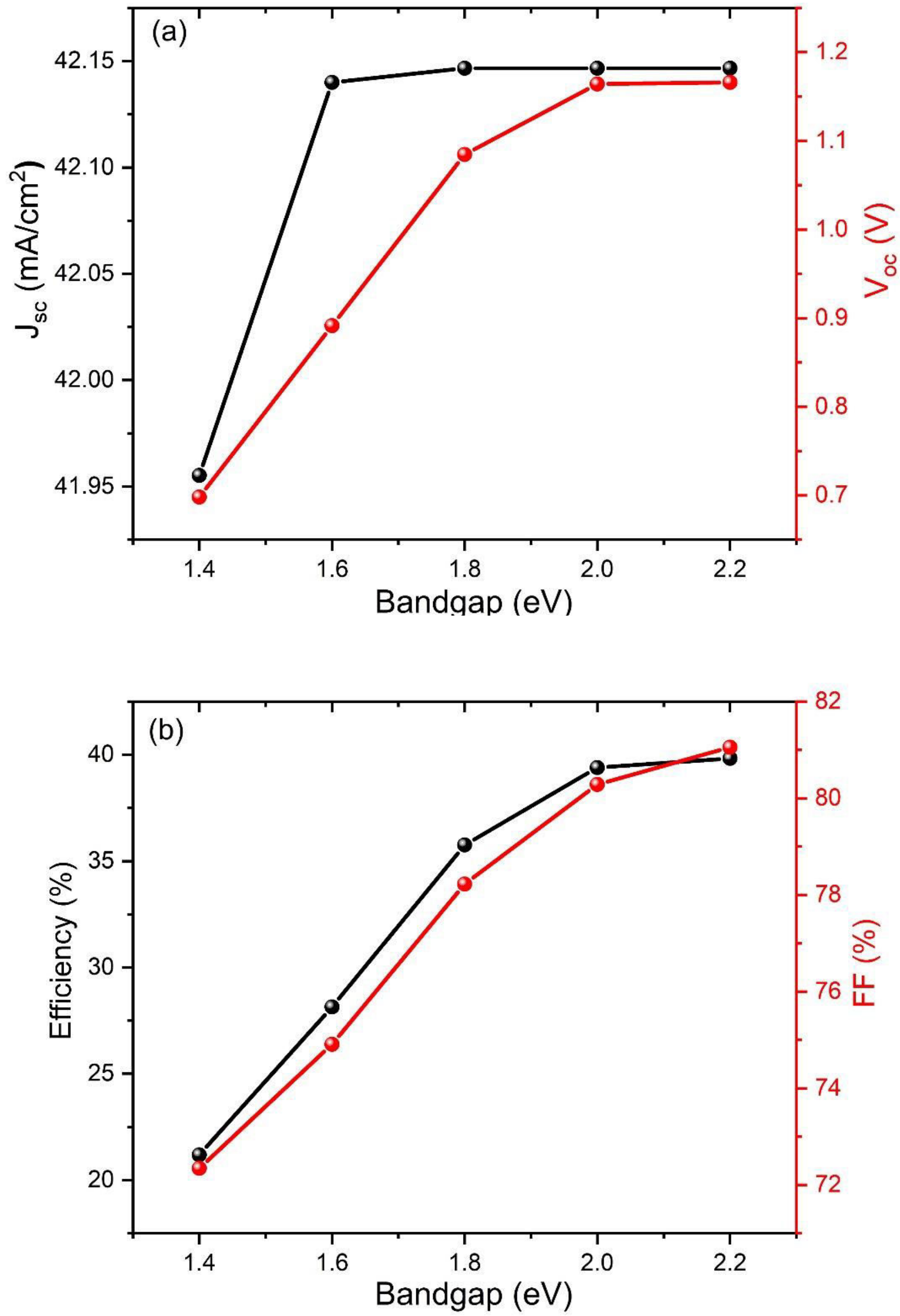

Fig 3.Effect of variation of bandgap of Cu_2O HTL on (a) Open-Circuit Voltage and Short-circuit current density (b) Power conversion efficiency andFill factor of CIGS solar cell.

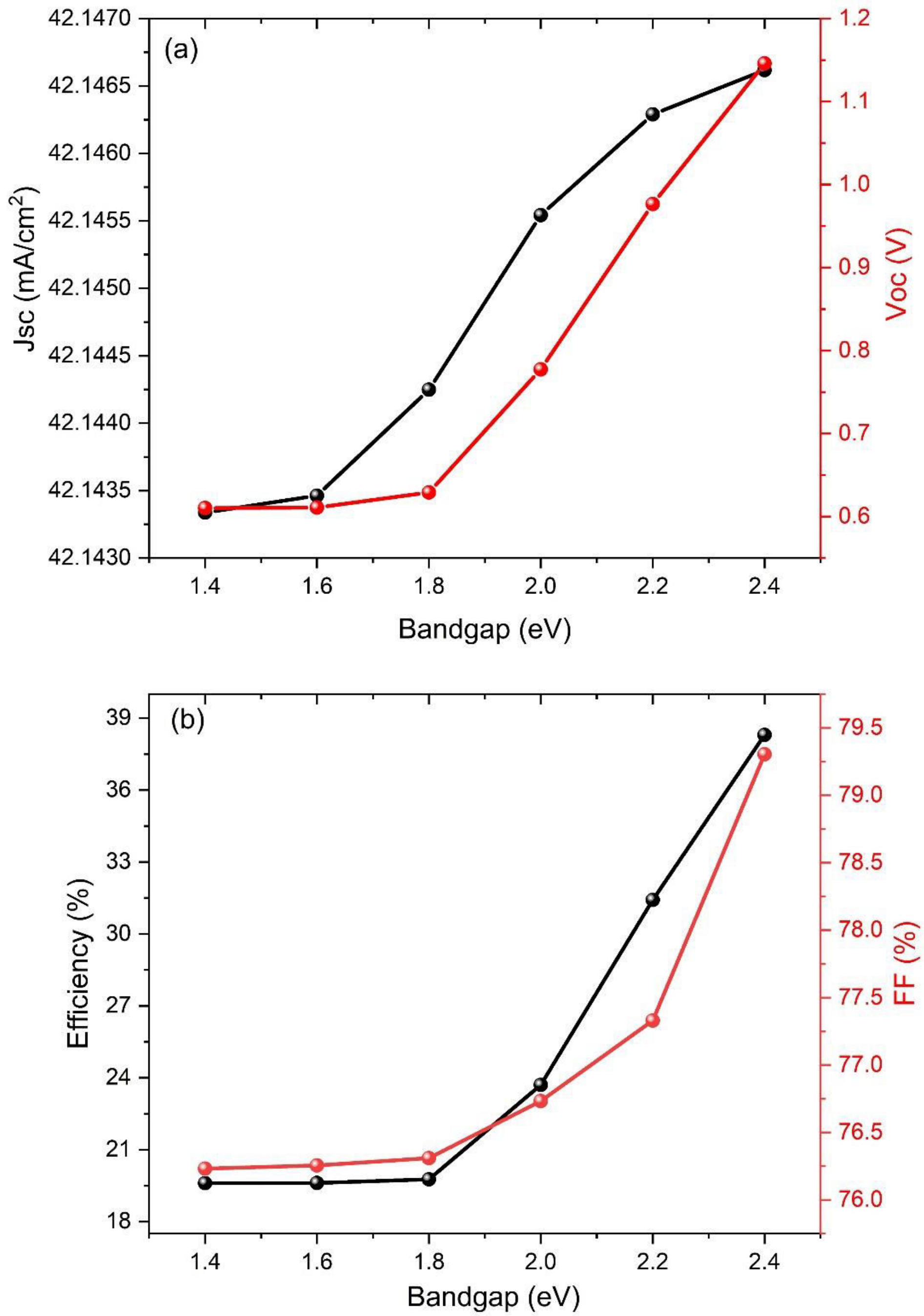

Fig 4.Effect of variation of bandgap of CuS HTL on (a) Short-circuit current density and Open-Circuit Voltage (b) Power conversion efficiency and Fill factorof CIGS solar cell.

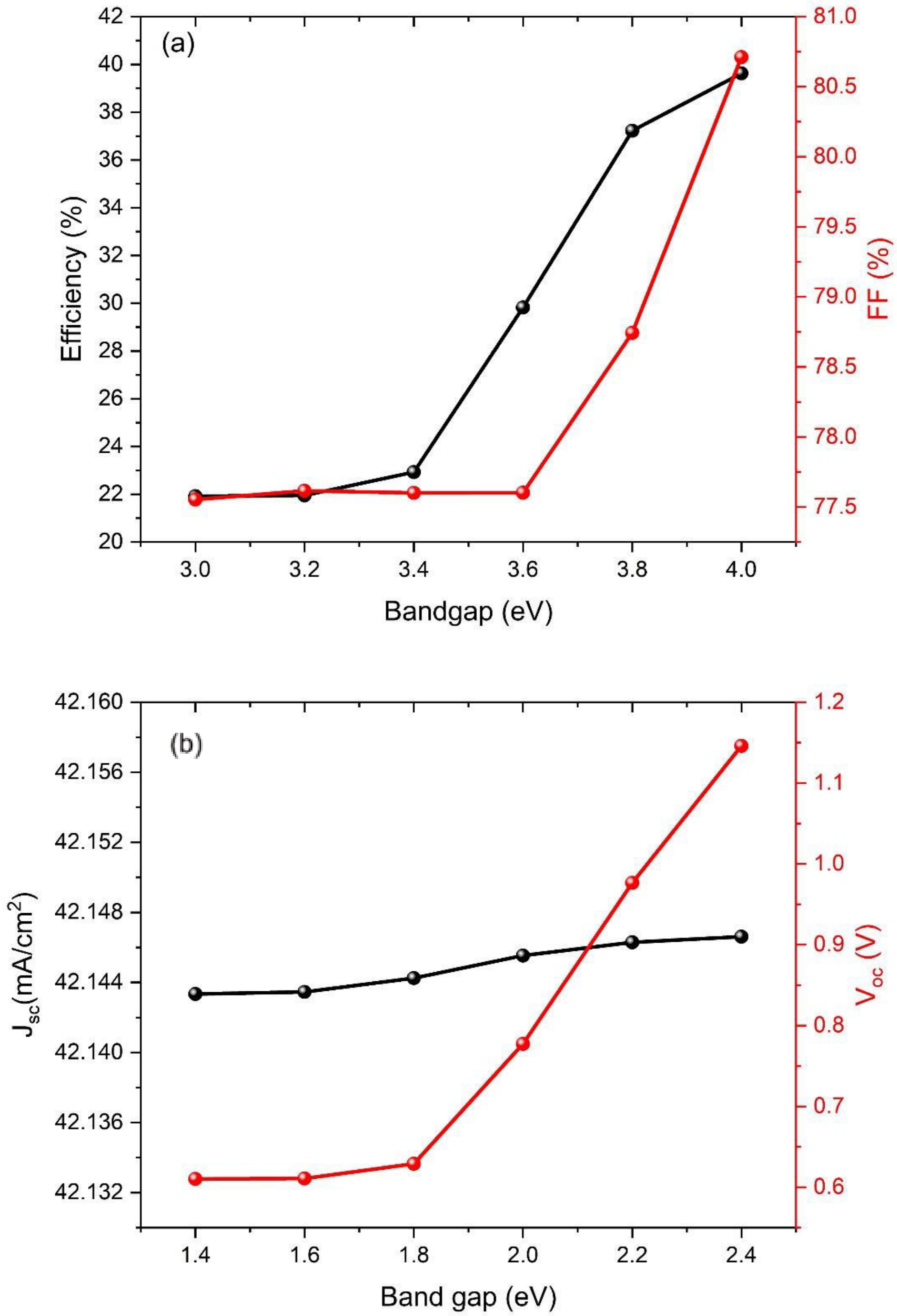

Fig 5.Effect of variation of bandgap of $CuSCN$ HTL on (a) Short-circuit current density and Open-Circuit Voltage (b) Power conversion efficiency and Fill factorof CIGS solar cell.

For CuS, the bandgap was varied from 1.4 to 2.4 eV and the highest efficiency of 38.30% was achieved at a 2.4 eV bandgap.Similar to Cu_2O, the performance of CuS as an HTL improves with an increasing bandgap due to the reduced recombination losses. At lower bandgaps, the HTL is less effective in blocking electrons, leading to higher recombination rates[17]. As the bandgap increases, the HTL becomes more efficient in hole transport and electron blocking. The maximum efficiency at a 2.4 eV bandgap indicates that this value provides the optimal trade-off between effective hole transport and minimal recombination, leading to enhanced solar cell performance.

CuSCN, with its naturally higher bandgap, exhibits a trend similar to Cu_2O and CuS, but with its efficiency peaks at a much higher bandgap of 4.0 eV. At lower bandgaps (3.0–3.4 eV), the alignment with the CIGS absorber is suboptimal, resulting in higher recombination losses. As the bandgap increases, CuSCN becomes highly selective for holes while effectively blocking electrons, reducing recombination and enhancing efficiency. The maximum effectiveness of the solar cell is ensured by the bandgap that offers the most favorable circumstances for charge carrier dynamics, as indicated by the peak efficiency at 4.0 eV.

Effect of thickness variation of Cu based HTLs

In this part, we evaluate the impact of altering the thickness of Cu_2O, CuS, and CuSCN hole transport layers (HTLs) on the efficiency of CIGS solar cells. As seen in Figure 6, the results reveal that there is no discernible difference in efficiency when the thickness of HTLs is changed fromo.06 to 0.22 μm.

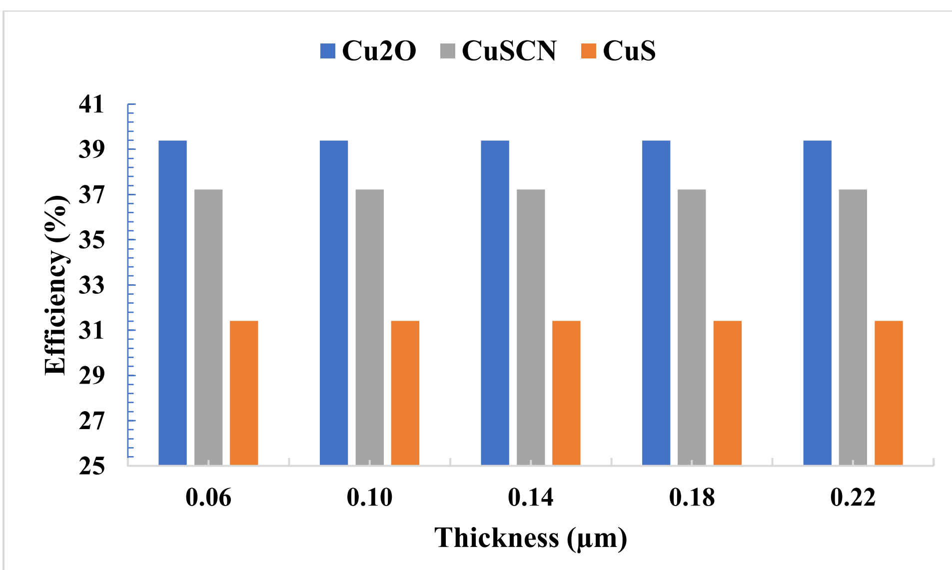

Fig 6.Effect of various Cu based HTLs on the solar cell efficiency with thickness variation.

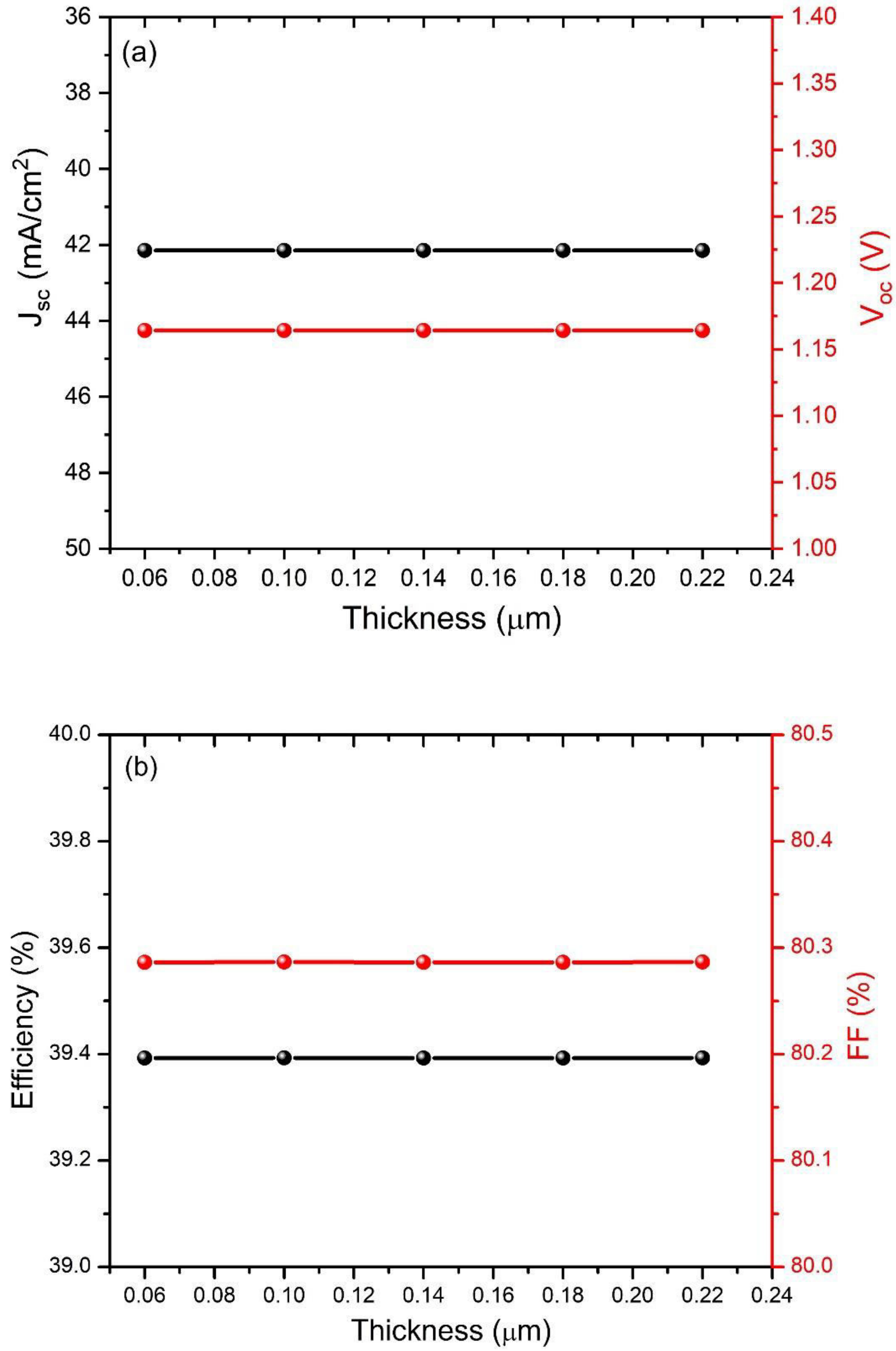

Fig 7.Effect of thickness variation of Cu_2O HTL on (a) Short circuit current density and Open Circuit Voltage (b) PCE and Fill factor of the solar cell.

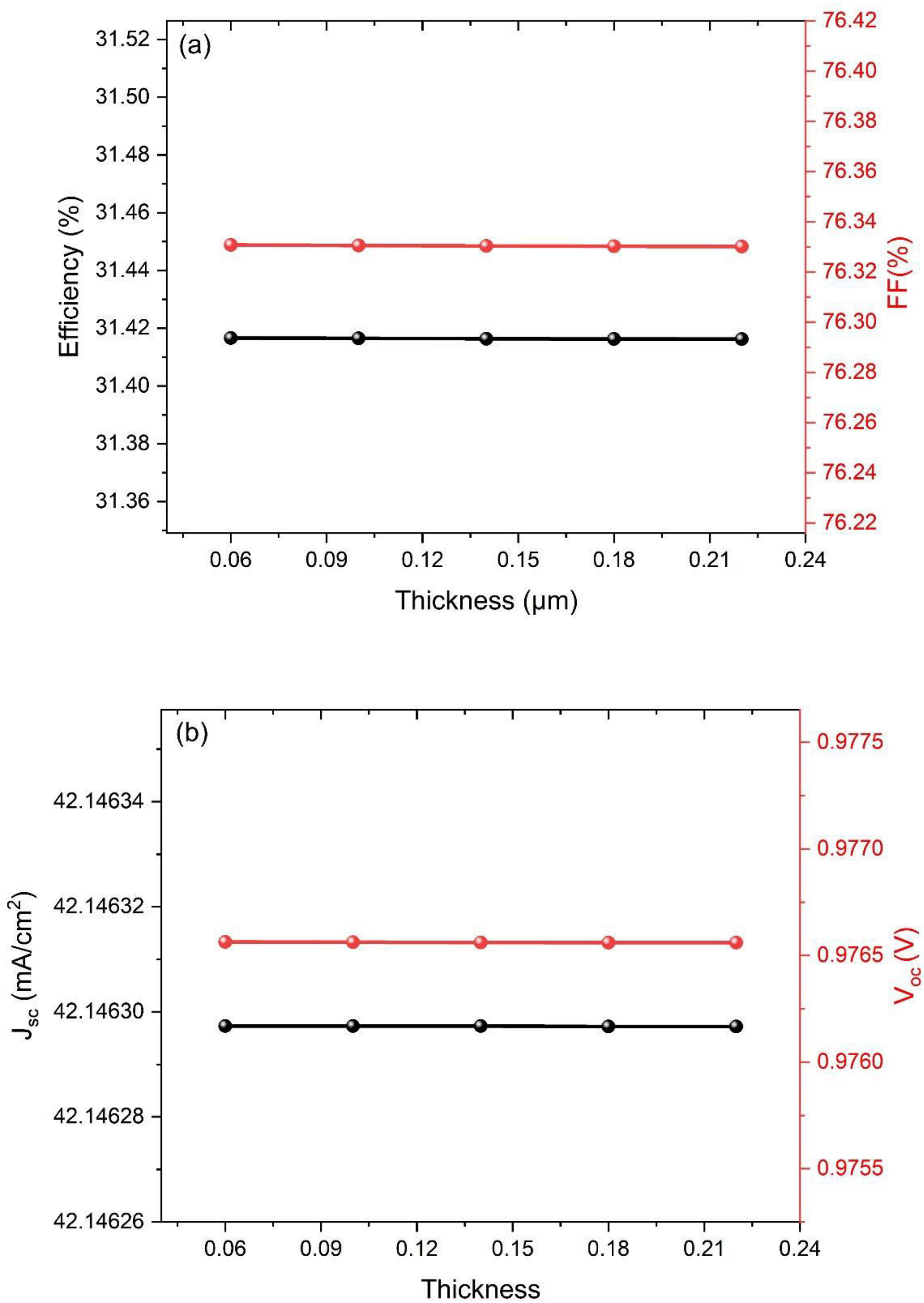

Fig 8.Effect of thickness variation of CuS HTL on (a) Short circuit current density and Open Circuit Voltage (b) PCE and Fill factor of the solar cell.

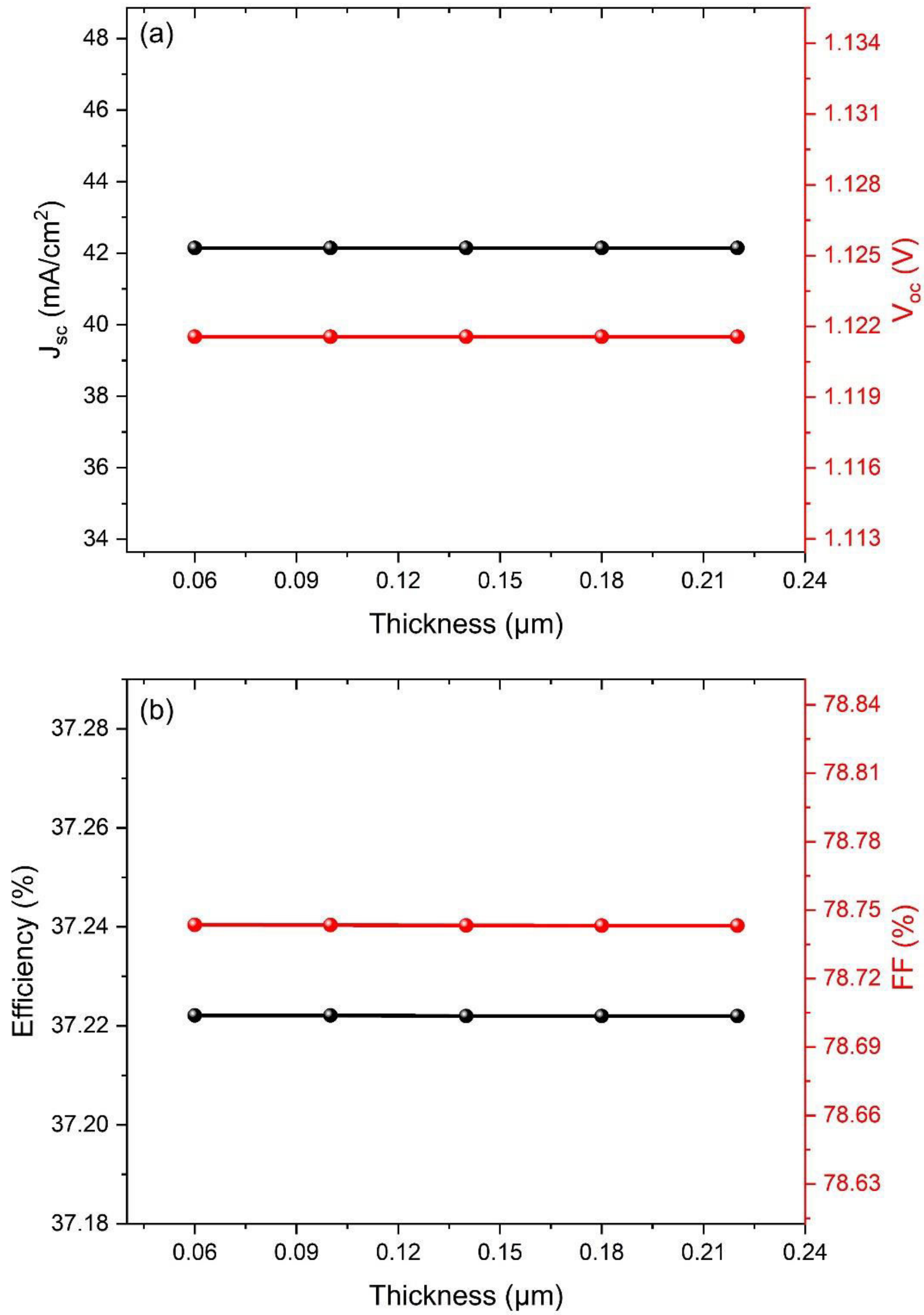

Fig 9.Effect of thickness variation of CuSCN HTL on (a) Short circuit current density and Open Circuit Voltage (b) PCE and Fill factor of the solar cell.

The negligible impact of thickness variation on efficiency can be attributed to the fact that thebasic function of the HTL is to facilitate hole transit while blocking electrons[10]. Once a sufficient thickness is achieved to establish an effective potential barrier for electrons, further increases in thickness do not substantially improve the device's performance. Additionally, since Cu_2O has a relatively high hole mobility, even a thinner layer is sufficient to transit holes efficiently to the back contact[18]. Thus, variations within the utilized thickness range do not significantly affect the efficiency and the other parameters (V_{oc}, J_{sc}, FF) almost remain same (Figure 7,8,9). Like Cu_2O, CuSdemonstrates that once an optimumthickness is achieved, further increases in thickness do not contribute to higher efficiencies. The consistent efficiency across different thicknesses can be explained by the fact that CuS effectively blocks electron transport and facilitates hole movement at all tested thicknesses. As long as the HTL thickness is sufficient to perform these functions, additional material does not significantly enhance the cell's performance, leading to the observed stability in efficiency.The lack of significant efficiency variation with CuSCN thickness is due to its high intrinsic hole mobility and the ability to form an effective potential barrier with even a thin layer. As a result, increasing the thickness beyond the necessary minimum does not provide additional benefits in terms of hole transport or electron blocking, leading to stable efficiencies across the tested thicknesses.

Effect of acceptor density variation of Cu based HTLs

In this section, we discuss the effect of varying the acceptor density (varied from 1E+14 to 1E+20 cm^{-3}) of the HTLs on the efficiency of CIGS solar cells. Thisstudy indicates that the PCE remains relatively constant at lower acceptor densities but begins to increase significantly after a certain threshold, eventually reaching a peak.

Figure 10 demonstrates the effect of acceptor density variation on PCE of CIGS solar cell with different Cu based HTL. At low acceptor densities (1E+14 to 1E+16 cm^{-3}), the HTL may not provide a strong enough electric field to effectively separate and transport the photogenerated holes from the absorber layer to the back contact. This results in minimal variation in efficiency, as the hole transport capability of the HTL is not fully optimized.As the acceptor density increases beyond 1E+16 cm^{-3}, the electric field within the HTL strengthens, enhancing the separation and transport of holes. This reduces recombination losses and improves charge carrier collection, leading to a noticeable increase in PCE. The peak efficiency observed at higher acceptor densities (around 1E+19 to 1E+20 cm^{-3}) suggests that the HTL is now highly effective in its role, ensuring optimal hole transport and minimal recombination.For Cu_2O HTL, beyond a certain point, further increases in acceptor density yield diminishing returns in terms of efficiency. This is because the HTL has already reached a level of optimal performance, where the electric field is sufficient to drive efficient hole transport. Additional increases in acceptor density do not significantly enhance this capability, leading to the observed almost plateau in efficiency gains. For CuS and CuSCN HTL, the peak efficiency also observed at 1E+20 cm^{-3}acceptor density.

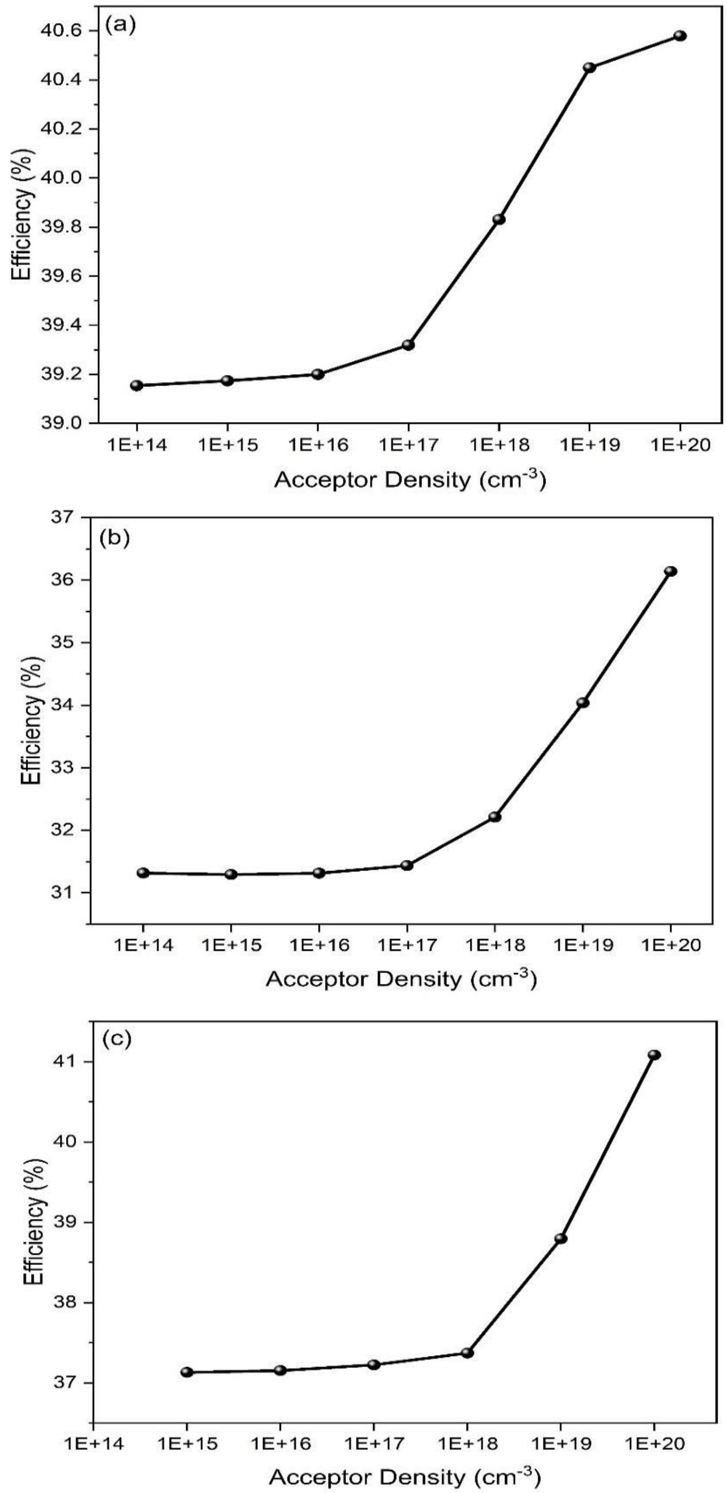

Fig 10.Effect of acceptor density variation ofdifferent Cubased HTLs on PCE of the solar cell.

Investigating how solar cells behave at different temperatures (T) is crucial because, in terrestrial applications [19], solar cells are often subjected to temperatures between 15 °C (288 K) and 50 °C (323 K), and in space and concentrator systems [20], they are exposed to much higher temperatures.Because the parameters such as V_{oc}, J_{sc}, FF, and efficiency are temperature dependent, the operating temperature has an impact on solar cell performance[21].

This section examines how temperature variations affect the CIGS solar cells' efficiency while using HTL. The effect of operational temperature change on the PCE of a solar cell is seen in Figure 11. The findings show that when the working temperature rises from 280K to 400K, PCE gradually decreases. The intrinsic carrier concentration of semiconductor materials, such as the CIGS absorber and HTLs, grows with temperature. The higher carrier recombination rates result from this, especially in the depletion region and at the device's interfaces. The short-circuit current (Jsc) and overall PCE are lowered when there are fewer charge carriers available for collection due to increased recombination[18].Furthermore, a decrease in the open-circuit voltage (Voc) may result from greater temperatures. Usually, the bandgap of semiconductor materials narrows with increasing temperature, lowering the Voc. This reduction in Voc adds even more to the overall decrease in PCE at high temperatures. These results highlight how critical temperature control is to CIGS solar cell effectiveness optimization, especially in environments with substantial temperature swings.

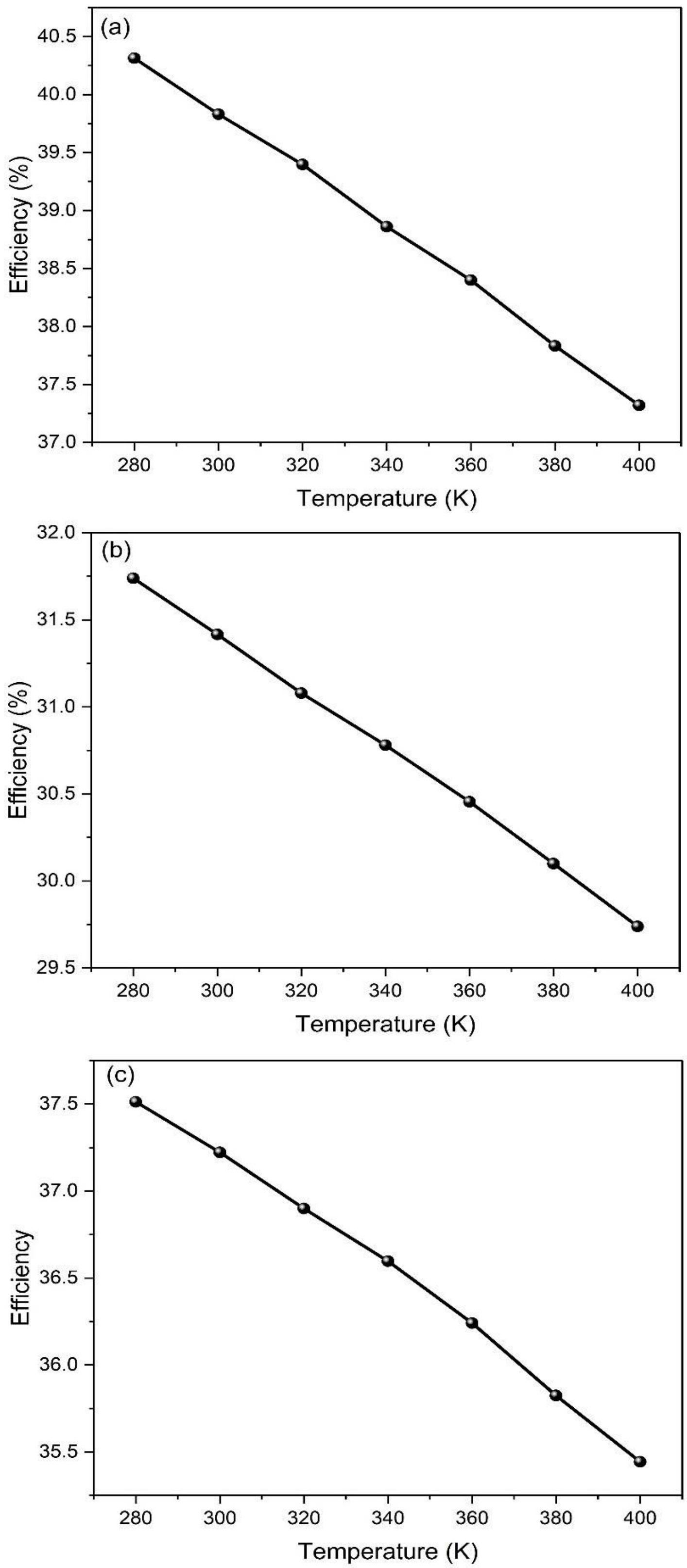

Fig 11.Effect of operating temperature variation on the efficiency (PCE) of CIGS solar cells with different CubasedHTLs.

Conclusions

In this work, we have used the SCAPS-1D modelling program to analyze the potential candidate Cu-based materials (Cu_2O, CuS, and CuSCN) as the hole transport layer (HTL) in CIGS solar cells. We investigated how different Cu-based HTLs have an impact on efficiency of CIGS solar cells in terms of bandgap, thickness, acceptor density, and operating temperature change.

The optimal bandgap values (2.2 eV for Cu_2O, 2.4 eV for CuS, and 4.0 eV for CuSCN) provided the best energy level alignment, minimize recombination losses, and maximize charge carrier extraction, thereby leading to the highest efficiencies observed in this study. The Cu_2O HTL achieved the highest PCE of 39.83% at an optimal bandgap of 2.2 eV.Furthermore, the thickness of Cu_2O, CuS, and CuSCN HTLs within the range of 0.06 to 0.22 micrometers did not significantly affect the PCE of CIGS solar cells because of the effective hole transport and electron blocking capabilities of these materials, which was already optimized at lower thicknesses. Besides, the influence of acceptor density variation of HTLs show that the efficiency remains almost constant at lower acceptor densities as the HTLs may not provide a strong enough electric field to effectively separate and transit the holes from the absorber layer to the back contact. But it starts to increase noticeably beyond a certain value due to decrease recombination losses and improves charge carrier collection.Moreover, thePCE of CIGS solar cells withHTLs decreases with enhancing operating temperature due to increased carrier recombination, reduced open-circuit voltage, and higher series resistance at elevated temperatures. The Cu_2O HTL emerges as the most promising candidate for the usage as an HTL in CIGS solar cells due to the highest PCE of 39.83% at an optimal bandgap of 2.2 eV, the strong performance across different bandgaps and acceptor densities, and its efficiency was less sensitive to thickness variation.CuSCN is also a strong candidate, achieving close efficiency values (39.62% at 4.0 eV bandgap), but the overall stability and better performance of Cu_2O HTL make it the most suitable choice among these materials.

Future research could focus on optimizing the interface properties between the HTL and CIGS absorber to minimize recombination lossesand investigating the better stability of these materials. Additionally, integrating these HTLs into tandem or multi-junction solar cells could offer pathways to even higher efficiencies, contributing to the advancement of next-generation photovoltaic technologies.

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Author Contributions:
Mimi Mondal: Writing– original draft, Writing– review &editing, Md. Salahuddin Mina: Conceptualization (lead); Investigation (lead); Methodology& editing (lead); Supervision (lead); Md Rakib Hasan: Visualization and editing (supporting).

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