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# Simulation of $SnO_2/Cs_2AgInBr_6/CuO$ heterojunction solar cell using AMPS-1D modeling

# Simulação da célula solar de heterojunção $SnO_2/Cs_2AgInBr_6/CuO$ usando a modelagem AMPS-1D

# Simulación de una célula solar de heterounión $SnO_2/Cs_2AgInBr_6/CuO$ mediante modelado AMPS-1D

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## ABSTRACT

Using the one-dimensional computer code AMPS-1D MPS-1D (Analysis of Microelectronic and Photonic Structures), we simulated a lead-free double perovskite cell made of $Cs_2AgInBr_6$. This study examines the influence of the thickness and acceptor density of the active layer ($Cs_2AgInBr_6$) on key solar cell parameters, including short-circuit current density ($J_{SC}$), efficiency ($E_{ff}$), fill factor (FF), open-circuit voltage ($V_{OC}$), current-voltage characteristics (J-V)). Our results suggest that an optimal active layer thickness of 500 nm yields good performance for the studied solar cell. Furthermore, the ideal acceptor density for enhancing output parameters is in the range of $10^{13}$-$10^{15}$ $cm^{-3}$. Post-optimization, our findings reveal a Voc of 0.969 V, a Jsc of 29.402 mA $cm^{-2}$, and an FF of 0.876, resulting in an efficiency of 24.959%. The results from AMPS-1D simulations for a $Cs_2AgInBr_6$ lead-free double perovskite solar cell suggest that this material and device structure can achieve high efficiency and good performance characteristics.

**Keywords:** AMPS-1D. $Cs_2AgInBr_6$ Solar Cells. Hetero-Junction. $SnO_2$. CuO. Efficiency.

**RESUMO**

Usando o código de computador unidimensional AMPS-1D MPS-1D (Analysis of Microelectronic and Photonic Structures), simulamos uma célula de perovskita dupla sem chumbo feita de Cs2AgInBr6. Esse estudo examina a influência da espessura e da densidade do aceitador da camada ativa (Cs2AgInBr6) nos principais parâmetros da célula solar, incluindo densidade de corrente de curto-circuito (JSC), eficiência (Eff), fator de preenchimento (FF), tensão de circuito aberto (VOC), características de tensão de corrente (J-V). Nossos resultados sugerem que uma espessura ideal da camada ativa de 500 nm produz um bom desempenho para a célula solar estudada. Além disso, a densidade ideal do aceitador para melhorar os parâmetros de saída está na faixa de $10^{13}$-$10^{15}$ $cm^{-3}$. Após a otimização, nossas descobertas revelam um Voc de 0,969 V, um Jsc de 29,402 mA $cm^{-2}$ e um FF de 0,876, resultando em uma eficiência de 24,959%. Os resultados das simulações AMPS-1D para uma célula solar de perovskita dupla sem chumbo Cs2AgInBr6 sugerem que esse material e a estrutura do dispositivo podem alcançar alta eficiência e boas características de desempenho.

**Palavras-chave:** AMPS-1D. Células Solares de $Cs_2AgInBr_6$. Heterojunção. $SnO_2$. CuO. Eficiência.

**RESUMEN**

Utilizando el código informático unidimensional AMPS-1D MPS-1D (Análisis de Estructuras Microelectrónicas y Fotónicas), hemos simulado una célula de doble perovskita sin plomo fabricada con Cs2AgInBr6. Este estudio examina la influencia del grosor y la densidad de aceptor de la capa activa (Cs2AgInBr6) en los parámetros clave de la célula solar, como la densidad de corriente de cortocircuito (JSC), la eficiencia (Eff), el factor de llenado (FF), el voltaje en circuito abierto (VOC) y las características corriente-voltaje (J-V). Nuestros resultados sugieren que un espesor óptimo de la capa activa de 500 nm proporciona un buen rendimiento para la célula solar estudiada. Además, la densidad de aceptor ideal para mejorar los parámetros de salida se encuentra en el rango de $10^{13}$-$10^{15}$ $cm^{-3}$. Tras la optimización, nuestros resultados revelan un Voc de 0,969 V, un Jsc de 29,402 mA $cm^{-2}$ y un FF de 0,876, lo que se traduce en una eficiencia del 24,959%. Los resultados de las simulaciones AMPS-1D para una célula solar de doble perovskita sin plomo Cs2AgInBr6 sugieren que este material y la estructura del dispositivo pueden alcanzar una alta eficiencia y buenas características de rendimiento.

**Palabras clave:** AMPS-1D. Células Solares de $Cs_2AgInBr_6$. Heterounión. $SnO_2$. CuO. Eficiencia.

## 1 INTRODUCTION

The exploration of renewable energies is a vital strategy for promoting sustainable development in response to the global energy crisis [1]. Among these alternatives, solar energy stands out as an exceptional solution, being clean,

silent, and capable of being converted into electricity through the sun's direct irradiation. It can be efficiently harnessed using panels that are easily installed in deserts and on buildings.

Perovskite materials have garnered significant interest from researchers owing to their remarkable performance in solar cells [2- 7]. This success is largely attributed to their exceptional optical and electronic properties. However, despite their efficiency, perovskite solar cells face instability issues and contain lead, a toxic element [8]. This unfortunately restricts their use in photovoltaic systems. In response, a new generation of dual perovskites has been proposed to address this challenge [2]. These stable, non-toxic, inorganic materials have been successfully synthesized [2], making them promising candidates for photovoltaic applications.

$Cs_2AgInBr_6$, a double perovskite, is considered a promising candidate for photovoltaic applications. Zhang *et al*. [2] investigated its optical absorption under stress and found it to be an excellent absorber layer for potential solar cell applications. Recently, $Cs_2AgInBr_6$ has been recognized for its favorable optical and electrical properties [3]. Its direct bandgap makes Cs2AgInBr$_6$ well-suited for high-efficiency solar cells [2- 4], [10]. Moreover, solar cells utilizing $Cs_2$AgInBr6 can achieve an optimal efficiency of 28%, closely approaching the theoretical maximum of 30% for $CH_3NH_3PbI_3$-based solar cells [11].

The need for renewable energy solutions has driven research into advanced solar cell materials and architectures. This study focuses on the SnO2/$Cs_2AgInBr_6$/CuO solar cell, aiming to enhance its performance through numerical simulation and optimization. The unique properties of these materials offer promising avenues for improving solar cell efficiency.

In this study, we employ the AMPS-1D software to conduct numerical simulations of a perovskite solar cell utilizing hole transport layer (CuO), based on $Cs_2AgBiBr_6$, under standard illumination conditions (AM1.5G, 100 mW/cm$^2$, 300 k).

The purpose of this research is to evaluate the performance of a heterojunction solar cell using $Cs_2AgInBr_6$, a double perovskite, as the absorber material. The primary objective is to analyze the impact of the active layer thickness and the modified acceptor density on cell performance, while also characterizing the structural parameters of each layer within the cell. By optimizing

these structural parameters, our aim is to enhance the performance of the hetero-junction solar cell and gain valuable insights into improving solar cell efficiency.

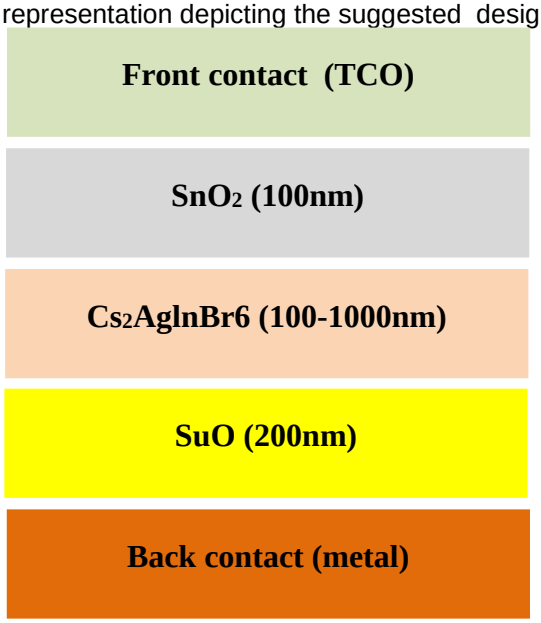
The presented work is structured into four sections. Section 2 discusses the architecture of the device and the parameters used for the simulation. Section 3 presents the properties of the voltage-current characteristics and the impact on the active layer, as well as the effect of acceptor density (NA) in the active layer. Finally, Section 4 provides the conclusions drawn from the study.

## 2 SIMULATION

### 2.1 ARCHITECTURE OF DEVICES

The solar cell was fabricated on a metal substrate serving as the back contact. A transparent conducting oxide (TCO) layer was deposited on the n-side to form the front contact. The device features an active $Cs_2AgInBr_6$ (p-type) layer, with thicknesses varying from 100 to 1000 nm, sandwiched between a 100 nm $SnO_2$ (n-type) layer and a 200 nm CuO (p-type) window layer, as illustrated in Figure 1.

Figure 1. A visual representation depicting the suggested design of the solar cell.




Source: Authors

## 2.2 PARAMETERS FOR SIMULATIONS

The materials parameters utilized in our simulations were meticulously selected based on existing literature and prior experimental research. Table 1, located below, presents the parameters and their respective values utilized in the simulation, encompassing (CuO), perovskite (absorber layer), and ($SnO_2$).

# 3 FINDINGS AND DISCUSSION

## 3.1 PROPERTIES OF VOLTAGE CURRENT

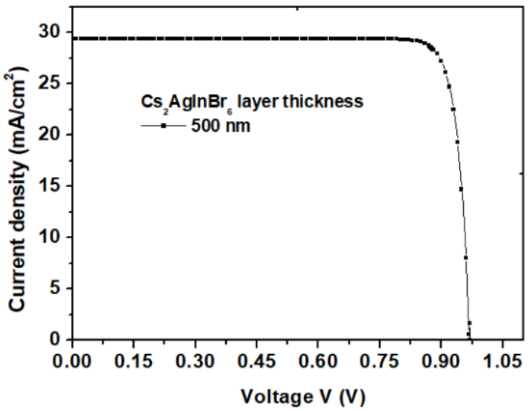
Following simulation using the AMPS-1D code with parameters listed in Table 1 (layer properties and interface characteristics affected by Gaussian defects), the resulting electrical characteristics are depicted in Figure 2.

Table 1. Adjustments for the SnO2, Cs2AgInBr6 and CuO layers used in the simulation.

| **Parameters** | **n-$SnO_2$ [ 12 – 15]** | **p-$Cs2AgInBr_6$ [3, 10, 16, 17]** | **p-CuO [12],[18-21]** |
|---|---|---|---|
| Thickness (nm) | 100 | 100-1000 | 200 |
| Dielectric constant | 9 | 4.37 | 18.1 |
| Electron mobility ($cm^2\ V^{-1}\ s^{-1}$) | 100 | 89.4 | 100 |
| Hole mobility ($cm^2\ V^{-1}\ s^{-1}$) | 25 | 3.3 | $10^{-1}$ |
| Effective conduction band density ($cm^{-3}$) | $2.2 \times 10^{18}$ | $1.26 \times 10^{18}$ | $2.2 \times 10^{19}$ |
| Effective valence band density ($cm^{-3}$) | $1.8 \times 10^{19}$ | $1.73 \times 10^{18}$ | $5.5 \times 10^{20}$ |
| Acceptor concentration ($cm^{-3}$) | 0 | $1 \times 10^{15}$ | $1 \times 10^{15}$ |
| Donor concentration ($cm^{-3}$) | $1 \times 10^{16}$ | 0 | 0 |
| Band gap (eV) | 3.6 | 1.57 | 1.4 |
| Electron affinity (eV) | 4.0 | 4.1 | 4.07 |
| Gaussian defect density ($cm^{-3}$)<br>Velocity SNL (cm/s)<br>Velocity SPL (cm/s) | $1 \times 10^{15}$<br>$10^7$<br>$10^7$ | $1 \times 10^{14}$<br>$10^7$<br>$10^7$ | $1 \times 10^{12}$<br>$10^7$<br>$10^7$ |

Source: A. Menedjhi *et al*, (2021), Y. Liu, *et al*. (2023), M. K.Hossain *et al*. (2022), J.P.C. Baena *et al*. (2015), V. Deswal *et al*, (2024), K.Q. Wang *et al*. (2021), I. Chandran *et al*. (2023), N. Benaissa *et al*., (2023), P. Sawicka-Chudy *et al*., (2019).

Figure 2. Characteristics of the solar cell.



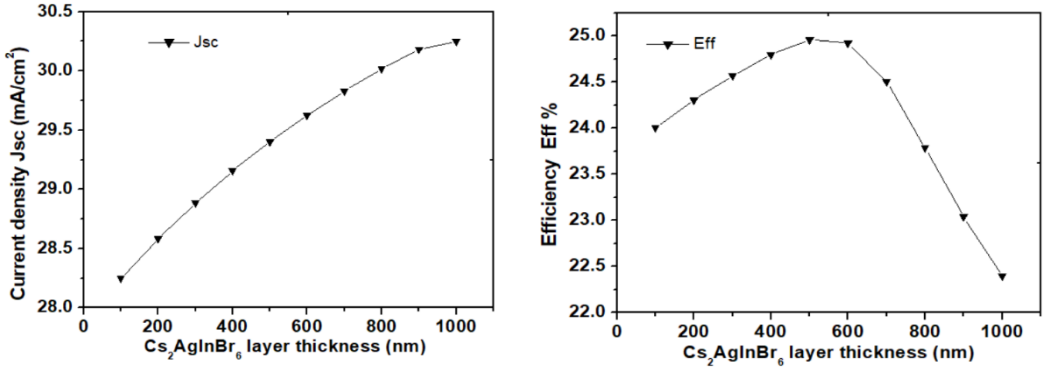

Source: Authors

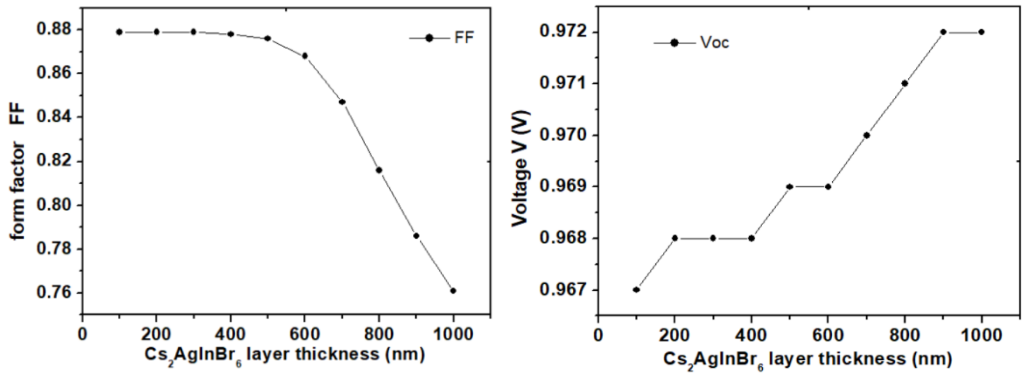
## 3.2 IMPACT OF THE ACTIVE LAYER'S THICKNESS $CS_2AGINBR_6$

In Figure 3, we present the four variations of the output characteristics of cell containing double perovskite $Cs_2AgInBr_6$, evaluated according to thickness.

Increasing the active layer's thickness leads to higher current density (Jsc) and voltage (Voc), while the fill factor (FF) gradually decreases. Moreover, the efficiency (Eff) improves as the thickness grows from 100 nm to 500 nm, but begins to decline beyond this range.

Figure 3. The impact of $Cs_2AgInBr_6$ layer thickness on cell characteristic parameters (JSC, Eff, FF, VOC).





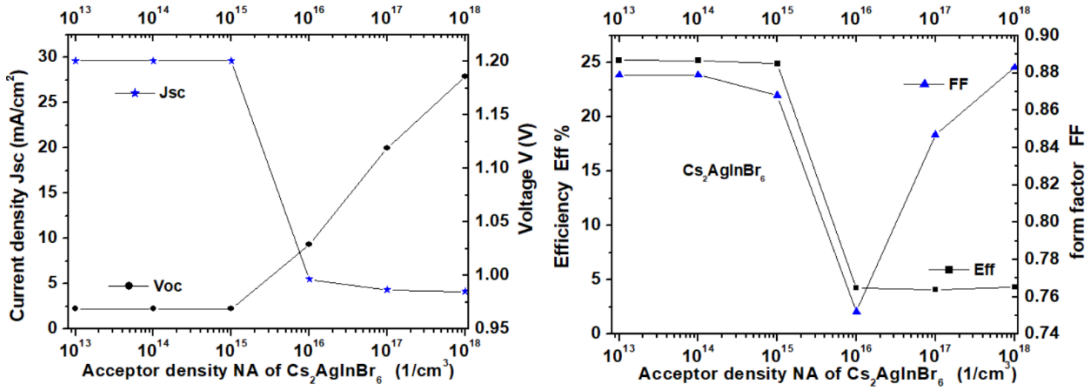

Source: Authors

## 3.3 THE IMPACT OF ACCEPTOR DENSITY (NA) IN THE ACTIVE LAYER ($CS_2AGINBR_6$)

The doping level of the active layer is essential for enhancing solar cell performance and optimizing efficiency. To evaluate the effect of different acceptor densities in the absorber layer on cell performance, the acceptor concentration was varied from $1\times10^{13}$ $cm^{-3}$ to $1\times10^{18}$ $cm^{-3}$. This range was analyzed for its impact on key device parameters, including ($V_{OC}$), ($J_{SC}$), (FF), and (Eff), as illustrated in Figure 4.

Figure 4 shows that increasing the doping concentration of the active layer keeps the performance parameters (FF, $V_{OC}$, $J_{SC}$, Eff) constant up to $1\times10^{15}$ $cm^{-3}$. Beyond this concentration, as the acceptor density increases, $V_{OC}$ rises between $1\times10^{15}$ $cm^{-3}$ and $1\times10^{18}$ $cm^{-3}$, peaking at 1.186 V at $1\times10^{18}$ $cm^{-3}$. Other performance metrics decline up to an acceptor density of $10^{16}$ $cm^{-3}$; beyond this point, $J_{SC}$ and Eff remain stable while FF increases. After acceptor doping, holes and electrons become the majority and minority carriers, respectively. Thus, with specific acceptor atom doping, the number of majority carriers (holes) increases, enhancing the device's charge capacity.

Figure 4. The impact of Acceptor density of Doule Perovskite ($Cs_2AgInBr_6$) layer.




Source: Authors

## 4 CONCLUSION

The AMPS-1D simulation software was used to model a heterojunction solar cell incorporating the double perovskite $Cs_2AgInBr_6$. The main objective of this study was to evaluate the impact of the thickness of the $Cs_2AgInBr_6$ (p) active level and the variation of the acceptor density in this layer, while determining the structural parameters of each cell component. Simulation results revealed that the optimum thickness for the active layer should be between 500 and 600 nm for technological applications. Furthermore, our models showed that ideal acceptor densities, leading to optimal cell performance, are generally between $10^{13}$ and $10^{15}$ $cm^{-3}$.

The study successfully demonstrated the potential of the $SnO_2/Cs_2AgInBr_6/CuO$ solar cell through numerical simulation and optimization. The optimized cell configuration achieved a notable increase in efficiency, suggesting that further research and development could lead to commercially viable solar cells.

Improving the efficiency of photovoltaic cells remains a critical pursuit in renewable energy research. By focusing on advancements in materials science, manufacturing techniques, and optical design, researchers aim to maximize light absorption and minimize energy loss, ultimately enhancing the conversion of sunlight into electricity. This multidimensional approach not only strives to boost energy output but also seeks to make solar technology more cost-effective and environmentally sustainable for widespread adoption in the global energy landscape.

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