

DEVICE-LEVEL SIMULATION OF $\text{Rb}_2\text{InSbCl}_6$ DOUBLE PEROVSKITES FOR EFFICIENT SOLAR CELL APPLICATIONS

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DOI: <https://doi.org/10.5281/zenodo.22913880>

Keywords

Lead-free perovskites; SCAPS-1D simulation; photovoltaic; Solar cells

Article History

Received: 01 June 2026

Accepted: 23 August 2026

Published: 23 September 2026

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Abstract

The investigation of lead-free double perovskites for third generation photovoltaic uses has been spurred by the quest for effective and eco-friendly photovoltaic materials. In this study, SCAPS-1D simulations were employed to estimate the photovoltaic efficiency of $\text{Rb}_2\text{InSbCl}_6$ double perovskites. This material was used as absorber layers in simulated solar cell architectures because of its excellent optical qualities and appropriate bandgap. To maximise the device performance, various electron transport layers (TiO_2 , IGZO, and SnO_2) were examined. For $\text{Au/CuO/Rb}_2\text{InSbCl}_6$ /ETL/FTO designs, photovoltaic metrics for instance open-circuit voltage V_{OC} , short-circuit current density J_{SC} , fill factor (FF), power conversion efficiency (η), and quantum efficiency (QE) were assessed. TiO_2 showed the most promising performance among the examined transport layers, indicating the possibility of $\text{Rb}_2\text{InSbCl}_6$ double perovskites as an effective lead-free absorber material for the future photovoltaic applications.

1 INTRODUCTION:

1.1 Motivation for studying $\text{Rb}_2\text{InSbCl}_6$ Double Perovskites

Due to rising demand and environmental harm, the world is currently experiencing a major energy crisis. It has made clean, effective, and sustainable energy solutions urgently necessary [1]. The switch from fossil fuels to renewable energy sources offers a chance to meet the world's expanding energy requirements in a relatively sustainable manner while shielding the environment from the harmful consequences of traditional fossil power sources that were

previously used to meet this demand (2). The acceptance of solar energy as a clean and renewable solution has accelerated due to the growing need for sustainable power and the limited supply of fossil fuels. Perovskite solar cells (PSCs) have captivated a lot of attention in photovoltaic research on account of their low cost of production and better optoelectronic behavior (3). Because of their tunable band gaps, high absorption coefficients, long carrier diffusion lengths, and solution-processable production approaches, metal halide perovskites have accumulated a lot of concern recently.

These characteristics have made it possible for perovskite solar cells (PSCs) to achieve impressive power conversion efficiencies (PCEs) of more than 26.95%, matching or surpassing those of well-known technologies like silicon-based photovoltaics(4). However, Pb-based perovskite's toxicity and environmental instability continue to be major barriers to their commercialization, which drives the hunt for sustainable, lead-free substitutes. Researchers are eager to advance solar cell technology to provide dependable and affordable energy solutions, emphasizing the potential of photovoltaic (PV) systems as crucial instruments for renewable energy generation. For many years, silicon-based solar cells have dominated the commercial solar energy market. Nevertheless, they have intrinsic disadvantages like low absorption coefficients, high production costs, and poor cost-effectiveness. The hunt for substitute solar materials has been prompted by these drawbacks(5). Researchers are becoming increasingly interested in perovskite materials due to their superior photovoltaic performance, inexpensive raw materials, and need for basic processing environment. The PSCs can be produced in labs utilizing wet chemistry and basic inexpensive methods including spin coating, dip coating, screen printing, dual source evaporation, etc., without the need for complex processing conditions. It is also possible to develop the perovskite materials on a flexible substrate. (6) An ABX_3 perovskite crystal structure in an organic metal-halide hybrid material was used as the light-absorbing layer in a recently published perovskite solar panel. As a next-generation solar cell, this kind of perovskite solar cell has garnered a lot of interest. A 3.8% efficient perovskite solar cell was initially reported by Kojima et al. in 2009(7). Nevertheless, due to the material's structural instability and ease of degradation upon exposure to air, moisture, and temperature, halide hybrid perovskites continue to face several unresolved problems in large-scale industrial applications. Furthermore, they frequently contain lead (Pb), which is poisonous and regarded as a serious environmental hazard. Thus, the development of stable, Pb-free,

nontoxic perovskites is essential for the advancement of perovskites-based technologies in the future (8). As a result, studies are focused on finding more environmentally friendly and reliable substitutes. Due to their high synthesizability, phase stability, and environmentally benign composition, cesium-based lead-free double perovskites have received more attention recently in halide perovskite research (9). Vacancy-ordered double perovskites, like Cs_2BiI_6 and related materials, offer a promising lead-free substitute for traditional lead-based perovskites, especially because of their improved stability and low toxicity. These materials are good candidates for sustainable energy harvesting because of their favorable thermal properties, which are linked to anharmonic lattice dynamics. They have also demonstrated potential in thermoelectric applications. Furthermore, perovskites like Mg_3NSb and Ca_3NSb illustrates an additional promising class of lead-free photovoltaic materials.(10) The development of lead-free halide double perovskites for large-scale solar applications is still fraught with difficulties, though. Stability problems including moisture and temperature instability continue to be a major obstacle that must be overcome. To increase the stability and dependability of lead-free perovskite solar cells, researchers are actively investigating several approaches, such as interface engineering, compositional tweaking, and device encapsulation techniques. While tackling these issues, it's critical to acknowledge lead-free halide perovskites wider potential to transform solar energy (11). Lead presents a significant threat to both human environmental and health concerns. It can hinder bone calcification and seriously harm the neurological and renal systems, even at low exposure limits. To address these issues, scientists are attempting to create more stable and less hazardous perovskite materials by substituting different homovalent and heterovalent cations for lead ions in the perovskite family (12). Bismuth and antimony-based materials are especially desirable from an environmental perspective because of their excellent stability and low toxicity. Nevertheless, their efficiency in solar cells is still

lower than that of Pb-based materials (13). It is a remarkable challenge to close the gap between high efficiency and long lifetimes by removing toxic materials, and new Pb-free perovskite materials can be crucial to achieving these lofty objectives (14). Perovskite materials have become attractive options to deal with these two issues (15). By utilizing the special qualities of these materials to develop sustainable and effective energy systems, our study on $\text{Rb}_2\text{InSbCl}_6$ opens the door to a new generation of solar energy solutions. This work puts halide compounds at the forefront of cutting-edge materials that have the potential to revolutionize solar energy. We are getting closer to the goal of having cheap, effective solar electricity that can light up the entire planet with every new development. Furthermore, $\text{Rb}_2\text{InSbCl}_6$ has the benefit of being a low-toxicity and earth-abundant material, which supports international efforts to find economical and ecologically sustainable energy options. Our goal in investigating these HDPs is to aid in the creation of cutting-edge optoelectronic devices and next-generation photovoltaics. Our results highlight the value of interdisciplinary research by demonstrating how materials science can result in ground-breaking developments in energy storage and conversion. We are about to make fascinating findings that could advance energy technology for coming generations as we dig deeper into these unique molecules. (16)

2. Simulation Software:

Enhancing a groundbreaking material instrument requires simulation of solar cell device performance. Such simulations of the suggested solar cell structure can forecast efficiency and dependability prior to fabricating, as solar cell fabrication is both convoluted and prolonged. Software programs that are applicable to model cell features employing device's input parameters incorporate SETFOS, SILVACO, ATLAS, AMPS, COMSOL, and SCAPS-1D. Researchers at Gent University

developed SCAPS-1D as a numerical simulation program. Initially, the program was used to perform the simulation and define the solar cell's structure, which included layers like RbGeBr_3 for the perovskite absorber, ETLs, and HTLs. Material variables comprising bandgap, electron affinity, different constants, and carrier mobilities were defined in addition to operational factors such as temperature, illumination intensity (AM 1.5G), and the bias voltage spectrum for J-V characteristics. Quantum efficiency, capacitance, Mott-Schottky characteristics, and J-V characteristics were among the measurements used. The data was then evaluated utilizing visual interfaces, for instance Origin, to determine the solar cell's efficiency. Additionally, the simulator program uses three coupled differential equations: the Poisson equation [Eq. (1)], the electron equation for continuity [Eq. (2)], and the hole equation for continuity [Eq. (3)]. For steady-state electron and hole continuity, the fourth and fifth equations [Eqs. (4) and (5)] are used. The sixth and seventh equations are utilized to calculate the densities of electrons and holes. [43][44][45]

2.1. Mathematical modeling

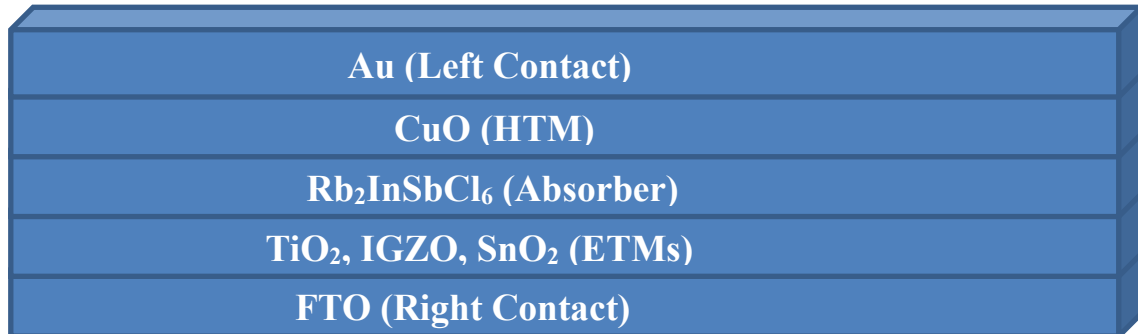
Poisson's equation, electron continuity equation, and hole continuity equation are used by the SCAPS-1D simulator to model semiconductor devices. These three related partial differential equations are analyzed by SCAPS-1D software to determine the concentrations of electrons and holes in the electrostatic potentials as a function of x .

The current density (J_{sc}), quantum efficiency (QE), energy band, and current-voltage characteristics are calculated using the subsequent three formulas.

Poisson's Equation:

$$-\frac{\partial}{\partial x}(-\epsilon(x)\frac{\partial V}{\partial x}) = q[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (1)$$

Continuity equation for electrons:



$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n \quad (2)$$

Continuity equation for holes:

$$\frac{\partial p}{\partial t} = \frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p \quad (3)$$

$$\frac{\partial n(x,t)}{\partial t} = G - R \quad (4)$$

$$\frac{\partial p(x,t)}{\partial t} = G - R \quad (5)$$

These formulas describe how recombination and generation processes affect the electron and hole densities over time.

Equations for Electron and Hole Current Density:

$$J_n(x) = qn(x)\mu_n E(x) + qD_n \frac{dn(x)}{dx} \quad (6)$$

The Au+ CuO+ Rb₂InSbCl₆ + ETLs + FTO simulated solar panel is displayed in Fig. 1. The productivity of these solar panels was determined using numerical simulation.

$$J_p(x) = qp(x)\mu_p E(x) + qD_p \frac{dp(x)}{dx} \quad (7)$$

where q= Charge, ϵ = Dielectric permittivity, V= Potential, $p(x)$ = Free holes concentration, $n(x)$ = Free electrons concentration, $N_D^+(x)$ = Ionized donor concentration, $N_A^-(x)$ = Ionized acceptor concentration, $p_t(x)$ = Trap density of hole, $n_t(x)$ = Trap density of electron, J_n = Current density of electron, J_p = Current density of holes, G_n = Rate of electrons generation, G_p = Rate of holes generation, R_n = Recombination rate of electron, R_p = Recombination rate of hole[44][45]

Standard AM 1.5 G, 1000 mW/cm² light was used to calculate electrical parameters.

Table 1 yields a thorough description of the CuO/ Rb₂InSbCl₆ /ETM input parameters.

Table.1: Material Parameters of HTM, ETMs and Absorber Layer

Material parameters	TiO ₂ (ETM)	IGZO (ETM)	SnO ₂ (ETM)	CuO (HTM)	Rb ₂ InSbCl ₆ (Absorber)
Thickness(μm)	0.065	0.060	0.070	0.1242	0.645
Band gap (eV)	3.2	3.05	3.6	1.5	1.06
Electron affinity (eV)	4.0	4.16	4.0	4.07	4.6
dielectric permittivity (relative)	9.0	10.0	9.0	18.1	4.089
CB effective density of states (cm ⁻³)	2.2×10 ¹⁸	5.0×10 ¹⁸	2.2×10 ¹⁸	2.2×10 ¹⁹	2.24×10 ¹⁸

VB effective density of states (cm^{-3})	1.8×10^{19}	5.0×10^{18}	1.8×10^{19}	5.5×10^{20}	7.09×10^{18}
electron thermal velocity ($cm s^{-1}$)	1.8×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
hole thermal velocity ($cm s^{-1}$)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
electron mobility ($cm^2 V^{-1} s^{-1}$)	2.0×10^1	1.5×10^1	1.0×10^2	1.0×10^1	5.0×10^1
hole mobility ($cm^2 V^{-1} s^{-1}$)	1.0×10^1	1.0×10^{-1}	2.5×10^1	1.0×10^{-1}	5.0×10^1
shallow uniform donor density ND ($1/cm^3$)	2.0×10^{19}	1.0×10^{16}	1.0×10^{19}	0	1.0×10^{15}
shallow uniform acceptor density NA ($1/cm^3$)	0	0	0	1.0×10^{18}	1.0×10^{15}

The input parameters of $Rb_2InSbCl_6$ (Absorber) are obtained from DFT calculation.

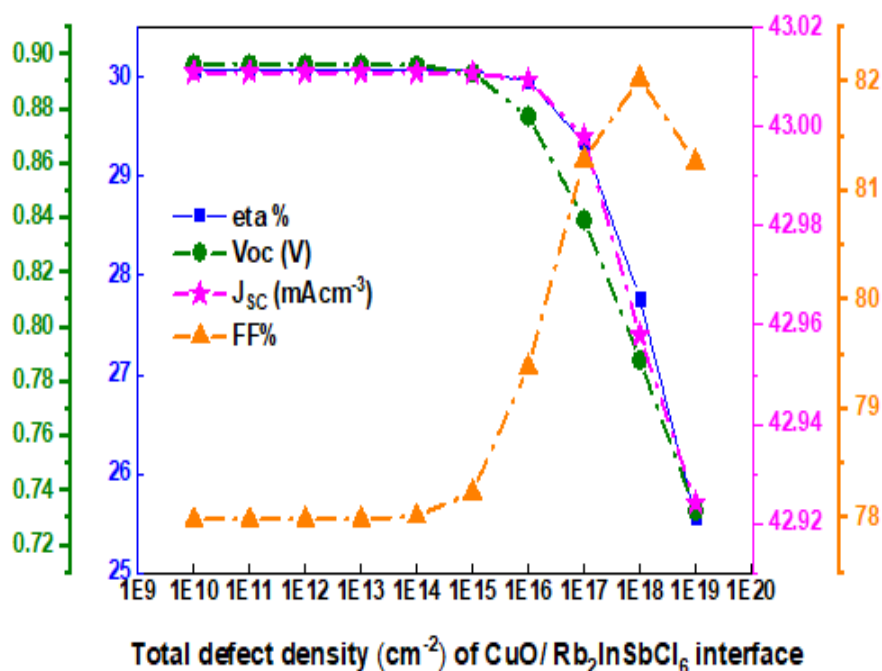


Fig.2: Simulated chart of Au + CuO + $Rb_2InSbCl_6$ + ETLs + FTO Solar cell

2.2 Numerical Simulations Result:

The device's photovoltaic characteristics are significantly influenced by variations in the total defect density at the $CuO/Rb_2InSbCl_6$ interface. V_{OC} , J_{SC} and FF stay almost constant at relatively low defect densities ($\sim 10^{10}$ - 10^{15} carrier recombination and hence lower solar performance [17]. The current graph shows a significant drop at high defect concentrations,

cm^{-2}), suggesting that the interface introduces relatively small recombination losses. The concentration of interface trap states rises with defect density, creating more recombination sites that interface encourage Fig.2. Total defect Density optimization of $CuO/Rb_2InSbCl_6$ which may be related to decreased quasi-Fermi-level splitting and increased interfacial non-radiative recombination. Similarly, because

interface traps can trap photogenerated carriers and prevent their effective collection at the electrodes, J_{SC} drops as the defect density increases. At even higher defect concentrations, the fill factor first rises and reaches a maximum before declining due to increasing recombination and worsening of carrier transport across the interface.[19] Thus, the findings show that maintaining high photovoltaic performance and preventing interfacial recombination require minimizing the CuO/Rb₂InSbCl₆ interface defect density. [17]

V_{OC} , J_{SC} , FF and efficiency (η) are nearly constant at low defect densities (10^9 - 10^{12} cm^{-3}), suggesting that the device is comparatively tolerant to a modest concentration of absorber flaws. [20]. All photovoltaic characteristics begin to drop when the defect density ascends over around 10^{12} cm^{-3} , with a noticeable degradation seen at $(10^{13}-10^{15}) \text{ cm}^{-3}$. Enhanced trap-assisted Shockley-Read-Hall recombination, which raises the recombination current and decreases the quasi-Fermi-level splitting, is primarily responsible for the decrease with increasing defect density.

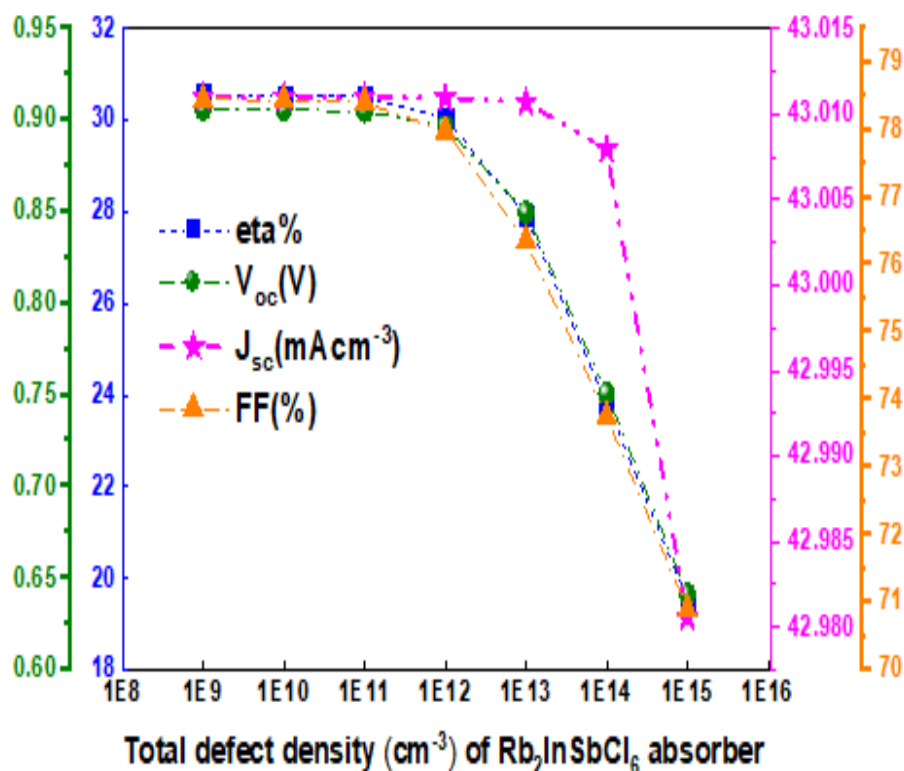


Fig.3. Total defect Density optimization of Rb₂InSbCl₆ Absorber.

Carrier trapping and decreased carrier lifetime and diffusion length, which impede the effective collection of photogenerated electrons and holes, are the causes of the drop in J_{SC} with greater defect concentrations. [21]. Because the higher density of defect states increases non-radiative recombination and charge-transport

losses within the absorber layer, FF and efficiency similarly decrease at large defect densities. Consequently, the graph shows that efficient Rb₂InSbCl₆ based solar cells require a low bulk defect density, with defect values of or lower typically being preferred in SCAPS-based simulations. [22]

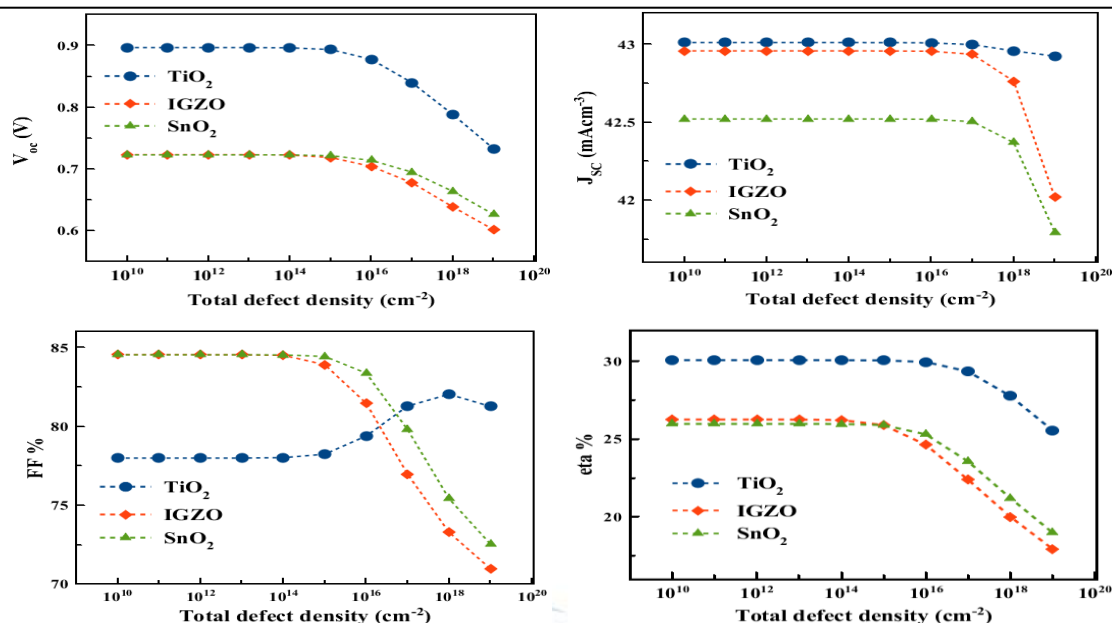


Fig.4. Total defect Density optimization of Rb₂InSbCl₆/ETL Interface

At low defect densities, TiO₂ has the greatest and most stable V_{oc} (≈ 0.90 V), whereas IGZO and SnO₂ stay close to 0.72 V; at high defect densities, V_{oc} falls because defect states encourage trap-assisted non-radiative recombination [23]. At low defect densities, J_{sc} is nearly constant, suggesting that defects have little effect in this area. However, at high defect densities, especially for IGZO and SnO₂, there is a discernible decrease because of higher carrier entrapment and recombination [24]. IGZO and SnO₂ show a significant decrease

after around 10^{16} cm^{-2} , whereas TiO₂ retains a reasonably high FF and shows a minor increase with increasing defect density in the estimated range. Increased recombination and charge-transport losses brought on by defect states are typically linked to such deterioration. For all three ETLs, efficiency declines as defect density rises; the decline is most noticeable at high defect densities. The combined degradation of V_{oc} , J_{sc} and FF causes this behaviour because flaws serve as recombination/trapping centers.[23] [24].

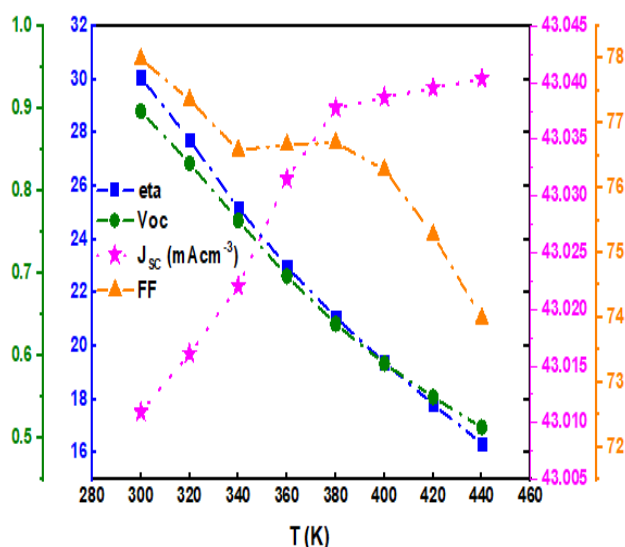


Fig.5. Temperature based performance of Au/CuO/Rb₂InSbCl₆/ETL/FTO solar cell device

Figure 5 shows how the photovoltaic parameters, V_{OC} , J_{SC} , fill factor (FF), and power conversion efficiency (η) change as the temperature increases from 300 to 440 K. V_{OC} significantly drops from roughly 30 to 16 as the temperature rises, suggesting a substantial negative temperature dependence. This decrease is typically linked to the rise in reverse saturation current and carrier recombination brought on by temperature, which reduces the open-circuit voltage. [25] J_{SC} , alternatively, increases slightly with temperature, from roughly 43.01 to 43.04 mAcm^{-2} . Although the temperature dependency of J_{SC} is often significantly smaller than that of V_{OC} this behaviour is commonly attributed to the lessening of the semiconductor band gap and the consequent rise in photogenerated charge carriers [26]. As the temperature rises, the FF likewise shows a general declining trend, going from roughly 78% to 74%. This suggests that the electrical quality of the solar-cell output characteristics deteriorates at high temperatures [27]. As a result, photovoltaic efficiency declines dramatically when the temperature rises because

the slight increase in J_{SC} is insufficient to offset the considerable decrease in V_{OC} and FF. At higher temperatures, the combined decrease in voltage and fill factor leads to general drop in device efficiency η is proportional to V_{OC} , J_{SC} and FF. [25]

The influence of absorber layer thickness on V_{OC} , J_{SC} , FF, and efficiency (η) for TiO_2 , IGZO, and SnO_2 based device topologies is shown in figure.

For all three device topologies, V_{OC} , J_{SC} , FF, and efficiency (η) often drop as the absorber thickness develop from 0 to 2 μm , whereas J_{SC} stays nearly constant. TiO_2 has the best photovoltaic performance among the ETLs under investigation, closely followed by IGZO, while SnO_2 shows somewhat lower values. Increased carrier recombination and transport losses are responsible for the decrease at higher thicknesses, suggesting that an ideal absorber thickness is necessary to attain optimal performance in lead-free double-perovskite solar cells. Studies of lead-free and double perovskite solar cells using SCAPS have shown similar thickness dependent behavior. [28][29][30][31]

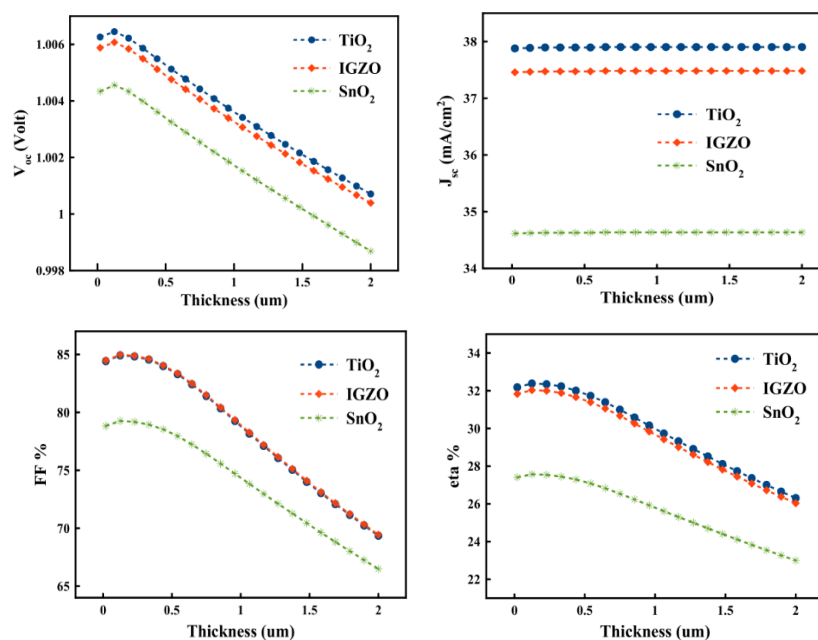


Fig.6: Thickness Optimization of CuO with Different ETLs.

Furthermore, tunable band alignment

Table 2: Optimized electrical parameters of $\text{Rb}_2\text{InSbCl}_6$ (Absorber) layer with different ETMs.

Device	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF %	Eta %	T/E & Ref.
Au/CuO/ $\text{Rb}_2\text{InSbCl}_6$ /IGZO/FTO	0.7225	42.95	84.50	26.23	This Study
Au/CuO/ $\text{Rb}_2\text{InSbCl}_6$ / SnO_2 /FTO	0.7215	42.52	84.43	25.90	This Study
Au/CuO/ $\text{Rb}_2\text{InSbCl}_6$ / TiO_2 /FTO	0.7230	43.00	84.54	26.28	This Study

The thickness-dependent results confirm that the selection of ETL has a profound impact on the photovoltaic efficiency of the $\text{Rb}_2\text{InSbCl}_6$ absorber. J_{sc} stays almost constant as the absorber thickness rises, suggesting that adequate photon absorption is already attained at comparatively low thickness. On the other hand, with greater thicknesses, V_{oc} , FF, and efficiency (η) fall mostly because of increased

bulk recombination and carrier-transport losses. While SnO_2 provides relatively lower photovoltaic characteristics, TiO_2 shows the best overall performance among the examined ETLs, closely followed by IGZO. These findings emphasise how crucial it is to concurrently optimise interfacial band alignment and absorber thickness for effective lead-free double-perovskite solar cells. [32][33][34][35].

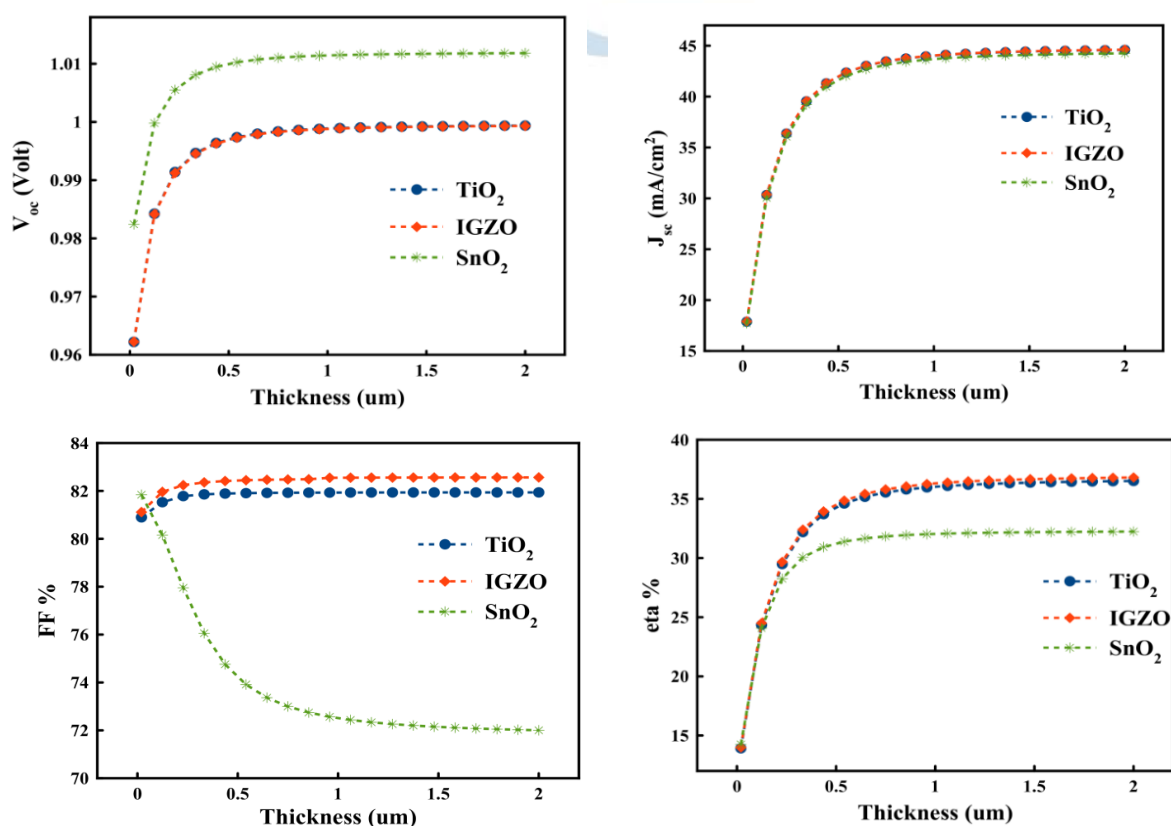


Fig. 7. Thickness of $\text{Rb}_2\text{InSbCl}_6$ with different ETLs

The Au/CuO/Rb₂InSbCl₆/ETL/FTO device's J-V parameters show how well it performs photovoltaically under light. The effective photogeneration and subsequent withdrawal and separation of charge carriers via the Rb₂InSbCl₆ absorber and transport layers are

responsible for the generated photocurrent. The curve's values for J_{sc}, V_{oc}, and FF are important measures of the device's performance; enhanced power-conversion efficiency is a result of effective interfacial charge transport and reduced recombination. [36][37][38][39].

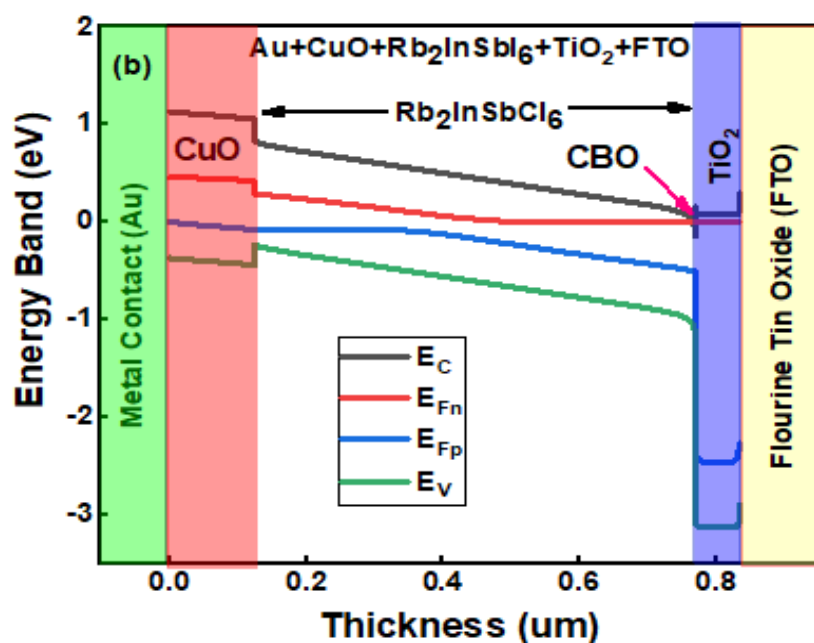


Fig.8. Current Density, of Au + CuO + Rb₂InSbCl₆ + ETL + FTO Solar Cell.

Efficiency is a result of effective interfacial charge transport and reduced recombination. [36][37][38][39].

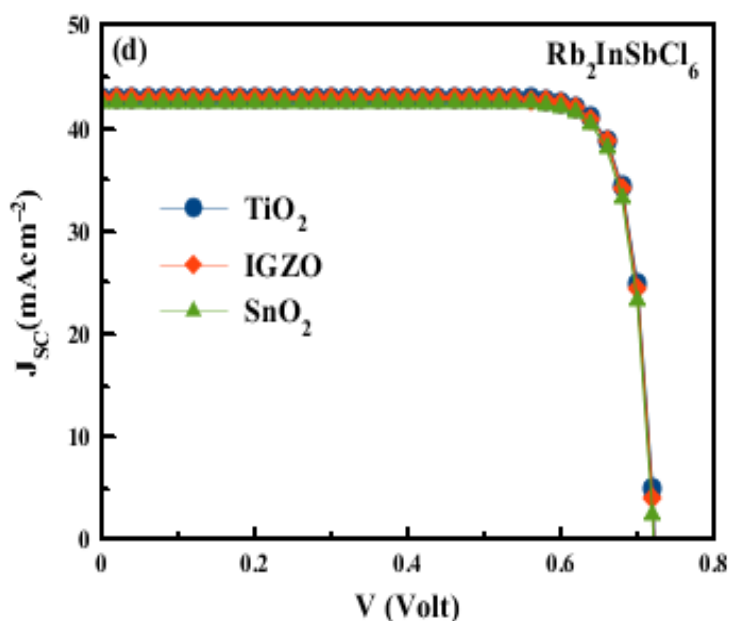


Fig.9: Energy band diagrams of Au + CuO + Rb₂InSbCl₆ + TiO₂ + FTO Solar Cell

The Au/CuO/Rb₂InSbCl₆/ETL/FTO device's J-V parameters show how well it performs photovoltaically under light. The effective photogeneration and subsequent withdrawal and separation of charge carriers via the Rb₂InSbCl₆ absorber and transport layers are responsible for the generated photocurrent. The curve's values for J_{sc}, V_{oc}, and FF are important measures of the device's performance; enhanced power-conversion

The Au/CuO/Rb₂InSbCl₆/TiO₂/FTO device exhibits favourable charge selective transport due to its energy-band alignment. When exposed to light, photogenerated holes migrate toward the CuO HTL and are collected by the Au electrode, while photogenerated electrons are preferentially conveyed from the Rb₂InSbCl₆ absorber to the TiO₂ ETL and then gathered by FTO. At the absorber/transport-layer interfaces, the proper band offsets promote charge separation, inhibit carrier recombination, and enhance solar efficiency. [40][41][42].

Conclusion:

Using the Au/CuO/Rb₂InSbCl₆/ETL/FTO device architecture, this study concludes with a thorough SCAPS-1D simulation evaluation of Rb₂InSbCl₆-based solar cells. To find the best ETL for effective carrier extraction, several electron transport layers, such as TiO₂, IGZO, and SnO₂, were thoroughly examined. To maximize the photovoltaic performance, the impacts of CuO as the hole transport layer, operating temperature, bulk defect density, interface defect density, and absorber-layer thickness were further examined. The optimised Rb₂InSbCl₆/TiO₂ device showed the best photovoltaic properties among the combinations under investigation, suggesting effective charge separation and transport. The gains in V_{oc}, J_{sc}, fill factor, and power conversion efficiency (PCE) that were obtained demonstrate the potential of Rb₂InSbCl₆ as a lead-free absorber layer. Overall, the simulation results indicate that the efficiency of Rb₂InSbCl₆-based solar cells can be greatly improved by carefully optimizing the ETL, absorber thickness, defect densities, and device operating requirements. This provides helpful

theoretical recommendations for the development of effective and eco-friendly photovoltaic devices.

Data availability:

The article and the Supplementary Material that goes with it contain the data that supports the study's conclusions.

Funding:

This study received no specific funding from any government, corporation, or nonprofit organizations.

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