

RESEARCH ARTICLE

Simulation–Driven Optimization of Charge Transport Layers in RbGeI₃–Based Lead–Free Perovskite Solar Cells Using SCAPS–1D

Saumya Vaish ^{1,*}, Shiv Kumar Dixit ¹, Sultan Ahmad ², Faheem Ahmed ², Zishan Husain Khan ²

ABSTRACT: The growing interest in perovskite photovoltaics has been tempered by concerns regarding the toxicity of lead-based compounds, prompting a concerted research effort toward developing environmentally benign alternatives. Among the promising candidates, germanium-based perovskites offer a compelling combination of suitable optoelectronic properties and reduced ecological impact. This study presents a comprehensive numerical investigation of a lead-free perovskite solar cell employing Rubidium Germanium iodide (RbGeI₃) as the absorber material within a planar n-i-p architecture. The proposed device configuration consists of Fluorine-doped tin oxide (FTO) as the transparent front contact, Tungsten disulfide (WS₂) as the electron transport layer, RbGeI₃ as the absorber, cuprous oxide (Cu₂O) as the hole transport layer, and gold (Au) as the back metal contact. Using the Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D), we systematically examined the influence of critical parameters including absorber layer thickness, bulk defect density, and operating temperature on the overall device performance. The simulation results demonstrate that careful optimization of these parameters yields a power conversion efficiency of 21.14 %, accompanied by a fill factor of 0.80, a short-circuit current density of 32.28 mA per square centimeter, and an open-circuit voltage of 0.8 V. Particular attention was devoted to understanding the role of the transport layers, with WS₂ and Cu₂O proving to be effective charge-selective contacts that facilitate efficient carrier extraction while minimizing recombination losses. The external quantum efficiency analysis revealed that the device maintains high photon conversion across the visible spectrum, reaching approximately 90 % in the wavelength range where the absorber operates most effectively. Energy band diagram analysis confirmed proper band alignment between the constituent layers, which is essential for minimizing energy barriers and promoting unidirectional charge flow. The findings from this simulation study suggest that RbGeI₃-based devices, when combined with appropriate transport materials, possess considerable potential for advancing the development of next-generation photovoltaics that are both high-performing and environmentally sustainable.

Keywords: Lead-free perovskite, Rubidium Germanium iodide, SCAPS-1D simulation, charge transport layers, photovoltaic optimization, inorganic absorber

Received: 21 July 2025; Revised: 17 September 2025; Accepted: 20 October 2025; Published Online: 07 November 2025

1. INTRODUCTION

The rapid advancement of photovoltaic technology over the

past two decades has been substantially driven by the emergence of perovskite solar cells as a compelling candidate for next-generation energy conversion devices. These materials, characterized by the general formula ABX₃ where A represents an organic or inorganic cation, B denotes a metal cation, and X signifies a halide anion, have demonstrated remarkable optoelectronic properties that make them exceptionally well-suited for solar energy harvesting [1]. The high absorption coefficient exhibited by perovskite materials ensures efficient photon capture even with relatively thin

¹ Department of Electronics and Communication Engineering, School of Engineering, Manav Rachna University, Faridabad, Haryana, 121004-India

² Department of Applied Sciences and Humanities, Jamia Millia Islamia University, New Delhi, 110025-India

* Author to whom correspondence should be addressed:
svaish91@gmail.com (Saumya Vaish)

absorber layers, while their low exciton binding energy facilitates effective charge separation upon illumination [2]. Additionally, the tunable bandgap achievable through compositional engineering allows for optimization of the spectral response, and the high carrier mobility observed in many perovskite compositions supports efficient charge transport toward the respective extraction layers [3].

The historical trajectory of perovskite solar cell development began with the pioneering work of Kojima and colleagues in 2009, who first demonstrated the potential of these materials by achieving a power conversion efficiency of 3.8 % using organometal halide perovskites as sensitizers in photovoltaic devices [4]. This initial breakthrough sparked intense research activity worldwide, leading to remarkable improvements in device performance over subsequent years. Through systematic optimization of material composition, deposition techniques, and device architectures, researchers have progressively elevated the power conversion efficiency of perovskite solar cells to exceed 25 % in laboratory-scale devices [5]. This rapid efficiency evolution, rivaling the performance of established technologies such as crystalline silicon and thin-film compounds, has positioned perovskite photovoltaics at the forefront of emerging solar energy research.

Despite these impressive achievements, the widespread commercialization of perovskite solar cells faces a significant obstacle in the form of lead toxicity [6]. The most efficient perovskite compositions to date incorporate lead at the B-site, raising legitimate environmental and health concerns regarding material synthesis, device operation, and end-of-life disposal. The water-soluble nature of lead compounds further exacerbates these concerns, as any breach in device encapsulation could potentially release toxic species into the environment [7]. This toxicity challenge has motivated extensive research efforts directed toward identifying suitable alternatives that can replicate the exceptional optoelectronic properties of lead-based perovskites while eliminating the associated environmental hazards [8].

Among the various candidates proposed as lead substitutes, tin and Germanium have emerged as particularly promising options due to their similar electronic configurations and ionic radii compared to lead [9]. Tin-based perovskites have attracted considerable attention and have demonstrated encouraging photovoltaic performance, with power conversion efficiencies reaching approximately 14 % in experimental devices [10]. However, the tendency of tin to oxidize from the divalent to the tetravalent state introduces stability challenges that have thus far limited the practical viability of tin-based devices under operational conditions [11]. This oxidation susceptibility leads to self-doping effects and increased recombination losses, compromising both efficiency and long-term stability.

Germanium presents an intriguing alternative to both lead and tin, offering several distinctive advantages that warrant careful investigation [12]. The ionic radius of germanium, approximately 0.73 Å, is substantially smaller than that of lead at 1.49 Å, yet the perovskite crystal structure can accommodate this size difference without significant

distortion when Germanium substitutes for lead at the B-site. This structural compatibility is essential for maintaining the desirable optoelectronic properties associated with the perovskite framework. Furthermore, the smaller ionic radius of Germanium contributes to enhanced orbital overlap and improved charge carrier transport characteristics, potentially enabling higher conductivities than those observed in lead-based analogs [13]. The Germanium 4s lone pair exhibits greater reactivity compared to the lead 6s lone pair, leading to favorable modifications in the electronic band structure that can benefit photovoltaic performance [14].

The first experimental demonstration of germanium-based perovskite solar cells was reported by Krishnamoorthy and coworkers, who fabricated devices using cesium Germanium iodide as the absorber layer and achieved a power conversion efficiency of 0.11% [15]. While modest in absolute terms, this proof-of-concept study established the fundamental viability of Germanium perovskites for photovoltaic applications and opened avenues for further optimization. Subsequent investigations have explored various germanium-based compositions, including those incorporating Rubidium at the A-site, which offers the advantage of an all-inorganic formulation that may enhance thermal and environmental stability compared to hybrid organic-inorganic alternatives [16].

The selection of appropriate charge transport layers represents a critical consideration in perovskite solar cell design, as these materials govern the selective extraction and collection of photogenerated charge carriers [17]. The hole transport layer, in particular, has been the subject of extensive investigation, with organic materials such as spiro-OMeTAD emerging as the most commonly employed option in high-efficiency devices [18]. However, spiro-OMeTAD suffers from several notable disadvantages, including high synthesis costs, complex molecular structure requiring elaborate purification procedures, and intrinsic instability that necessitates the use of hygroscopic dopants [19]. These dopants, while improving conductivity, can accelerate degradation of the perovskite absorber through moisture ingress and ion migration, ultimately compromising device longevity [20]. The search for stable, cost-effective inorganic alternatives to organic hole transport materials has therefore become a priority research direction.

Cuprous oxide has emerged as a particularly attractive candidate for inorganic hole transport layers due to its favorable optoelectronic properties and earth-abundant composition [21]. This p-type semiconductor exhibits a direct bandgap of approximately 2.17 eV, providing high optical transparency across the visible spectrum while maintaining sufficient conductivity for efficient hole extraction [22]. The valence band edge of cuprous oxide aligns favorably with the ionization potential of many perovskite absorbers, facilitating unidirectional hole transfer while blocking electron flow [23]. Recent advances in deposition techniques, including bidirectional pulsed electrodeposition, have enabled the fabrication of cuprous oxide films with enhanced phase purity, reduced defect densities, and improved carrier mobilities exceeding 46 cm²/vs [24]. These developments position

cuprous oxide as a viable alternative to organic hole transport materials for high-performance perovskite solar cells.

On the electron transport side, Tungsten disulfide has attracted increasing attention as a promising inorganic electron transport material [25]. As a transition metal dichalcogenide, Tungsten disulfide exhibits excellent electron mobility on the order of 100 cm²/vs, which facilitates rapid extraction of photogenerated electrons and minimizes recombination losses at the electron transport layer-absorber interface [26]. The conduction band minimum of Tungsten disulfide provides appropriate energetic alignment with the conduction band of germanium-based perovskites, creating a favorable gradient for electron extraction while effectively blocking holes [27]. Additionally, Tungsten disulfide can be deposited using scalable techniques compatible with large-area manufacturing, enhancing its practical appeal for commercial applications [28].

The scientific literature contains several important contributions to the understanding of germanium-based perovskite solar cells through numerical simulation approaches. Saikia and colleagues systematically investigated the influence of various device parameters on the performance of germanium-based perovskite solar cells, providing valuable insights into the relationships between material properties and device outcomes [29]. Pindolia and coworkers conducted an extensive simulation study examining the effects of different electron transport materials and hole transport materials on Rubidium Germanium iodide-based devices, identifying promising material combinations for further investigation [30]. Mary and colleagues explored the possibility of hole transport layer-free device architectures, demonstrating that Titanium dioxide alone could serve as an effective charge transport layer in Rubidium Germanium iodide devices, albeit with some performance trade-offs [31]. More recently, Rahman and collaborators achieved simulated power conversion efficiencies exceeding 30 % through comprehensive optimization of Rubidium Germanium iodide devices incorporating various transport layer combinations [32]. Neupane and colleagues specifically investigated Tungsten disulfide as an electron transport layer for Rubidium-based halide perovskites, confirming its superior performance compared to alternative electron transport materials [32].

The present study contributes to this growing body of knowledge by investigating a previously unexplored device architecture combining Tungsten disulfide as the electron transport layer and cuprous oxide as the hole transport layer with a Rubidium Germanium iodide absorber in a planar n-i-p configuration. While individual components of this architecture have been studied in various contexts, the specific combination of Tungsten disulfide and cuprous oxide as complementary transport layers for Rubidium Germanium iodide-based devices has not been systematically investigated. This work addresses this gap by providing a comprehensive numerical analysis of the Fluorine-doped tin oxide, Tungsten disulfide, Rubidium Germanium iodide, cuprous oxide, gold device structure using SCAPS-1D simulation software. The study examines the influence of

critical parameters including absorber layer thickness, defect density, and operating temperature on device performance, with the objective of identifying optimal design parameters for maximizing power conversion efficiency. The simulation results demonstrate that this carefully engineered device architecture achieves a power conversion efficiency of 21.14 %, accompanied by a fill factor of 0.80, a short-circuit current density of 32.28 mA per square centimeter, and an open-circuit voltage of 0.8 V. These findings establish the viability of this material combination and provide guidance for experimental efforts aimed at realizing high-performance, environmentally sustainable perovskite solar cells based on Rubidium Germanium iodide.

2. SIMULATION METHODOLOGY

2.1. Simulation Tool and Governing Equations

The numerical simulations presented in this work were performed using the Solar Cell Capacitance Simulator in One Dimension, commonly referred to as SCAPS-1D, which was developed at the Department of Electronics and Information Systems of the University of Gent in Belgium under the supervision of Professor Marc Burgelman [17]. This software has been extensively validated and widely adopted within the photovoltaic research community for the analysis and optimization of thin-film solar cells, including perovskite-based devices. The SCAPS-1D program operates by solving the fundamental semiconductor equations that govern charge transport and recombination within multilayer device structures under steady-state conditions and illuminated operation.

The core mathematical framework of the simulator encompasses three coupled differential equations that collectively describe the electrodynamic behavior of semiconductor devices. The Poisson equation relates the electrostatic potential to the spatial distribution of charge densities, including free carriers, ionized dopants, and trapped charges within defect states. The continuity equations for electrons and holes account for the generation, recombination, and transport of charge carriers throughout the device layers [18]. These equations are solved numerically under appropriate boundary conditions that reflect the properties of the front and back contacts, as well as the interfaces between adjacent layers. The simulator employs an iterative approach to achieve self-consistent solutions that satisfy all three equations simultaneously, thereby providing a physically realistic description of device operation under specified illumination and bias conditions.

2.2. Device Structure and Material Parameters

The proposed device architecture adopts a planar n-i-p configuration consisting of five distinct layers arranged in sequence from the illuminated side to the back contact (Figure 1). The transparent conductive oxide layer comprises

Fluorine-doped tin oxide, which serves as the front contact and allows incident light to enter the device while providing lateral conductivity for current collection. Upon this substrate, the electron transport layer of Tungsten disulfide is deposited, followed by the Rubidium Germanium iodide absorber layer, the cuprous oxide hole transport layer, and finally the gold back contact. This architecture was designed to facilitate efficient charge separation by establishing appropriate band alignments between successive layers, with the electron transport layer positioned to selectively extract photogenerated electrons and the hole transport layer positioned to selectively extract photogenerated holes.

The optical and electrical parameters assigned to each layer in the simulation were compiled from previously published experimental and theoretical studies to ensure physical realism and consistency with established material properties. Table 1 presents the complete set of input parameters employed in the baseline simulation, including layer thicknesses, bandgap energies, electron affinities, dielectric constants, effective densities of states in the conduction and valence bands, thermal velocities for electrons and holes, charge carrier mobilities, doping concentrations, and total defect densities [19]. The thickness values were initially set to 0.05 μm for all layers except the absorber, which was assigned a thickness of 0.5 μm for the baseline case, with subsequent parametric studies examining the influence of varying the absorber thickness over a broader range. The defect densities were uniformly initialized at $1 \times 10^{15} \text{ cm}^{-3}$ across all layers, representing a reasonable approximation of material quality achievable through contemporary fabrication techniques.

The doping concentrations reflect the intended conductivity types of the respective layers, with the Fluorine-doped tin oxide and Tungsten disulfide layers assigned donor-type doping to function as electron transport materials, while the cuprous oxide layer was assigned acceptor-type doping to function as a hole transport material. The Rubidium

Germanium iodide absorber was modeled with a low background doping concentration consistent with intrinsic or near-intrinsic semiconductor behavior, which is appropriate for the active layer in which photogenerated carriers are produced and separated.

2.3. Simulation Conditions and Contact Properties

All simulations were conducted under standard illumination conditions corresponding to the AM1.5G solar spectrum, which represents the typical spectral distribution and intensity of sunlight at the earth's surface after passing through 1.5 atmosphere thickness at a zenith angle of 48 degrees. This spectrum is the internationally accepted reference for characterizing photovoltaic device performance under terrestrial operating conditions and enables direct comparison of simulation results with experimental measurements reported in the literature.

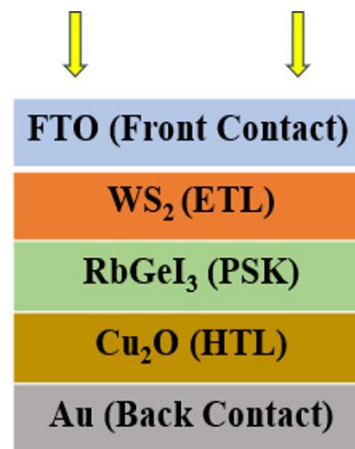


Fig. 1. Device architecture of Solar Cell.

Table 1. Optoelectronic parameters employed in the SCAPS-1D simulation for each layer of the FTO/WS₂/RbGeI₃/Cu₂O/Au device architecture. The values are compiled from previously reported experimental and theoretical studies [Adapted from ref. 27, 29, 30, 32].

Parameter	FTO	WS ₂	RbGeI ₃	Cu ₂ O
Thickness (μm)	0.05	0.05	0.5	0.05
Bandgap (eV)	3.6	2.1	1.31	2.0
Electron affinity (eV)	4.0	4.05	3.9	3.2
Dielectric permittivity (relative)	9.0	13.6	23.31	7.6
CB effective density of states ($1/\text{cm}^3$)	2.2×10^{18}	2.0×10^{18}	2.8×10^{19}	2.2×10^{18}
VB effective density of states ($1/\text{cm}^3$)	1.8×10^{18}	2.0×10^{18}	1.4×10^{19}	1.8×10^{19}
Electron thermal velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Hole thermal velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Electron mobility (cm^2/Vs)	100	100	1.61	20
Hole mobility (cm^2/Vs)	25	25	1.42	80
Shallow donor density N_a ($1/\text{cm}^3$)	1.0×10^{18}	1.0×10^{18}	0	0
Shallow acceptor density N_a ($1/\text{cm}^3$)	0	0	1.0×10^9	1.0×10^{18}
Total defect density N_t ($1/\text{cm}^3$)	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}

The front contact formed by the Fluorine-doped tin oxide layer was modeled assuming flat band conditions, which implies ideal electrical contact without significant barrier formation or band bending at the interface. This assumption is justified by the highly doped nature of transparent conductive oxides, which typically form ohmic contacts with adjacent layers when appropriate work function matching is achieved. The back contact was implemented using gold with an assigned work function of 5.1 eV, which provides favorable energetics for hole extraction from the cuprous oxide layer and is consistent with common practice in experimental perovskite solar cell fabrication [20].

The simulations were performed at a default temperature of 300 K for the baseline optimization studies, with additional temperature-dependent simulations conducted over the range from 250 K to 600 K to investigate thermal effects on device performance. Series resistance and shunt resistance effects were included in the simulations to capture the influence of non-ideal contact behavior and leakage pathways on the current-voltage characteristics. The software's built-in defect modeling capabilities were utilized to account for bulk recombination through Shockley-Read-Hall statistics, while interface recombination was addressed through appropriate surface recombination velocity parameters at the heterojunction boundaries.

2.4. Simulation Procedure and Analysis Approach

The simulation procedure involved systematically entering the material parameters for each layer into the SCAPS-1D panel interface, followed by defining the illumination spectrum, contact properties, and operating conditions. The software was then executed to compute the current density versus voltage characteristics under both dark and illuminated conditions, from which the key performance parameters including open-circuit voltage, short-circuit current density, fill factor, and power conversion efficiency were extracted.

Parametric studies were conducted by varying specific input parameters while holding all others constant, thereby isolating the influence of each variable on device performance. The absorber layer thickness was varied from 0.1 μm to 1000 μm to identify the optimal value for maximizing efficiency. Temperature-dependent simulations were performed at 75 K intervals from 300 K to 600 K to assess thermal stability and determine the temperature sensitivity of the device. The external quantum efficiency spectra were computed over the wavelength range relevant to the absorber bandgap to evaluate the spectral response and identify limitations in carrier collection efficiency. All simulations were repeated with appropriate convergence criteria to ensure numerical stability and reproducibility of the results.

3. RESULTS AND DISCUSSION

3.1. Optimized Device Performance

The current density versus voltage characteristic of the optimized device architecture under standard AM1.5G illumination is presented in Figure 2. This simulation was conducted after systematic optimization of the layer thicknesses and material parameters to maximize power conversion efficiency. The J-V curve exhibits the typical shape expected for a well-functioning solar cell, with clear diode behavior in the dark and substantial photocurrent generation under illumination. From this characteristic, the key performance parameters were extracted, yielding a power conversion efficiency of 21.14 %, a fill factor of 0.80, a short-circuit current density of 32.28 mA per square centimeter, and an open-circuit voltage of 0.81 V.

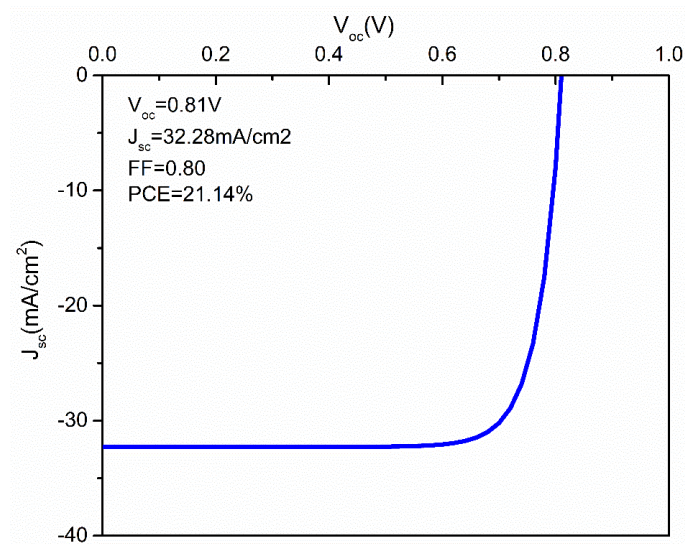


Fig. 2. Current density versus voltage characteristic of the optimized FTO/WS₂/RbGeI₃/Cu₂O/Au device under AM1.5G illumination, showing a power conversion efficiency of 21.14 % with a fill factor of 0.80.

The achievement of 21.14 % efficiency with an all-inorganic, lead-free absorber material is particularly significant when considered in the context of previous reports on germanium-based perovskite devices. Krishnamoorthy and colleagues reported an experimental efficiency of only 0.11% for CsGeI₃-based devices in their pioneering work, highlighting the substantial gap between initial demonstrations and the potential predicted by simulation studies [15]. The efficiency obtained in the present work compares favorably with other simulation studies of RbGeI₃-based devices, including the work of Pindolia and coworkers who reported efficiencies in the range of 18 to 22 % depending on the specific transport layer combination employed [30]. The fill factor of 0.80 indicates that series resistance losses are well-controlled and that the charge transport layers are effectively extracting photogenerated carriers with minimal recombination losses at the interfaces. The short-circuit current density of 32.28 mA per square centimeter reflects efficient light absorption

across the solar spectrum, which is consistent with the direct bandgap and high absorption coefficient of RbGeI₃. The open-circuit voltage of 0.81 volts represents approximately 62 % of the radiative limit for a material with a 1.31 eV bandgap, suggesting that further improvements may be possible through reduction of non-radiative recombination pathways [32].

3.2. External Quantum Efficiency Analysis

The external quantum efficiency spectrum of the optimized device is shown in Figure 3, plotted as a function of wavelength across the range relevant to the absorber bandgap. The quantum efficiency represents the ratio of collected charge carriers to incident photons at each wavelength, providing valuable insight into the spectral regions where the device operates most effectively. The spectrum reveals that the device maintains high quantum efficiency throughout the visible region, with values approaching 90% between approximately 400 nm and 700 nm. This broad plateau of high efficiency indicates that photogenerated carriers are efficiently collected across most of the visible spectrum, with minimal losses due to recombination or incomplete absorption.

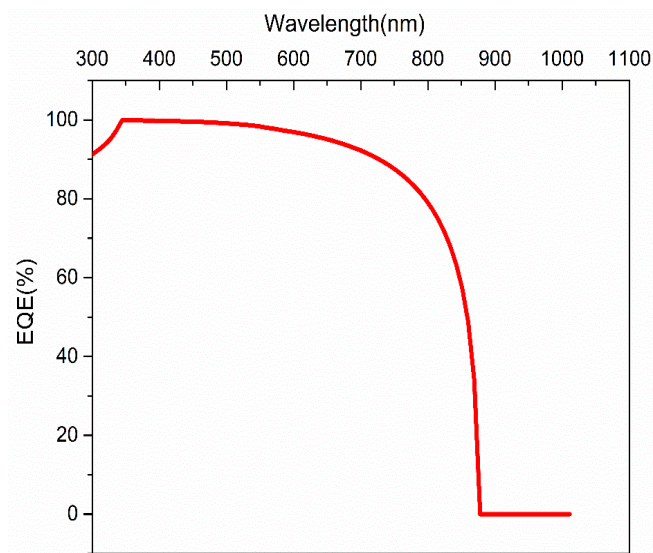


Fig. 3. External quantum efficiency spectrum of the optimized RbGeI₃-based device plotted as a function of wavelength, demonstrating peak efficiency approaching 90% across the visible region.

The onset of photoresponse occurs at approximately 950 nm, which corresponds to the bandgap of RbGeI₃ at 1.31 eV. Photons with wavelengths longer than this threshold possess insufficient energy to excite electrons across the bandgap and therefore do not contribute to photocurrent generation. The gradual rather than abrupt decline near the band edge suggests some degree of band tailing or the presence of sub-bandgap states that extend the absorption edge, which is

commonly observed in perovskite materials and can be attributed to slight variations in local composition or structural disorder [19].

The high quantum efficiency values observed in the visible region carry important implications for the practical applicability of this device architecture. Because the solar spectrum peaks in the visible range, efficient conversion in this region is essential for achieving high overall power conversion efficiency. The 90% quantum efficiency indicates that optical losses due to reflection and transmission are minimal and that electrical losses due to recombination are well-suppressed. This level of performance compares favorably with that of lead-based perovskite devices and suggests that RbGeI₃-based absorbers are capable of matching the carrier collection efficiency of their toxic counterparts [22].

Figure 4 presents the same quantum efficiency data plotted against photon energy rather than wavelength, providing an alternative perspective that facilitates direct correlation with the electronic band structure of the absorber material. When plotted in this manner, the quantum efficiency spectrum reveals that the maximum photon conversion occurs in the energy range from approximately 1.6 eV to 3.5 eV.

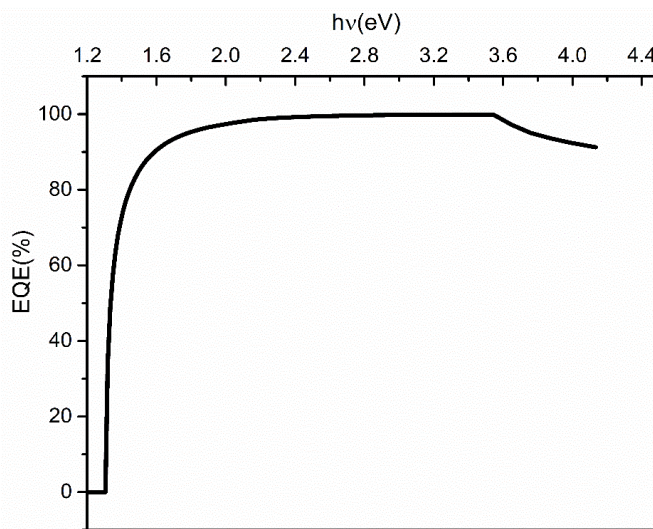


Fig. 4. External quantum efficiency spectrum plotted as a function of photon energy, clearly showing the bandgap onset at approximately 1.3 eV and the high-efficiency plateau extending from 1.6 to 3.5 eV.

The gradual increase in quantum efficiency with increasing photon energy above the bandgap reflects the energy-dependent absorption coefficient of the material, which typically rises as photons become more energetic and the density of available states for optical transitions increases. The plateau region above 2 eV indicates that absorption has become sufficiently strong that essentially all incident photons are absorbed within the thickness of the absorber layer, and the collection efficiency is limited primarily by transport and recombination rather than by incomplete absorption [27].

3.3. Energy Band Diagram Analysis

The energy band diagram of the complete device structure under equilibrium conditions is presented in Figure 5, showing the spatial variation of the conduction band minimum, valence band maximum, and Fermi level throughout the multilayer stack. This diagram provides essential information about the energetic alignment between adjacent layers and the resulting barriers or favorable gradients that influence charge transport and collection. The simulated band diagram reveals that the chosen materials form a coherent heterojunction system with appropriate band offsets to facilitate selective carrier extraction.

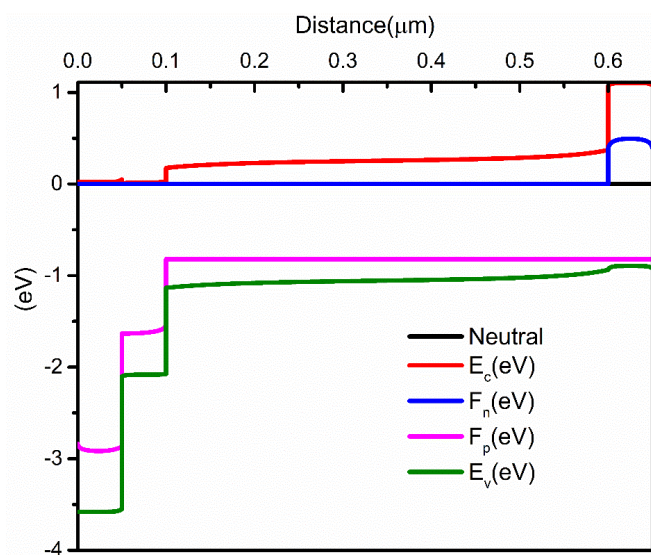


Fig. 5. Energy band diagram of the FTO/WS₂/RbGeI₃/Cu₂O/Au device under equilibrium conditions, showing the conduction band minimum (E_c), valence band maximum (E_v), and Fermi level (E_f) throughout the structure.

At the front interface between the Fluorine-doped tin oxide transparent conductive oxide and the Tungsten disulfide electron transport layer, the conduction band alignment exhibits a slight downward step from the transport layer to the contact, which promotes electron extraction while presenting no significant barrier to electron flow. The valence band offset at this interface is substantial, effectively blocking holes from reaching the front contact and thereby suppressing recombination at the illuminated side of the device. This favorable asymmetry in band alignment is essential for maintaining high collection efficiency and minimizing carrier losses [23].

The interface between the Tungsten disulfide electron transport layer and the Rubidium Germanium iodide absorber shows a conduction band offset that facilitates electron transfer from the absorber to the transport layer while the valence band offset prevents holes from entering the electron transport layer. The magnitude of these offsets is critical for device performance, as excessively large offsets can create

barriers that impede carrier extraction while insufficient offsets may fail to provide adequate carrier confinement. The values used in this simulation, based on the electron affinities presented in Table 1, produce offsets that fall within the range generally considered optimal for perovskite solar cells [28].

At the opposite side of the absorber, the interface with the cuprous oxide hole transport layer exhibits the complementary behavior, with a valence band offset that promotes hole extraction and a conduction band offset that blocks electrons. This selective contact behavior ensures that electrons remain confined within the absorber and electron transport layer while holes are efficiently transferred to the hole transport layer and subsequently to the back contact. The Fermi level remains constant throughout the structure under equilibrium conditions, and its position relative to the band edges in each layer confirms the intended doping type and carrier concentrations. The flat Fermi level across the entire device, despite variations in band edge positions, indicates that the structure has reached thermal equilibrium with appropriate charge transfer between layers to align the electrochemical potentials [30].

3.4. Influence of Absorber Layer Thickness on Device Performance

The thickness of the absorber layer represents one of the most critical design parameters in perovskite solar cell optimization, as it directly influences the trade-off between light absorption and charge carrier collection. To investigate this relationship systematically, the thickness of the RbGeI₃ layer was varied from 0.1 μm to 1000 μm while holding all other parameters constant at their baseline values. The resulting effects on the four primary performance metrics are presented in Figure 6 and tabulated in Table 2.

The open-circuit voltage exhibited a monotonic decrease with increasing absorber thickness throughout the investigated range, declining from 0.86 volts at 0.1 μm to 0.74 V at 1.0 μm . This behavior can be attributed to several factors that become more pronounced in thicker absorber layers. As the thickness increases, the series resistance of the device rises proportionally, leading to increased voltage drops under operating conditions. Additionally, thicker layers provide a larger volume within which recombination can occur, and the increased path length that carriers must traverse to reach the extraction layers raises the probability of recombination before collection. Both effects contribute to a reduction in the quasi-Fermi level splitting that determines the achievable open-circuit voltage [24].

In contrast to the declining voltage, the short-circuit current density showed a progressive increase with absorber thickness, rising from 17.7 mA per square centimeter at 0.1 μm to 34.5 mA/cm² at 1.0 μm . This trend reflects the fundamental relationship between absorber thickness and light absorption, with thicker layers capturing a larger fraction of the incident photons across the solar spectrum. At the smallest thickness of 0.1 μm , absorption is incomplete, particularly for photons with energies near the bandgap that

have longer penetration depths. As the thickness increases, more photons are absorbed within the active layer, generating additional charge carriers that contribute to the photocurrent provided they can be collected before recombining [25].

The power conversion efficiency, which represents the product of voltage, current, and fill factor divided by the incident power density, exhibited a distinct optimum at an absorber thickness of 0.7 μm . At this thickness, the efficiency reached 21.5 %, representing the best compromise between the competing trends of increasing current and decreasing voltage. Below this optimum, the efficiency was limited by insufficient light absorption and consequently low current generation. Above the optimum, the benefits of additional current from enhanced absorption were outweighed by the penalties of reduced voltage and increased recombination losses, leading to a gradual decline in efficiency. The fill factor remained relatively stable across most of the thickness

range, fluctuating between 0.79 and 0.81, though minor variations were observed that can be attributed to changes in the balance between series and shunt resistances as the absorber geometry was modified [32].

The identification of 0.5 μm as the optimal thickness carries practical significance for experimental efforts aimed at realizing high-efficiency RbGeI₃ devices. This thickness is readily achievable through common deposition techniques such as spin-coating, thermal evaporation, or chemical vapor deposition, and it falls within the range typically employed for lead-based perovskite absorbers. The existence of a clear optimum rather than a plateau of near-constant efficiency underscores the importance of precise thickness control in device fabrication and suggests that significant performance penalties may result from deviations of even a few hundred nanometers from the optimal value [29].

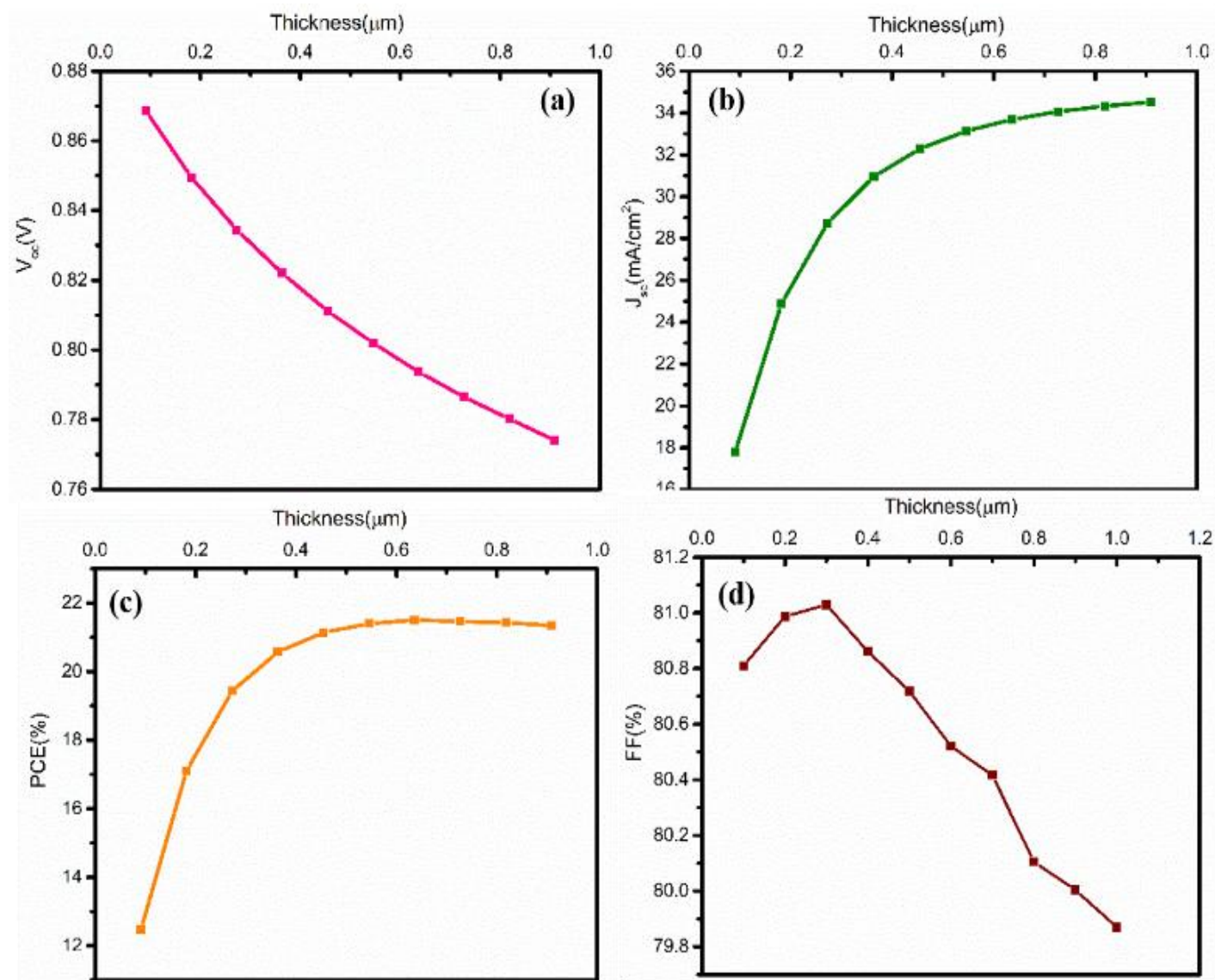


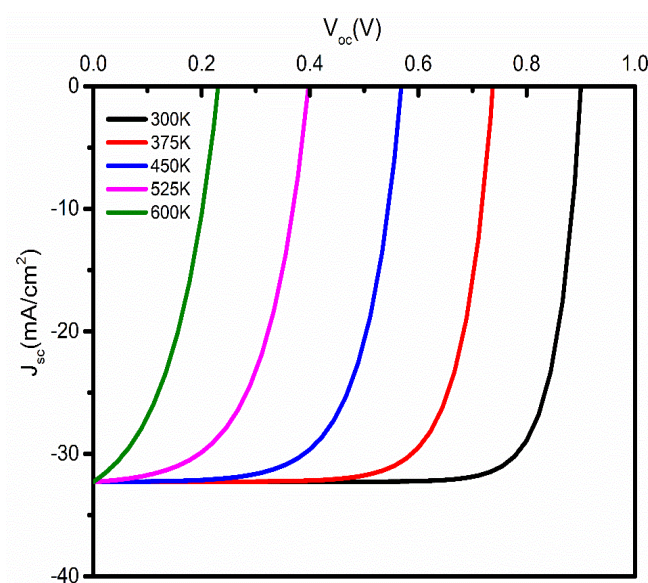
Fig. 6. Variation of key photovoltaic parameters with RbGeI₃ absorber layer thickness: (a) open-circuit voltage, (b) short-circuit current density, (c) power conversion efficiency, and (d) fill factor.

Table 2. Summary of photovoltaic parameters extracted from simulations as a function of RbGeI₃ absorber layer thickness.

Thickness (μm)	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF
0.1	0.86	17.7	12.40	0.80
0.2	0.84	24.8	17.12	0.80
0.3	0.83	28.7	19.40	0.81
0.4	0.82	30.9	20.52	0.80
0.5	0.81	32.2	21.14	0.80
0.6	0.80	33.1	21.33	0.80
0.7	0.79	33.6	21.50	0.80
0.8	0.78	34.0	21.48	0.80
0.9	0.77	34.3	21.41	0.80
1.0	0.74	34.5	21.39	0.79

3.5 Temperature Dependence of Device Performance

The operating temperature of photovoltaic devices in real-world applications can vary widely depending on geographic location, seasonal conditions, and mounting configuration. Understanding the temperature dependence of device performance is therefore essential for predicting energy yield under realistic operating conditions and for identifying potential stability concerns. To address this consideration, the optimized device was simulated over a temperature range from 250 K to 600 K, with the resulting current-voltage characteristics presented in Figure 7 and the extracted parameters summarized in Table 3.

**Fig. 7.** Current density versus voltage characteristics of the optimized device at different operating temperatures from 300 K to 600 K, illustrating the progressive degradation of performance with increasing temperature.

Simulations at temperatures below 300 K failed to achieve numerical convergence, indicating that the charge carrier

generation at reduced temperatures is insufficient to sustain stable device operation under the modeled conditions. This behavior can be understood in terms of the temperature dependence of carrier statistics and transport properties. At lower temperatures, the thermal energy available for ionization of dopants and for promoting carriers across energetic barriers is reduced, leading to lower effective carrier concentrations and reduced conductivities. Additionally, the capture cross-sections of defect states may exhibit temperature dependence that influences recombination rates. The inability to obtain converged solutions suggests that the modeled material parameters, which were primarily derived from room-temperature measurements, may not accurately represent the low-temperature behavior of these materials [18].

Table 3. Summary of photovoltaic parameters extracted from simulations as a function of operating temperature.

Temperature (K)	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF
300	0.81	32.28	21.14	0.80
375	0.66	32.28	16.00	0.74
450	0.51	32.29	11.00	0.65
525	0.82	32.29	6.30	0.55
600	0.20	32.29	2.80	0.42

At 300 K, which represents approximately room temperature, the device achieved its peak efficiency of 21.14% with the fill factor of 0.80 and short-circuit current density of 32.28 milliamperes per square centimeter noted previously. As the temperature was increased to 375 K, the efficiency declined to 16 %, primarily driven by a reduction in open-circuit voltage from 0.81 V to 0.66 V. This voltage reduction with increasing temperature is expected from fundamental semiconductor physics, as the intrinsic carrier concentration increases exponentially with temperature, leading to enhanced recombination currents that reduce the achievable quasi-Fermi level splitting under illumination [20].

Further increasing the temperature to 450 K reduced the efficiency to 11 %, with the open-circuit voltage declining further to 0.51 V while the fill factor dropped to 0.65. The short-circuit current density remained essentially constant across this temperature range, indicating that the generation and collection of photogenerated carriers is relatively insensitive to temperature compared to the voltage-determining recombination processes. At 525 K, the efficiency fell to 6.30 %, and at 600 K, it reached only 2.8 % with an open-circuit voltage of just 0.20 V and a fill factor of 0.42.

The progressive degradation of performance with increasing temperature carries important implications for practical applications of RbGeI₃-based devices. The strong temperature sensitivity suggests that thermal management strategies may be necessary to maintain high efficiency under real-world operating conditions where module temperatures can substantially exceed ambient temperature. The results also highlight the importance of material stability at elevated temperatures, as the simulated performance degradation reflects only the fundamental thermodynamic effects on carrier statistics and recombination, without considering additional degradation mechanisms such as thermally activated ion migration or chemical decomposition that would further compromise device performance in experimental systems [31].

The temperature dependence observed in this study is generally consistent with that reported for other perovskite materials, though the magnitude of the voltage decline and the absolute efficiency at elevated temperatures may differ based on the specific material parameters and device architecture. The results underscore the importance of conducting temperature-dependent characterization in experimental studies and of considering operating temperature in the design of modules and systems for specific deployment scenarios.

4. CONCLUSION

This study employed SCAPS-1D simulation software to conduct a systematic numerical investigation of RbGeI₃-based lead-free perovskite solar cells incorporating WS₂ as the electron transport layer and Cu₂O as the hole transport layer. The primary objective was to evaluate the viability of this environmentally benign material combination while maintaining competitive photovoltaic performance. The simulation results demonstrate that the thickness of the RbGeI₃ absorber layer critically influences device performance, with increasing thickness from 0.1 μ m to 1.0 micrometer producing opposing effects on key parameters. Open-circuit voltage exhibited a gradual decline due to enhanced series resistance and increased bulk recombination, while short-circuit current density showed progressive improvement from greater photon absorption and charge carrier generation. The power conversion efficiency reached an optimum value of 21.14 % at an absorber thickness of 0.7 μ m, where the competing mechanisms of light absorption and

recombination achieve favorable balance. Beyond this thickness, efficiency diminished as recombination losses began to dominate over photocurrent gains. Temperature-dependent simulations revealed optimal device performance at 300 K, with efficiency declining substantially at elevated temperatures. At 600 K, efficiency dropped to approximately 2.8 %, representing a dramatic reduction from the room-temperature peak. This degradation arises from increased thermal carrier generation and enhanced recombination, which collectively impair photovoltaic response. The inability to achieve simulation convergence below 300 K further emphasizes the importance of thermal management for stable device operation. The selection of WS₂ and Cu₂O as charge transport layers proved advantageous, with energy band diagram analysis confirming appropriate band alignment that minimizes energy barriers and facilitates efficient carrier extraction. This proper alignment contributes directly to the respectable open-circuit voltage and high fill factor observed in the optimized device. These findings establish that RbGeI₃-based lead-free perovskite solar cells, when properly engineered with suitable transport layers, can achieve efficiencies exceeding 21 percent, positioning them as credible alternatives to toxic lead-based counterparts. The results underscore the critical importance of layer thickness optimization and thermal management in realizing the full potential of this material system. Future research should focus on experimental validation of these simulation results, exploration of alternative transport layer combinations, and comprehensive investigation of long-term device stability under operational conditions. The continued advancement of lead-free perovskite photovoltaics represents a meaningful step toward sustainable solar energy conversion technologies.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

Availability of data and material

The datasets generated and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Authors' contributions

All authors contributed equally to this work.

ACKNOWLEDGEMENTS

The authors would like to thank Professor Marc Burgelman for providing the SCAPS-1D software for carrying out this analysis.

REFERENCES

- [1] Zhou, D., Zhou, T., Tian, Y., Zhu, X. and Tu, Y., **2018**. Perovskite-based solar cells: materials, methods, and future perspectives. *Journal of Nanomaterials*, 2018(1), p.8148072.
- [2] Snaith, H.J., **2018**. Present status and future prospects of perovskite photovoltaics. *Nature Materials*, 17(5), pp.372-376.
- [3] Grätzel, M., **2017**. The rise of highly efficient and stable perovskite solar cells. *Accounts of Chemical Research*, 50(3), pp.487-491..
- [4] Kojima, A., Teshima, K., Shirai, Y. and Miyasaka, T., **2009**. Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. *Journal of the American Chemical Society*, 131(17), pp.6050-6051.
- [5] Shen, W., Zhao, Y. and Liu, F., **2024**. Highlights of mainstream solar cell efficiencies in 2023. *Frontiers in Energy*, 18(1), pp.8-15.
- [6] Ke, W. and Kanatzidis, M.G., **2019**. Prospects for low-toxicity lead-free perovskite solar cells. *Nature Communications*, 10(1), p.965.
- [7] Babayigit, A., Ethirajan, A., Muller, M. and Conings, B., **2016**. Toxicity of organometal halide perovskite solar cells. *Nature Materials*, 15(3), pp.247-251.
- [8] Ju, M.G., Dai, J., Ma, L. and Zeng, X.C., **2017**. Lead-free mixed tin and Germanium perovskites for photovoltaic application. *Journal of the American Chemical Society*, 139(23), pp.8038-8043.
- [9] Noel, N.K., Stranks, S.D., Abate, A., Wehrenfennig, C., Guarnera, S., Haghighirad, A.A., Sadhanala, A., Eperon, G.E., Pathak, S.K., Johnston, M.B. and Petrozza, A., **2014**. Lead-free organic-inorganic tin halide perovskites for photovoltaic applications. *Energy & Environmental Science*, 7(9), pp.3061-3068.
- [10] Cao, J. and Yan, F., **2021**. Recent progress in tin-based perovskite solar cells. *Energy & Environmental Science*, 14(3), pp.1286-1325.
- [11] Meng, X., Wu, T., Liu, X., He, X., Noda, T., Wang, Y., Segawa, H. and Han, L., **2020**. Highly reproducible and efficient FASnI₃ perovskite solar cells fabricated with volatilizable reducing solvent. *The Journal of Physical Chemistry Letters*, 11(8), pp.2965-2971.
- [12] Houari, M., Bouadjemi, B., Matougui, M., Haid, S., Lantri, T., Aziz, Z., Bentata, S. and Bouhafs, B., **2019**. Optoelectronic properties of Germanium iodide perovskites AGeI₃ (A= K, Rb and Cs): first principles investigations. *Optical and Quantum Electronics*, 51(7), p.234.
- [13] Minemoto, T., Kawano, Y., Nishimura, T., Shen, Q., Yoshino, K., Iikubo, S., Hayase, S. and Chantana, J., **2020**. Theoretical analysis of band alignment at back junction in Sn-Ge perovskite solar cells with inverted pin structure. *Solar Energy Materials and Solar Cells*, 206, p.110268.
- [14] Lakhdar, N. and Hima, A., **2020**. Electron transport material effect on performance of perovskite solar cells based on CH₃NH₃GeI₃. *Optical Materials*, 99, p.109517.
- [15] Sherburne, M., Li, S., Asta, M., Mathews, N. and Mhaisalkar, S.G., **2015**. Lead-free Germanium iodide perovskite materials for photovoltaic application. *Journal of Materials Chemistry A*, 3(47), pp.23829-23832.
- [16] Samaki, S., Tchangnwa Nya, F., Dzifack Kenfack, G.M. and Laref, A., **2023**. Materials and interfaces properties optimization for high-efficient and more stable RbGeI₃ perovskite solar cells: optoelectrical modelling. *Scientific Reports*, 13(1), p.15517.
- [17] Moyofola, O.O. and Emetere, M.E., **2025**. Improving the performance conversion efficiency of perovskite solar cells through optimization of charge transport layers: A review. *Renewable and Sustainable Energy Reviews*, 222, p.115943.
- [18] Sajid, S., Elseman, A.M., Huang, H., Ji, J., Dou, S., Jiang, H., Liu, X., Wei, D., Cui, P. and Li, M., **2018**. Breakthroughs in NiO_x-HTMs towards stable, low-cost and efficient perovskite solar cells. *Nano Energy*, 51, pp.408-424.
- [19] Hawash, Z., Ono, L.K. and Qi, Y., **2018**. Recent advances in spiro-MeOTAD hole transport material and its applications in organic-inorganic halide perovskite solar cells. *Advanced Materials Interfaces*, 5(1), p.1700623.
- [20] Wang, S., Sina, M., Parikh, P., Uekert, T., Shahbazian, B., Devaraj, A. and Meng, Y.S., **2016**. Role of 4-tert-butylpyridine as a hole transport layer morphological

- controller in perovskite solar cells. *Nano letters*, 16(9), pp.5594-5600.
- [21] Miao, X., Wang, S., Sun, W., Zhu, Y., Du, C., Ma, R. and Wang, C., **2019**. Room-temperature electrochemical deposition of ultrathin CuOx film as hole transport layer for perovskite solar cells. *Scripta Materialia*, 165, pp.134-139.
- [22] Nian, J.N., Hu, C.C. and Teng, H., **2008**. Electrodeposited p-type Cu₂O for H₂ evolution from photoelectrolysis of water under visible light illumination. *International Journal of Hydrogen Energy*, 33(12), pp.2897-2903.
- [23] Hossain, M.K., Toki, G.I., Kuddus, A., Rubel, M.H., Hossain, M.M., Bencherif, H., Rahman, M.F., Islam, M.R. and Mushtaq, M., **2023**. An extensive study on multiple ETL and HTL layers to design and simulation of high-performance lead-free CsSnCl₃-based perovskite solar cells. *Scientific Reports*, 13(1), p.2521.
- [24] Dolai, S., Das, S., Hussain, S., Bhar, R. and Pal, A.K., **2017**. Cuprous oxide (Cu₂O) thin films prepared by reactive DC sputtering technique. *Vacuum*, 141, pp.296-306.
- [25] Sajid, M., Ali, K., Shah, H.S., Shahid, A., Bakar, S.A., Yousaf, M. and Lee, S.L., **2024**. Boosting solar cell performance: optimization of WS₂ absorber with Cu₂O HTL & ZnSe ETL using SCAPS-1D simulation. *Journal of Optics*, pp.1-12.
- [26] Neupane, K., Dakua, P.K., Sahu, J.K., Polamuri, S.R., Ved, A., Chethan, M., Ananth, D.V.N., Kumar, R., Karri, H. and Bhattarai, S., **2025**. Empowering Rubidium-Based Halide PSCs: A Deep Dive into ETL Material Performance. *Journal of Physics and Chemistry of Solids*, p.112897.
- [27] Araújo, V.H.D., Nogueira, A.F., Tristão, J.C. and dos Santos, L.J., **2025**. Advances in lead-free perovskite solar cell design via SCAPS-1D simulations. *RSC Sustainability*, 3(10), pp.4314-4335.
- [28] Kanoun, A.A., Kanoun, M.B., Merad, A.E. and Goumri-Said, S., **2019**. Toward development of high-performance perovskite solar cells based on CH₃NH₃GeI₃ using computational approach. *Solar Energy*, 182, pp.237-244.
- [29] Vaish, S., Dixit, S.K., Aljubairi, F., Ahmad, S., Ahmed, F. and Khan, Z.H., **2025**. Numerical Simulation and Performance Optimization of CsGeI₃-Based Lead-Free Perovskite Solar Cells Using SCAPS-1D. *Journal of Nanoelectronics and Optoelectronics*, 20(4), pp.407-414.
- [30] Pindolia, G., Shinde, S.M. and Jha, P.K., **2022**. Optimization of an inorganic lead free RbGeI₃ based perovskite solar cell by SCAPS-1D simulation. *Solar Energy*, 236, pp.802-821.
- [31] Ekwu, M.T., Danladi, E., Tasie, N.N., Haruna, I.S., Okoro, O.E., Gyuk, P.M., Jimoh, O.M. and Obasi, R.C., **2023**. A Qualitative Theoretical Study of Inorganic HTM-Free RbGeI₃ Based Perovskite Solar Cells Using SCAPS 1D as a Pathway Towards 3.601% Efficiency. *East European Journal of Physics*, (1), pp.118-124.
- [32] Rahman, M.M., Ali, M.H., Haque, M.D. and Islam, A.Z.M.T., **2024**. Numerical modeling and extensive analysis of an extremely efficient RbGeI₃-based perovskite solar cell by incorporating a variety of ETL and HTL materials to enhance PV performance. *Energy Advances*, 3(9), pp.2377-2398.