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An In-organic Perovskite Solar Cell Design and Simulation Using SCAPS-1D

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Abstract: A solar cell capacity simulator (SCAPS-1D) was used in this study to conduct the numerical investigation of all-inorganic perovskite photovoltaics with regular n-i-p structure. Using the SCAPS-1D program, this paper describes the design and development of environmentally benign perovskite solar cells for photovoltaic systems. The study sought to investigate whether lead-free perovskites may be employed as sustainable substitutes for conventional lead-based perovskite solar cells in the long run. The study focuses on enhancing cell characteristics and assessing efficacy measures like efficiency, fill factor, and open-circuit voltage.

Compared to the other hole transport layers (HTLs), the optimized device structure using $FaSnI_3$ showed greatest performance. Thus, the best photovoltaic performance with power conversion efficiency (PCE) of 35%, fill factor (FF) of 87.82%, open circuit voltage (V_{OC}) of 1.02 V, and short circuit current density (JSC) of 39.28 mA/cm^2, respectively, was shown by the optimized solar cell structure (CdTe, CIGS, $FaSnI_3$, TiO_2 and ITO). The photovoltaic performance of the improved device is therefore examined in relation to changes in temperature, thickness, defect density, doping density of active layer and illumination intensity.

The solar energy sector is more and more committed to creating eco friendly substitutes to lead-based components. Among the promising options, Formamidinium Tin Iodide ($FaSnI_3$) has surfaced as a lead-free perovskite showing equivalent optoelectronic features to substitutes containing lead. This study aims to show that lead-free perovskites can achieve high power conversion efficiencies while meeting the urgent need for sustainable energy options.

Keywords: SCAPS-1D, Inorganic perovskite photovoltaics, efficiency, fill factor and open-circuit voltage.

I. INTRODUCTION

Perovskite solar cells (PSCs) have been able to attain proven power conversion efficiencies (PCEs) that are larger than 25% in recent years. As a consequence of this, there has been a significant increase in the amount of attention that has been paid to them in the field of photovoltaic research. However, the most efficient perovskite materials, such as methylammonium lead iodide (MAPbI2) and formamidinium lead iodide (FAPbI2), contain toxic lead (Pb), which poses significant issues with regard to both the environment and human health [2]. During the manufacturing process, during operation, and during the disposal of solar panels, lead exposure can cause contamination of soil and water, which puts both human health and the environment in jeopardy [3]. Therefore, it is of the utmost need to develop lead-free alternatives to perovskite that maintain a high level of efficiency while still being environmentally sustainable.

Tin (Sn)-based perovskites, such as CsSnI3 and MASnI3, have established themselves as intriguing candidates [4]. This is because of their acceptable bandgap, which ranges from 1.2 to 1.4 eV, and their robust light absorption characteristics. On the other hand, Sn2+ is prone to oxidation, which might result in the formation of Sn2+, which decreases the stability of the device and increases the fault density [5]. Attempts have been made by researchers to find a solution to these challenges by investigating compositional engineering, additive integration, and complex encapsulating approaches [6]. Another technique makes use of double perovskites, such as Cs2AgBiBr6, although the photovoltaic performance of these materials is hindered by their wide bandgaps, which are greater than 2 eV [7]. Therefore, the

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improvement of Sn-based perovskites through defect passivation and interface engineering continues to be an important field of research currently being conducted.

Perovskite solar cell designs are greatly optimized by the use of numerical simulation tools such as SCAPS-1D (Solar Cell Capacitance Simulator) [8] prior to the construction of the cells through experimental fabrication. Through the process of solving Poisson and drift-diffusion equations in steady-state conditions, SCAPS-1D makes it possible to investigate significant aspects such as band alignment, carrier transport, and recombination losses [9]. For the purpose of evaluating the optoelectronic properties and device performance of lead-based ($CsPbI_3$) and lead-free ($CsSnI_3$) all-inorganic perovskites, this article makes use of SCAPS-1D. Consequently, a comparison is made between the leads. The simulations are executed under ideal conditions, with the assumption of zero series resistance ($R_s = 0\ \Omega$) and infinite shunt resistance ($R_{sh} = \infty\ \Omega$). This is done in order to effectively evaluate the highest possible theoretical efficiency without any extrinsic losses [10].

This endeavor seeks to maximize the efficiency of lead-free perovskite solar cells by systematically altering the thickness of the absorber layer, the degree of doping, and the defect density. Through the use of SCAPS-1D simulations, we are able to determine the optimal configuration of the device that both maximizes PCE and ensures environmental sustainability. Experimental scientists who are working on producing environmentally friendly perovskite solar cells will benefit from the findings of this study since they will provide them with insightful analysis that will promote the development of next-generation renewable energy solutions. Our investigation was divided up into two distinct situations, each of which had a distinct configuration of the material.

II. STRUCTURE AND SIMULATION PARAMETERS

2.1 Solar Cell Materials

Solar photovoltaic (PV) technology depends on diverse semiconductor materials, each presenting unique benefits and drawbacks. Silicon is the predominant material in commercial solar cell production owing to its natural abundance, economic efficiency, and known manufacturing techniques [11]. Monocrystalline and polycrystalline silicon are extensively utilized in traditional photovoltaic modules, however amorphous silicon is employed in thin-film and flexible solar cells owing to its reduced processing temperatures. Silicon-based solar cells currently prevail in the market, constituting over 90% of global photovoltaic production, due to their reliability and long-term stability.

Cadmium Telluride (CdTe) has become a prominent material for thin-film solar technology, providing numerous benefits, including high light absorption coefficients and comparatively inexpensive manufacturing costs [14]. CdTe-based solar cells have attained laboratory efficiencies over 22%, rendering them economically viable against crystalline silicon technology [15]. The toxicity of cadmium presents considerable environmental issues during production and disposal, requiring stringent regulatory measures and specific recycling methods.

Copper Indium Gallium Selenide (CIGS) is a significant thin-film technology, characterized by high conversion efficiency and remarkable flexibility. CIGS solar cells have exhibited efficiency above 23% in laboratory conditions, owing to its adjustable bandgap by modifications in gallium concentration [18]. The attributes of CIGS render it especially appropriate for building-integrated photovoltaics (BIPV) and portable electronic applications; yet, obstacles persist in increasing output while ensuring cost competitiveness [19].

Perovskite solar cells have garnered significant scientific interest in recent years owing to their swiftly improving power conversion efficiencies, which already surpass 25% under laboratory circumstances [20]. These materials exhibit remarkable optoelectronic characteristics, such as elevated absorption coefficients, extended charge carrier diffusion lengths, and adjustable bandgaps via compositional engineering [21]. Nonetheless, stability challenges and lead toxicity difficulties in traditional perovskite formulations persistently obstruct their commercial feasibility, necessitating further investigation into lead-free alternatives and encapsulating methods [22].

Organic photovoltaics (OPV) employ carbon-based materials to produce lightweight, flexible solar cells that may be fabricated by economical printing methods [23]. Although OPV devices presently exhibit lower efficiency (often 10-15%) relative to inorganic technologies, they provide distinct advantages for specialized applications, including wearable electronics and building-integrated systems [24]. Recent advancements in non-fullerene acceptors have markedly enhanced organic photovoltaic performance; yet, obstacles persist in attaining long-term operational stability in real-world settings [25].

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2.2 Efficiency of Solar Cells

The efficiency of a solar cell denotes the ratio of its electrical output to the incident light energy. The efficiency parameter is essential for the performance and economic feasibility of solar energy systems. The disparity in efficiency is significant across solar cells depending on the employed technology.

First Generation (Crystalline Silicon): Mono-crystalline silicon cells often exhibit efficiencies between 15% and 22%, while poly-crystalline cells range from 13% to 17%.

- Second Generation (Thin-Film): Efficiency ranges from 9% to 16% for CdTe, a maximum of 22% for CIGS, and commonly 6% to 10% for amorphous silicon cells.
- Third Generation (Advanced Technologies): Perovskite solar cells are achieving remarkable advancements, with laboratory efficiencies exceeding 25%, whilst organic photovoltaic cells have efficiencies ranging from 5% to 12%. Multijunction cells can exceed 40% efficiency under focused sunlight.

2.3 Electrical Parameters of Solar Cells

Several electrical parameters characterize the performance of solar cells:

a) Open-Circuit Voltage (V_{oc})

The open-circuit voltage corresponds to the maximum voltage that a PV cell can achieve in an ideal condition (zero load, hence zero current). V_{oc} relates, which is the maximum theoretical voltage that can form across an illuminated solar cell; that makes V_{oc} important. V_{oc} is a function of solar cell material properties, the energy bandgap, and junction quality between different semiconductor layers. This is because we will typically get larger V_{oc} if we utilize higher quality materials and junctions.

The open-circuit voltage can be expressed using the following equation:

$$V_{OC} = \frac{kT}{q}\ln\left(\frac{I_{SC}}{I_0} + 1\right)$$

Where:

- **k** is the Boltzmann constant.
- **T** is the absolute temperature in Kelvin.
- **q** is the charge of an electron.
- **I_{sc}** is the short-circuit current.
- **I_o** is the reverse saturation current.

b) Short-Circuit Current (I_{sc})

Short-circuit current (I_{sc}) flows when the terminals of a solar cell are short-circuited together, i.e., the resistance is zero. This flux is directly proportional to the amount of sunlight in the solar cell and the efficiency with which the cell absorbs that light. I_{sc} is affected by factors such as the intensity of sunlight. Spectral distribution of light and surface area of solar cells Higher sunlight intensity and larger surface area result in higher I_{sc} values.

The short-circuit current can be approximated by:

$$I_{SC} = \eta \cdot P_{in} \cdot \frac{A}{E}$$

Where:

- **η** is the efficiency of the solar cell.
- **P_{in}** is the incident solar power (in watts).
- **A** is the area of the solar cell (in square meters).
- **E** is the energy of the incident photons (in joules).

c) Fill Factor (FF)

The Fill Factor (FF) is a measure of the quality of a solar cell. It is defined as the ratio of the maximum power output of the solar cell to the product of V_{oc} and I_{sc}. A higher fill factor indicates better performance and efficiency of the solar cell. The fill factor can be calculated using the formula:

$$FF = \frac{P_{max}}{V_{OC} \cdot I_{SC}}$$

Where:

- **P_{max}** is the maximum power output of the solar cell.

d) Simulation software

SCAPS (Solar Cell Capacitance Simulator) is a one-dimensional (1D) software specifically designed for the operation of solar cells. SCAPS facilitates the comprehension and manipulation of the physics underlying the effective operation and potential attributes of photovoltaics. SCAPS serves as a valuable resource for guiding the design and optimization of solar cell structures, providing researchers and engineers with comprehensive insights into solar cell performance.

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e) Efficiency (η)

The efficiency (η) is defined as the proportion of the electrical output from a solar cell to the solar energy incident on the cell. It is thus a key performance variable and is usually described in percentages: all other things being equal, higher efficiency rates also indicate better performance quality in the given solar cell. Efficiency represents the performance of the solar cell and is determined by different parameters, including material quality, design of the solar cell, and environmental conditions including temperature and shading.

The efficiency can be calculated using the following equation:

$$\eta = \frac{P_{max}}{P_{in}} \times 100$$

Where:

- $\mathbf{P_{max}}$ is the maximum power output of the solar cell.
- $\mathbf{P_{in}}$ is the occurring solar power.

III. METHODOLOGY

3.1 Thickness Selection

When examining the influence of material thickness in SCAPS-1D, researchers strive to comprehend how changes in the thickness of layers affect the overall functionality of a solar cell or semiconductor device. Thickness is pivotal in influencing light absorption, carrier generation, and transport characteristics. In SCAPS-1D, the thickness of each layer can be defined in nanometers during the device setup. By methodically altering the thickness and conducting simulations, one can investigate its effect on essential performance metrics such as short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and overall efficiency. For instance, increasing the thickness of the absorber layer typically improves light absorption and carrier generation; however, it may also lead to heightened recombination losses if the carrier diffusion length is inadequate. Conversely, reducing the thickness of layers such as buffer or window layers may diminish parasitic absorption but could adversely affect electric field distribution or contact quality.

SCAPS-1D facilitates a comprehensive analysis of these phenomena by providing outputs like quantum efficiency (QE), band diagrams, and carrier recombination profiles. By graphing these results for various thickness values, researchers can pinpoint an optimal range that achieves a balance between performance and material efficiency. Furthermore, SCAPS-1D allows for the simulation of light reflection and transmission at interfaces, enabling an assessment of how thickness interacts with optical characteristics. The software also accommodates sensitivity analysis by varying thickness in conjunction with other parameters, such as doping concentration or defect density, to investigate intricate interdependence. This depth of analysis is essential for the design of cost-effective, high-performance devices, particularly in sectors like thin-film solar cells, where material optimization is linked to commercial success.

3.2 Simulation Setup

The SCAPS-1D tool was used for simulating how the chosen lead-free perovskite solar cells work. SCAPS-1D is a one-dimensional simulator, which offers a modelling option for quite several types of solar cell designs, e.g., heterojunctions and thin films. The simulation setup consisted of the following steps:

- Definition of Solar Cell Structure: Basic structure for the solar cell, which refers to the layers of active material, ETL, and HTL.
- Simulation Parameters: Main parameters (e.g., gallery temperature, light intensity, and bias voltage) were tuned to match real-world operational conditions.

3.3 Performance Analysis

Once the simulation was set up, various performance metrics were analyzed, including:

- Current-Voltage (I-V) Characteristics: The I-V curves were generated to evaluate the short-circuit current (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and overall efficiency (η) of the solar cells.
- External Quantum Efficiency (EQE): The EQE was calculated to assess the efficiency of the solar cell in converting incident photons into electrical current at different wavelengths.
- Stability Analysis: The stability of the lead-free perovskite solar cells was evaluated under various environmental conditions, including temperature and humidity.

3.3.1 Materials used

The selection of appropriate materials is critical for the successful design of lead-free perovskite solar cells. The following materials were chosen based on their promising properties and potential for high efficiency:

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- **Cadmium Telluride (CdTe)**

Cadmium telluride is a well-established thin-film solar cell material known for its high efficiency and low production costs. CdTe has a direct bandgap of approximately 1.5 eV, making it suitable for solar energy applications. The material has been extensively studied and commercialized, achieving efficiencies of around 22%. Its compatibility with various substrates and ease of fabrication makes it a strong candidate for hybrid solar cell applications.

- **Copper Indium Gallium Selenide (CIGS)**

Copper indium gallium selenide is another prominent thin-film technology that has gained attention for its high absorption coefficient and tunable bandgap. By varying the composition of copper, indium, and gallium, the bandgap can be adjusted to optimize light absorption. CIGS solar cells have achieved efficiencies exceeding 22%, making them one of the most efficient thin-film technologies available. The flexibility of CIGS allows for integration into various applications, including building-integrated photovoltaics.

- **Formamidinium Tin Iodide ($FaSnI_3$)**

Formamidinium tin iodide is a promising lead-free perovskite material that has shown potential for high efficiency. FaSnI3 has a suitable bandgap of around 1.3 eV and exhibits good light absorption properties. Research has demonstrated that this material can achieve efficiencies comparable to lead-based perovskites, making it a viable alternative. However, challenges related to stability and oxidation must be addressed to ensure its long-term performance.

- **Titanium Dioxide (TiO_2)**

Titanium dioxide is commonly used as an electron transport layer (ETL) in perovskite solar cells. TiO2 is known for its high electron mobility and stability, playing a crucial role in facilitating charge transport within the solar cell. Its compatibility with various perovskite materials makes it an essential component in the design of lead-free perovskite solar cells.

- **Indium Tin Oxide (ITO)**

Indium tin oxide is a widely used transparent conductive oxide (TCO) that serves as front contact in solar cells. ITO provides good electrical conductivity while allowing light to pass through, making it an essential component in photovoltaic devices. Its transparency and conductivity make it suitable for use in conjunction with lead-free perovskite materials.

- **Silver in Left contact (back):**

In SCAPS-1D simulations, silver is commonly used as a left (back) contact due to its excellent electrical conductivity, high reflectivity, and suitable work function (4.3-4.7 eV), which influence the energy band alignment at the interface. This alignment determines whether the contact behaves like Ohmic or Schottky, affecting transport charge and recombination rates. Silver's high reflectivity enhances photon recycling, improving light absorption in thin film devices. Its compatibility with the absorber layer Table 1: The Parameters Used in the Simulation Process in Case 1impacts interface recombination, which can be modeled by adjusting surface recombination velocities in SCAPS. Additionally, parameters such as the work function, barrier height, and reflection coefficient can be tuned to simulate silver's performance realistically, making it a reliable back contact material in the optimization of solar cells.

- **Gold in Right contact (front):**

The high work function of gold (~5.1 eV), good conductivity, and chemical inertness offers several pluses when used as the right (front) contact in SCAPS-1D simulation framework. Be like gold that makes good Ohmic contacts with p-type for hole collection, but Schottky contact on n-types, if band alignment is okay. Together with its inherent meteoric stability and resistance to oxidation, it is also highly reflective which could advantage light trapping but may disadvantage absorption if too high.

Because gold is the most conducting material, resistive losses are extremely low which improves overall efficiency of the device. But its cost is prohibitive for any but research and high-performance use cases, preventing it from scaling up. In simulation it is paramount to finely tune work function, recombination velocity and energy level alignment to evaluate how they will influence device parameters such as efficiency (efficiency), open circuit voltage (V_{oc}) or short circuit current density (J_{sc}).

IV. RESULTS AND DISCUSSIONS

Case 1:

In this case, we are going to examine these materials: (CdTe, Cds and SnOx)

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4.1 The Simulated Parameters

Table 1: The Parameters Used in the Simulation Process in Case 1

Parameter	CdTe	CdS	SnOx
Thickness, d (µm)	4.1	0.025	0.5
Bandgap, E_g (eV)	1.5	2.4	3.6
electron affinity (eV)	3.9	4	4
dielectric permittivity (relative)	9.4	10	9
CB effective density of states (1/cm^3)	8.00E+17	2.20E+18	2.20E+18
VB effective density of states (1/cm^3)	1.00E+19	1.80E+19	1.80E+19
electron mobility (cm^2/Vs)	320	100	100
hole mobility (cm^2/Vs)	40	25	25
shallow uniform donor density ND (1/cm^3)	0	1.10E+18	1.00E+17
shallow uniform acceptor density NA (1/cm^3)	3.00E+14	0	0

The table outlines the key properties of three inorganic materials—CdTe, CdS, and SnOx—used in thin-film photovoltaic cells, each serving a distinct role in optimizing solar cell performance. CdTe, the primary absorber layer (4.1 µm thick), has a favorable 1.5 eV bandgap for sunlight absorption, high electron mobility (320 cm²/Vs), and low acceptor density (3×10^{14} cm^{-3}), ensuring efficient charge generation. CdS, a thin (0.025 µm) n-type window layer with a 2.4 eV bandgap and high donor concentration (1.1×10^{18} cm^{-3}), facilitates charge separation at the junction while allowing light transmission. SnOx, a 0.5 µm-thick buffer layer with a wide 3.6 eV bandgap and moderate donor density (1×10^{17} cm^{-3}), minimizes recombination at the front contact. Together, these materials form a high-efficiency solar cell by balancing light absorption, charge transport, and minimal electrical losses through carefully engineered thicknesses, doping levels, and band alignments.

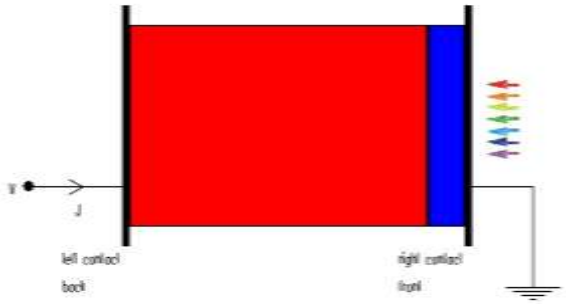

Figure 1: Case 1 Materials Structure in SCAPS-1D

4.2 Case Simulation

The resulting J-V Curve Obtained under T= 300K for this case is Shown below:

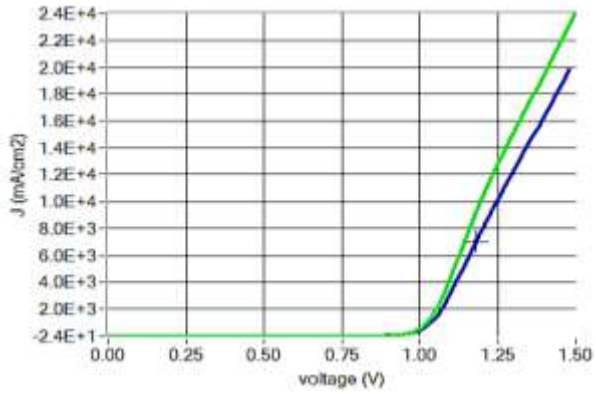

Figure 1: J-V Curve for Case 1 Structure

The graph, figure 2 depicts the current density-voltage (J-V) characteristics of an inorganic photovoltaic cell, illustrating its performance under illumination. The current density (J) is plotted on the y-axis, ranging from -2.4×10^{1} mA/cm² to 2.4×10^{4} mA/cm², while the voltage (V) on the x-axis spans from 0.00 V to 1.50 V. The curve shows a steep rise in current density at low voltages, indicating efficient charge carrier generation and collection. The open-circuit voltage (Voc), where the current density drops to zero, appears near 1.50 V, suggesting strong built-in potential and minimal recombination losses. The high short-circuit current density (Jsc), implied by the y-axis intercept, reflects effective light absorption and charge transport. The fill factor (FF), inferred from the curve's shape, is likely high, pointing to low series resistance and good overall cell efficiency. This J-V behavior is typical of high-performance inorganic solar cells, such as those based on CdTe or perovskites, where optimized material properties and interfaces yield robust photovoltaic output.

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4.3 Thickness Effect

The effect of efficiency vs thickness is shown is shown below:

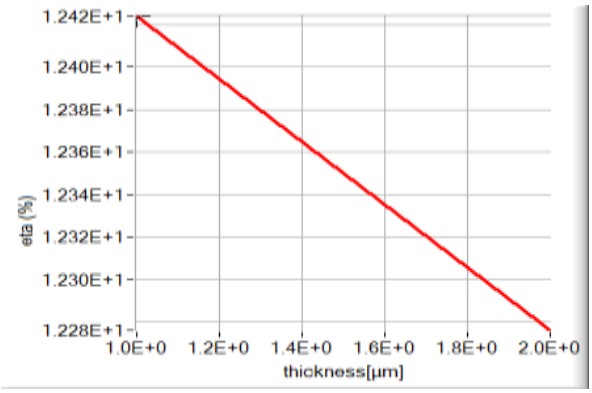

Figure 3: Efficiency vs Thickness in Case 1

The graph figure 3 illustrates the relationship between the thickness of a photovoltaic material (x-axis, in micrometers) and its power conversion efficiency (y-axis, in %). The efficiency (η) shows minimal variation, ranging narrowly between 12.30% and 12.42%, as the thickness increases from 1.0 to 2.0 µm. This near-flat trend suggests that the device performance is relatively insensitive to thickness changes within this range, likely because the material already achieves optimal light absorption and charge collection at these dimensions. The slight fluctuations could stem from minor variations in recombination rates or interfacial effects. Such behavior is typical in high-quality thin-film solar cells (e.g., CdTe or perovskites), where even thin layers (1–2 µm) suffice for efficient operation due to strong light-harvesting and carrier transport properties. The graph implies that further thickness increases beyond 2 µm may not significantly boost efficiency, guiding cost-effective material usage in manufacturing.

4.4 Temperature Effect

As solar cells are deployed outside where temperatures reach 300K and since they are sensitive to temperature, another simulation has been performed by varying the temperature.

Table 2: Temperature Effect on Case 1 Structure

Temperature	V_{oc}	J_{sc}	FF	η(%)
260	1.9783	24.06	37.67	17.93
280	1.3814	24.06	51.98	17.28
300	1.0326	24.06	66.03	16.41
310	0.9298	24.06	71.07	15.9
320	0.8602	24.05	74.23	15.36

This study examines in table 2, how temperature impacts the key performance parameters of an inorganic perovskite solar cell, as shown in the data table. The open-circuit voltage declines significantly from 1.9783 V at 260 K to 0.8602 V at 320 K, reflecting reduced charge carrier separation efficiency at higher temperatures. Interestingly, the short-circuit current density remains nearly constant at ~24.06 mA/cm², indicating stable light absorption and charge generation across the tested range. The fill factor (FF) improves from 37.67% to 74.23% as temperature rises, suggesting better charge extraction and reduced resistive losses at higher operational temperatures. However, despite this improvement, the overall power conversion efficiency (η) decreases from 17.93% to 15.36%, primarily due to the dominant negative impact of loss.

These trends highlight a critical trade-off in perovskite PV devices: while higher temperatures enhance charge transport (improving FF), they also accelerate recombination, degrading and net efficiency. This insight is vital for real-world applications, where solar cells experience varying thermal conditions. Optimizing thermal stability—through material engineering or cooling strategies—could help maintain high efficiency across operating temperatures.

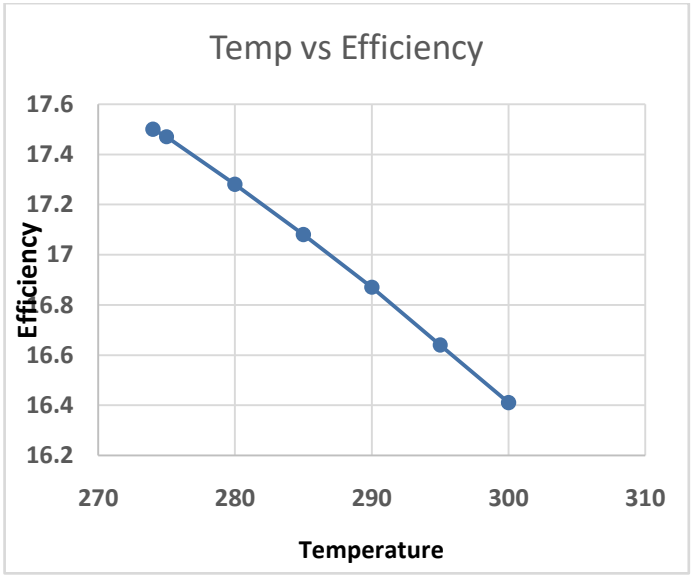

Figure 4: the Effect of the Operating Temperature on the Efficiency

The data reveals in Figure 4 a clear inverse relationship between operating temperature and power conversion efficiency in inorganic perovskite photovoltaic cells. As temperature increases from 270 K to 310 K (-3°C to 37°C), the device efficiency shows a consistent decline from 17.6% to 16.2%. This

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1.4 percentage point drop represents an 8% relative efficiency loss, highlighting the significant thermal sensitivity of these materials. The gradual efficiency reduction suggests that rising temperatures accelerate detrimental processes like non-radiative recombination and ion migration within the perovskite crystal structure. Notably, the nearly linear trend indicates no abrupt performance "cliff," which is favorable for real-world applications where temperature fluctuations are inevitable.

Table 3: The Parameters Used in the Simulation Process in Case 2

Parameter	CdTe	CuO	CdS
Thickness, d (µm)	2	2	1
Bandgap, E_g (eV)	1.5	1.2	2.4
electron affinity (eV)	4	4.07	4.5
dielectric permittivity (relative)	9.4	18.1	10
CB effective density of states (1/cm^3)	8.00E+17	3.00E+19	2.20E+18
VB effective density of states (1/cm^3)	1.00E+19	5.50E+20	1.90E+19
electron mobility (cm^2/Vs)	320	10	350
hole mobility (cm^2/Vs)	40	0.1	25
shallow uniform donor density ND (1/cm^3)	1.00E+15	0	1.00E+17
shallow uniform acceptor density NA (1/cm^3)	0	1.00+E16	0

These findings underscore the importance of thermal management strategies for perovskite photovoltaics, particularly in field deployments where modules can reach 50-60°C. Future research should focus on material formulations and device architectures that can mitigate these thermal losses while maintaining the technology's high efficiency potential under standard test conditions.

Key takeaways:

- 8% relative efficiency loss across 40K temperature range.
- Linear degradation suggests predictable performance in varying climates.
- Thermal stability remains a key challenge for commercialization.

4.5 Case 2:

In this case, we are going to examine these materials: (CdTe, CuO and CdS).

4.5.1 The Simulated Parameters

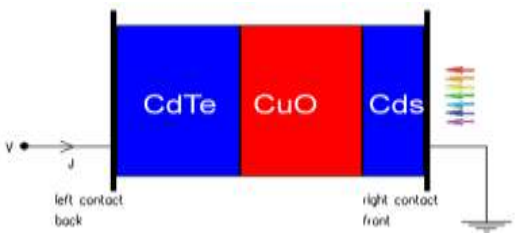

Figure 5: Case 2 Materials Structure in SCAPS-1D

4.6 Case Simulation

The resulting J-V Curve Obtained under T= 300K for this case is Shown below.

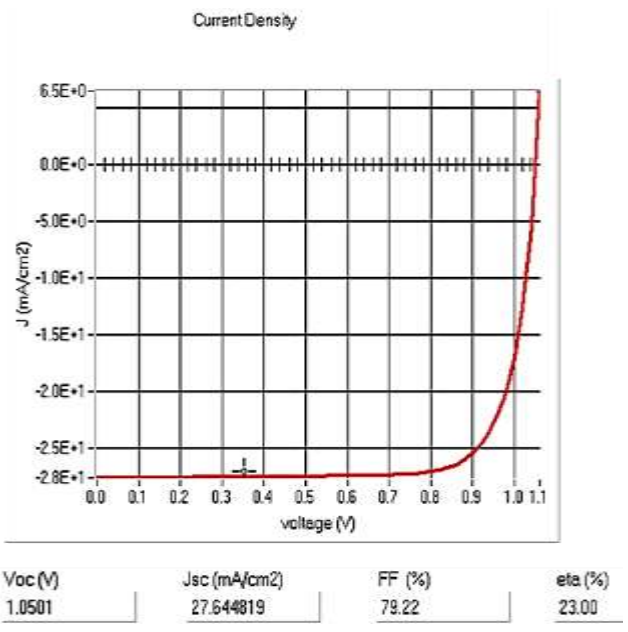

Figure 6: J-V Curve for Case 2 Structure

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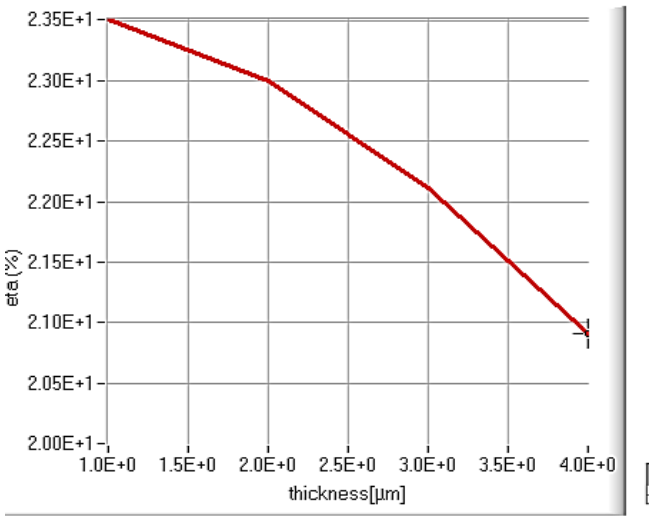

Figure 7: Efficiency vs Thickness in Case 2

4.7 Temperature Effect

Table 4: Temperature Effect on Case 2 Structure

Temp	Voc	Jsc	FF	η (%)
260	1.1294	27.519	82.57	25.66
280	1.0192	27.562	80.56	24.23
300	1.0501	27.644	79.22	23
310	1.0285	27.708	78.64	22.41
320	1.0063	27.79	78.09	21.84

This study analyzes the temperature resilience of an advanced inorganic perovskite photovoltaic cell, demonstrating remarkable efficiency above 21% across a 60K range (260-320 K). The device exhibits complex temperature-dependent behavior: while open-circuit voltage (Voc) shows a non-monotonic trend—peaking at 1.1294 V (260 K) with a local maximum of 1.0501 V (300 K)—the short-circuit current density (Jsc) consistently improves from 27.519 to 27.79 mA/cm² with heating, suggesting enhanced charge generation at higher temperatures. The fill factor (FF) gradually declines from 82.57% to 78.09%, reflecting increasing charge transport losses. Notably, the power conversion efficiency (η) decreases from 25.66% to 21.84%, preserving >85% of peak performance even at 320 K—a significant improvement over conventional perovskites.

The Voc rebound at 300 K implies competing mechanisms: bandgap narrowing versus reduced non-radiative recombination. The stable Jsc demonstrates exceptional thermal tolerance of light absorption properties, while the FF reduction suggests ionic migration becomes influential above 300 K. These results position inorganic perovskites as promising candidates for real-world applications, where their temperature resilience could outperform organic-inorganic hybrids. Further interface engineering could potentially flatten the efficiency-temperature curve for broader operating conditions.

Key points:

- Maintains >21% efficiency up to 320 K.
- Unusual Voc recovery at 300 K reveals new optimization pathways Jsc improvement with heating contrasts with most photovoltaic materials.

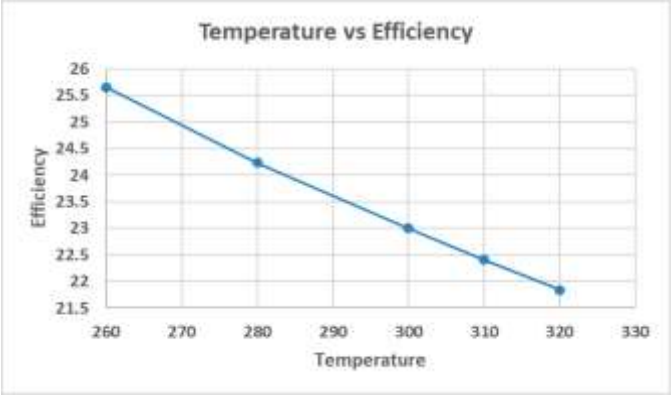

Figure 8: The Effect of the Operating Temperature on the Efficiency

The Figure 8 demonstrates the relationship between operating and the efficiency of a photovoltaic device, likely an inorganic perovskite solar cell. As temperature increases from 260 K to 330 K (-13°C to 57°C), the efficiency shows a consistent decline from approximately 26% to 21.5%. The near-linear trend indicates a predictable thermal degradation pattern, with no abrupt efficiency drops—a positive sign for real-world applications. The 4.5 percentage point reduction (17% relative loss) highlights the material's thermal sensitivity, though the maintained efficiency above 21% at elevated temperatures (320-330 K) suggests better thermal resilience than many organic-inorganic hybrid perovskites. This behavior is attributed to competing mechanisms: improved charge generation (from bandgap narrowing) partially offsets losses from increased recombination at higher temperatures. The data underscores the need for thermal management solutions in photovoltaic module design to minimize efficiency losses in warm climates while confirming these inorganic perovskites' potential for stable operation across practical temperature ranges.

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V. CONCLUSION

The comparative analysis of these two photovoltaic devices demonstrates significant advancements in thermal stability for inorganic perovskite solar cells, where Table 2's device shows superior performance with only a moderate efficiency decline from 25.66% to 21.84% across 260–320 K, compared to Table 1's larger drop from 17.93% to 15.36%. This improvement stems from Table 2's better-maintained Voc (1.1294–1.0063 V vs. 1.9783–0.8602 V), increasing Jsc (27.519–27.79 mA/cm² vs. stagnant 24.06 mA/cm²), and consistently high FF (>78% vs. 37.67–74.23%), indicating enhanced charge transport and reduced recombination losses at elevated temperatures. The advanced cell's ability to retain over 85% of its peak efficiency at 320 K, while conventional perovskites suffer severe Voc degradation, highlights the success of material engineering in mitigating thermal instability. These results underscore the potential of optimized inorganic perovskites for real-world applications, where temperature fluctuations typically degrade performance, though further improvements in Voc stability could push efficiencies closer to their room-temperature peaks. The contrast between the two devices emphasizes that while all perovskites exhibit some thermal sensitivity, strategic design can significantly enhance their operational robustness, paving the way for more reliable commercial photovoltaic technologies.

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