

Numerical Investigation of Defect–Temperature Effects on the Operational Reliability of Lead-Free FASnI₃ Perovskite Solar Cells

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ABSTRACT

The long-term performance of perovskite solar cells is limited by thermal stress and defect-assisted recombination, which accelerate degradation during operation. This study presents a reliability-oriented modeling approach using defect–temperature phase diagrams to identify stable operating conditions for lead-free FASnI₃ perovskite solar cells using SCAPS-1D. Simulations were conducted over an operating temperature range of 300–400 K and a bulk defect density of 1×10^{10} to $1 \times 10^{17} \text{ cm}^{-3}$. Normalized power conversion efficiencies were used to construct reliability phase diagrams, and sensitivity coefficients were determined to assess their relative impact on performance. The simulated device maintained stable performance across temperatures when bulk defect density remained low. However, performance declined rapidly once defect density exceeded $\sim 1 \times 10^{14}$ – $1 \times 10^{15} \text{ cm}^{-3}$ due to enhanced trap-assisted recombination. The reliability maps categorized operating conditions into four regions—Robust, Reliable, Critical, and Failure—showing that variations in defect density affect performance significantly more than operating temperature. The proposed framework offers a practical method for evaluating defect tolerance, setting safe thermal limits, and designing durable, long-lasting lead-free perovskite solar cells for sustainable energy deployment.

Keywords:

Perovskite solar cells,
Reliability phase diagram,
Defect density,
Thermal stability,
Green energy.

INTRODUCTION

As countries push to replace fossil fuels, the shift toward low-carbon energy has driven a massive surge in the rollout of photovoltaic (PV) technologies (dos Santos & Pacca, 2026; International Energy Agency, 2023). Pushing the boundaries of energy-conversion efficiency is a primary objective in photovoltaic research; however, achieving long-term operational lifespan, resource efficiency, and sustainable end-of-life management is equally critical for ensuring overall environmental and economic viability (Paç & Gok, 2024). When solar modules degrade prematurely, frequent replacement becomes necessary, driving up demand for raw materials, increasing energy consumption during manufacturing and transport, and generating substantial electronic waste (Bhandari & Sekimuli, 2026). Consequently, extending the operational lifetime of photovoltaic systems represents one of the most effective strategies for reducing the environmental footprint of renewable

energy technologies (Paç & Gok, 2024; Ovaitt et al., 2021).

The rapid development of perovskite solar cells (PSCs) has transformed photovoltaic research. Within a short period, power conversion efficiencies (PCEs) have increased remarkably due to advances in absorber composition, interface engineering, and device architecture (Green et al., 2026; Zuo et al., 2016). Coupled with low-temperature solution processability, tunable bandgaps, and high absorption coefficients, PSCs have emerged as promising candidates for next-generation photovoltaics. Despite these achievements, commercial deployment remains fundamentally constrained by a critical research problem: maintaining long-term operational reliability and stability under real-world operating conditions (Baumann et al., 2024). Prior studies have established that performance loss in PSCs is intrinsically linked to trap state formation within the absorber layer and at charge-transport interfaces.

These defect states function as non-radiative recombination centres via Shockley–Read–Hall (SRH) mechanisms, which severely shorten carrier lifetimes and impede charge collection efficiency (Chen & Park, 2019). Degradation is further compounded under thermal stress, where elevated operating temperatures accelerate ion migration, phase instability, and interfacial deterioration (López-González et al., 2023; Tang et al., 2025). Together, defect formation and thermal stress cause progressive reductions in open-circuit voltage, fill factor, and overall PCE. To systematically analyze these coupled physical processes, numerical simulation platforms such as SCAPS-1D are widely utilized to evaluate charge transport, interface recombination, and solar cell performance across varied environmental conditions (Araújo et al., 2025; Ouslimane et al., 2021). Experimental studies provide valuable information on degradation behaviour, but investigating every possible combination of material properties and operating conditions is both time-consuming and expensive. Numerical simulation offers an efficient alternative by allowing individual parameters to be controlled systematically. Among the available simulation platforms, SCAPS-1D has become one of the most widely used tools for analysing the electrical behaviour of perovskite solar cells, including the effects of defects, transport layers, interface properties, and environmental conditions (Araújo et al., 2025). Previous SCAPS studies have successfully identified favourable absorber thicknesses, operating temperatures, and defect concentrations that improve photovoltaic performance (Ouslimane et al., 2021). However, these investigations usually focus on optimizing efficiency rather than determining the conditions under which a device can continue to operate reliably over time.

Although numerical modeling has successfully identified optimal layer thicknesses and doping levels to maximize baseline efficiency, a significant gap in knowledge persists. Most existing SCAPS-1D literature focuses predominantly on initial performance optimization, leaving a clear lack of a practical framework for identifying operating regimes—specifically the dynamic interaction between bulk defect density and elevated temperature—that distinguish between safe, reliable operation and accelerated device degradation or failure (Peters & Sinha, 2021; Saidarsan et al., 2025).

Establishing such boundaries is essential for defining acceptable defect tolerances during manufacturing and establishing safe thermal operating thresholds for deployment in high-temperature environments.

The choice of the FASnI₃ absorber paired with a SnO₂ electron transport layer and a CuI hole transport layer is uniquely justified by their highly favorable energy band alignment, the superior charge carrier mobilities of SnO₂ and CuI, and the enhanced suppression of non-radiative recombination at the heterojunction interfaces compared to alternative lead-free perovskite configurations.

To address this gap, this study develops a novel, reliability-oriented modeling approach and introduces a defect–temperature reliability phase diagram framework to define acceptable operating limits for lead-free PSCs. The primary objective of this work is to investigate the combined effects of operating temperature and bulk defect density on device performance using SCAPS-1D simulations, and to classify device operation into distinct robustness regimes (Robust, Reliable, Critical, and Failure). By quantifying sensitivity coefficients and establishing clear operational boundaries, this study provides actionable design criteria to enhance defect tolerance, extend service life, and advance the sustainable deployment of lead-free perovskite photovoltaics.

MATERIALS AND METHODS

A planar heterojunction Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell was simulated using SCAPS-1D (version 3.3.12, ELIS-UGent). SnO₂ served as the electron transport layer (ETL), FASnI₃ as the lead-free absorber layer, and CuI as the hole transport layer (HTL), while the front and back contacts were assumed to be ideal ohmic contacts. Bulk defects in the FASnI₃ absorber layer were modeled using a Gaussian energy distribution with a characteristic energy width of 0.1 eV centered at 0.60 eV above the valence band. The schematic device architecture is presented in Figure 1, and the material properties used in the simulations, including layer thickness, bandgap, electron affinity, dielectric constant, carrier mobilities, doping concentrations, and Shockley–Read–Hall (SRH) defect parameters, are summarized in Table 1.

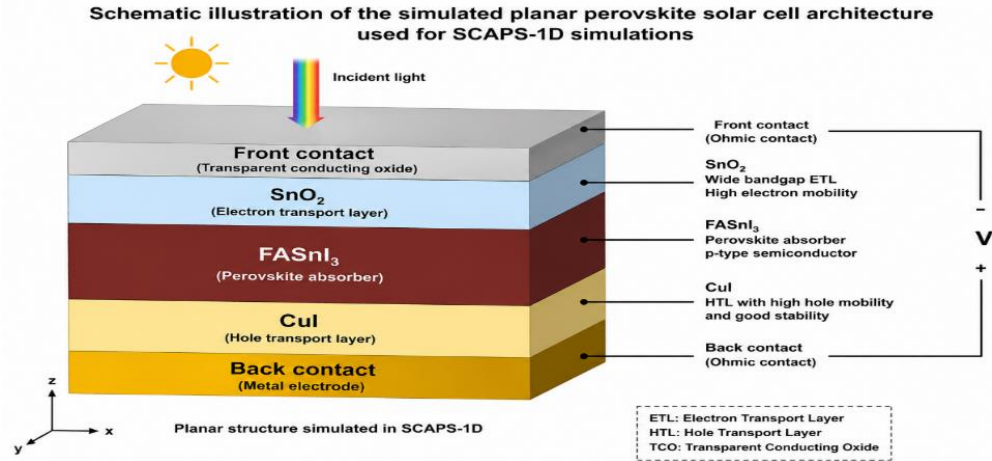


Figure 1: Schematic illustration of the simulated planar perovskite solar cell architecture consisting of Front contact/SnO₂/FASnI₃/CuI/Back contact used for the SCAPS-1D simulations.

Source: Authors' illustration

Table 1: Material Parameters used for the SCAPS-1D Simulation of the Front contact/SnO₂/FASnI₃/CuI/Back Contact Perovskite Solar Cell

Parameter	SnO ₂ (ETL)	FASnI ₃ (Absorber)	CuI (HTL)
Thickness (nm)	50	500	50
Bandgap, E_g (eV)	3.60	1.41	2.98
Electron affinity, χ (eV)	4.00	4.17	2.10
Relative dielectric constant, ϵ_r	9.0	8.2	6.5
Electron mobility, μ_n (cm ² V ⁻¹ s ⁻¹)	100	4	1
Hole mobility, μ_p (cm ² V ⁻¹ s ⁻¹)	10	5	20
Donor concentration, N_d (cm ⁻³)	1×10^{17}	0	0
Acceptor concentration, N_a (cm ⁻³)	0	0	1×10^{19}
Bulk defect density, N_t (cm ⁻³)	1×10^{15}	Variable (10^{10} – 10^{17})	1×10^{14}
Defect type	Neutral	Neutral (Gaussian, $\sigma = 0.1$ eV)	Neutral
Defect energy level, E_t (eV)	0.60	0.60	0.60
Electron capture cross-section, σ_n (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}
Hole capture cross-section, σ_p (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}

All simulations were performed under standard AM1.5G illumination (100 mW cm⁻²) using the internal SCAPS optical generation model under steady-state conditions. The series resistance was fixed at 1×10^{-9} $\Omega \cdot \text{cm}^2$, while a shunt resistance of 1×10^6 $\Omega \cdot \text{cm}^2$ was assumed to suppress leakage currents (Sabbah et al., 2024). Except for the investigated variables, all material parameters remained unchanged throughout the simulations.

To evaluate device reliability, two independent parameters were varied systematically: the operating temperature (300, 325, 350, 375, and 400 K) and the bulk defect density of the FASnI₃ absorber (1×10^{10} – 1×10^{17} cm⁻³). This produced a total of 40 simulation conditions,

from which the photovoltaic parameters (V_{oc} , J_{sc} , FF, and PCE) were extracted.

The normalized power conversion efficiency was calculated as (Snaith & Hacke, 2018):

$$P_{norm} = \frac{PCE}{PCE_{max}} \quad (1)$$

Where PCE_{max} the maximum efficiency obtained among all simulations. Based on the normalized efficiency, device operation was classified into four reliability regimes: Robust ($P_{norm} \geq 0.90$), Reliable ($0.80 \leq P_{norm} < 0.90$), Critical ($0.60 \leq P_{norm} < 0.80$), and Failure ($P_{norm} < 0.60$), as summarized Table in Table 2.

Table 2: Reliability Classification Criteria Based on Normalized Power Conversion Efficiency

Reliability Region	Normalized PCE (P_{norm})
Robust	≥ 0.90
Reliable	$0.80 - < 0.90$
Critical	$0.60 - < 0.80$
Failure	< 0.60

The simulated photovoltaic parameters were exported for post-processing in Python, where the normalized efficiencies were used to generate contour plots and a categorical reliability phase diagram illustrating the transitions between the Robust, Reliable, Critical, and Failure regions. In addition, the temperature sensitivity is (Afrin et al., 2024):

$$S_T = \frac{\partial PCE}{\partial T} \quad (2)$$

And defect sensitivity is (Abdulsalam & Lariski, 2026):

$$S_N = \frac{\partial PCE}{\partial \log_{10} N_t} \quad (3)$$

Were calculated from the simulated data to quantify the relative influence of thermal stress and bulk defects on device performance and reliability.

RESULTS AND DISCUSSION

The baseline photovoltaic performance of the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell was first evaluated under standard AM1.5G illumination (100 mW cm⁻²) at 300 K. The device exhibited an open-circuit voltage (Voc) of 1.0051 V, a short-circuit current density (Jsc) of 28.5199 mA cm⁻², a fill factor (FF) of 70.81%, and a power conversion efficiency (PCE) of 20.30%, demonstrating excellent baseline photovoltaic performance (Table 3 and Figure 2).

Table 3: Baseline Photovoltaic Parameters of the Optimized Front contact/SnO₂/FASnI₃/CuI/Back Contact Perovskite Solar Cell under AM1.5G Illumination

Voc (V)	Jsc (mA cm ⁻²)	FF (%)	PCE (%)
1.0051	28.5199	70.81	20.30

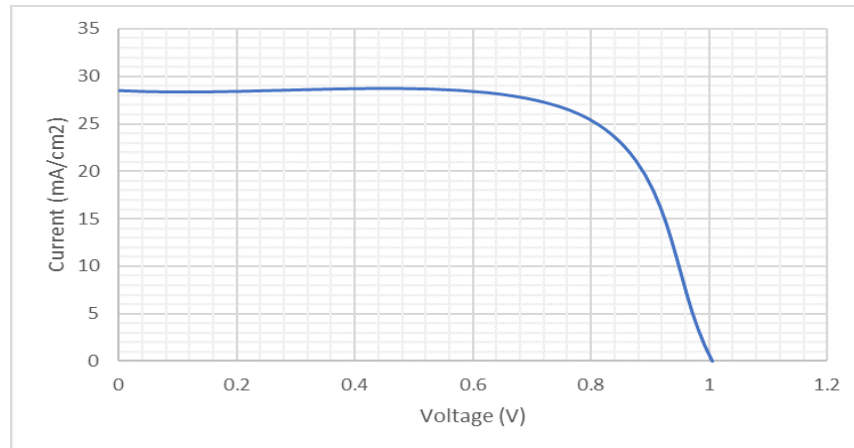


Figure 2: Current density–voltage (J–V) characteristics of the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell under AM1.5G illumination (100 mW cm⁻²) at 300 K

The effect of operating temperature was subsequently investigated over the range of 300–400 K at a bulk defect density of 1×10^{10} cm⁻³. As shown in Figure 3(a–d), the device maintained stable photovoltaic performance throughout the investigated temperature range. The Voc increased slightly from 1.0405 V to 1.0446 V, while Jsc remained nearly constant at approximately 28.54 mA

cm⁻². The FF increased from 80.30% to a maximum of 81.54% at 350 K before decreasing slightly to 80.54% at 400 K (Afrin et al., 2024). Similarly, the PCE increased from 23.85% to 24.29% at 350 K and then decreased marginally to 24.01% at 400 K, indicating good thermal stability of the optimized device (Figure 3).

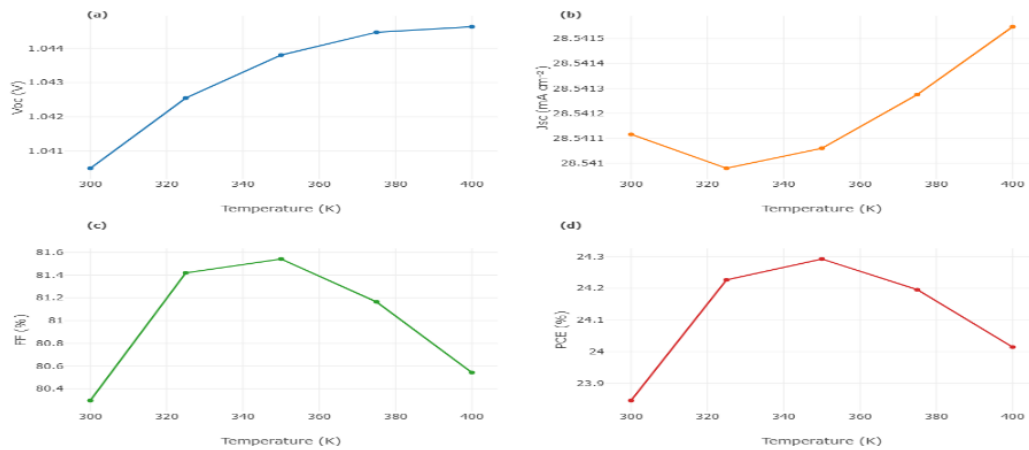


Figure 3: Effect of operating temperature on the photovoltaic performance of the optimized perovskite solar cell at a bulk defect density of 10^{10} cm^{-3} : (a) open-circuit voltage (V_{oc}), (b) short-circuit current density (J_{sc}), (c) fill factor (FF), and (d) power conversion efficiency (PCE)

The influence of bulk defect density (1×10^{10} – $1 \times 10^{17} \text{ cm}^{-3}$) was examined at 300 K. The photovoltaic parameters remained nearly unchanged up to approximately $1 \times 10^{13} \text{ cm}^{-3}$, indicating high defect tolerance (Abdulsalam & Lariski, 2026). Beyond $1 \times 10^{14} \text{ cm}^{-3}$, a pronounced degradation in device performance was observed. The V_{oc} decreased from 1.0405 V to

0.9876 V at $1 \times 10^{15} \text{ cm}^{-3}$, while J_{sc} remained nearly constant up to $1 \times 10^{15} \text{ cm}^{-3}$ before decreasing to 24.75 mA cm^{-2} at $1 \times 10^{17} \text{ cm}^{-3}$. Likewise, the FF decreased from 80.30% to 67.84%, and the PCE declined sharply from 23.85% to 6.94%, demonstrating that device performance deteriorates rapidly at high defect concentrations (Figure 4).

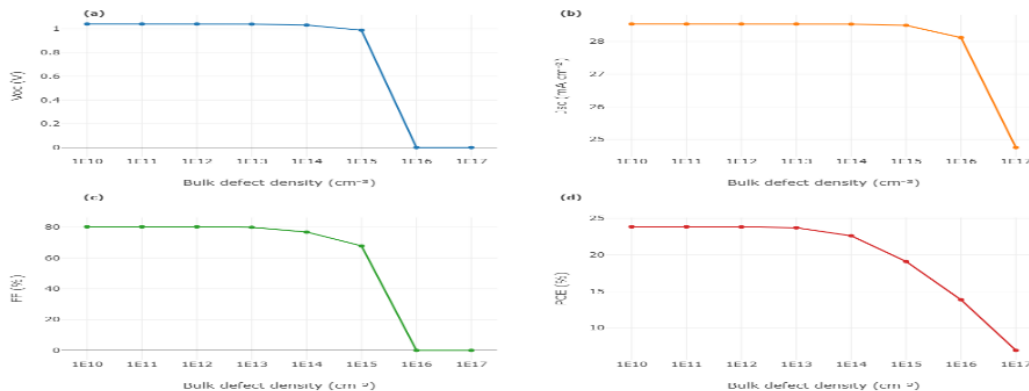


Figure 4: Dependence of the photovoltaic parameters of the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell on the bulk defect density at 300 K: (a) open-circuit voltage (V_{oc}), (b) short-circuit current density (J_{sc}), (c) fill factor (FF), and (d) power conversion efficiency (PCE)

To evaluate the combined influence of operating temperature and bulk defect density, the PCE values were normalized with respect to the maximum simulated efficiency. The contour plot (Figure 5) shows that the normalized PCE remained close to unity at low defect densities (1×10^{10} – $1 \times 10^{13} \text{ cm}^{-3}$) across the entire

temperature range, whereas a rapid decline occurred once the defect density exceeded approximately $1 \times 10^{14} \text{ cm}^{-3}$. The largest reduction in normalized efficiency occurred in the 1×10^{16} – $1 \times 10^{17} \text{ cm}^{-3}$ region, indicating that bulk defect density has a substantially greater influence on device performance than operating temperature.

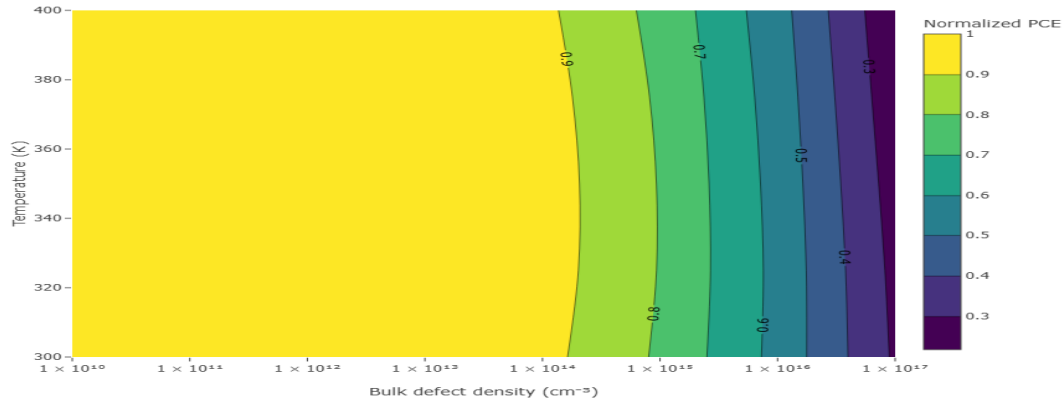


Figure 5: Contour plot showing the variation of normalized power conversion efficiency (PCE/PCE_{max}) as a function of operating temperature (300–400 K) and bulk defect density (1×10^{10} – $1 \times 10^{17} \text{ cm}^{-3}$) for the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell

Based on the normalized efficiency, a reliability phase diagram (Figure 6) was constructed to classify the operating conditions into Robust, Reliable, Critical, and Failure regions (Rijal et al., 2025). The Robust region was observed at low defect densities (1×10^{10} – $1 \times 10^{13} \text{ cm}^{-3}$) over the entire temperature range, while increasing

the defect density shifted the device successively into the Reliable and Critical regions. At defect densities of approximately $1 \times 10^{16} \text{ cm}^{-3}$ and above, the device entered the Failure region regardless of operating temperature, demonstrating that defect density primarily governs the transition between reliability regimes.

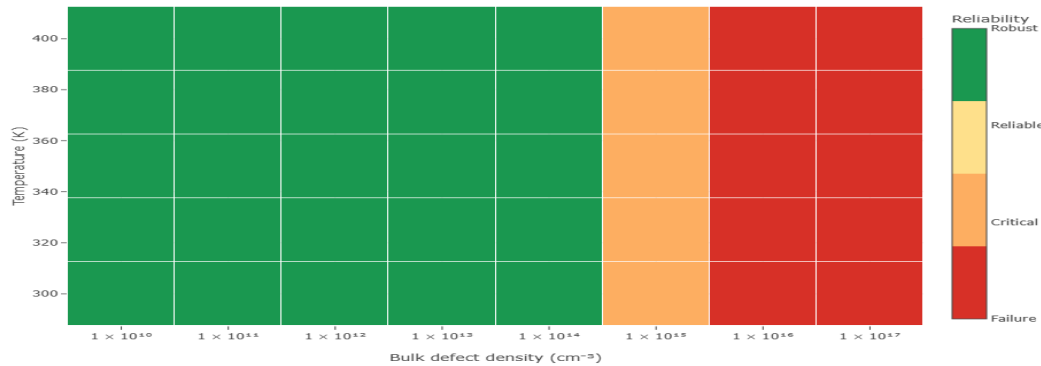


Figure 6: Reliability phase diagram of the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell showing the Robust, Reliable, Critical, and Failure operating regions as functions of operating temperature and bulk defect density based on normalized power conversion efficiency

To quantify the relative influence of operating temperature and bulk defect density on the photovoltaic performance of the optimized Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell, temperature and defect sensitivity coefficients were estimated from the simulated power conversion efficiency (PCE) data. The temperature sensitivity (S_T) and defect sensitivity (S_N) were defined in Equation (2) and (3).

Using the simulated data at the lowest defect density ($1 \times 10^{10} \text{ cm}^{-3}$), the PCE changed only slightly from 23.85% at 300 K to 24.01% at 400 K, corresponding to an average temperature sensitivity of

$$S_T \approx \frac{24.0144 - 23.8460}{400 - 300} = 1.68 \times 10^{-3} \% K^{-1}$$

This very small value indicates that the device performance is only weakly affected by temperature within the investigated operating range when the defect density is low (Afrin et al., 2024).

In contrast, at 300 K, increasing the bulk defect density from 1×10^{10} to $1 \times 10^{17} \text{ cm}^{-3}$ reduced the PCE from 23.85% to 6.94%. Since this corresponds to a seven-decade increase in defect density, the average defect sensitivity is

$$S_N \approx \frac{6.9442 - 23.8460}{17 - 10} = -2.41\% \text{ per decade of } N_t$$

The calculated sensitivity coefficients shown in Table 4, demonstrate that the magnitude of the defect sensitivity is several orders of magnitude greater than that of the

temperature sensitivity over the investigated operating range. While moderate temperature variations produce only marginal changes in device efficiency, increasing the bulk defect density causes a rapid deterioration in photovoltaic performance. These findings confirm that bulk defect density is the dominant parameter controlling the reliability of the simulated FASnI₃ perovskite solar cell, whereas temperature plays a secondary role under the examined conditions.

Table 4: Calculated Sensitivity Coefficients for the Optimized Perovskite Solar Cell

Sensitivity parameter	Expression	Calculated value	Interpretation
Temperature sensitivity, (S_T)	$(\partial PCE / \partial T)$	$1.68 \times 10^{-3} \% \text{ K}^{-1}$	Very weak dependence on temperature
Defect sensitivity, (S_N)	$(\partial PCE / \partial \log_{10} N_t)$	$(-2.41) \% \text{ per decade}$	Strong degradation with increasing defect density

These quantitative results are consistent with the reliability phase diagram, which shows that the transition from Robust to Failure operation is governed primarily by increasing bulk defect density, with temperature exerting only a comparatively minor influence over the range of 300–400 K (Abdulsalam & Lariski, 2026).

The simulation results indicate that both operating temperature and bulk defect density influence the behaviour of the Front contact/SnO₂/FASnI₃/CuI/Back contact perovskite solar cell, although their effects differ considerably. Within the investigated temperature range of 300–400 K, the device maintained nearly constant photovoltaic performance provided that the bulk defect density remained between 1×10^{10} and $1 \times 10^{13} \text{ cm}^{-3}$. Only small variations were observed in Voc, Jsc, FF, and PCE. A slight improvement in FF and PCE up to about 350 K is likely associated with enhanced carrier transport at moderate temperatures, which promotes more efficient charge extraction. Beyond this point, however, the benefit becomes less evident because thermal activation increases the participation of defect states in non-radiative recombination processes, producing a modest decline in performance (Shao et al., 2017). The calculated temperature sensitivity coefficient ($S_T = 1.68 \times 10^{-3} \% \text{ K}^{-1}$) supports this observation, indicating that moderate heating has only a limited influence when the absorber contains relatively few defects.

Changing the defect density produced a much stronger response. Performance remained almost unchanged at low defect concentrations, suggesting that the simulated FASnI₃ absorber can tolerate a moderate number of defects without significant electrical degradation. Once the defect density exceeded approximately $1 \times 10^{14} \text{ cm}^{-3}$, the electrical characteristics deteriorated rapidly. This behaviour is consistent with an increase in Shockley–Read–Hall (SRH) recombination, where additional trap

states shorten carrier lifetime and reduce the probability of successful charge collection (Sherkar et al., 2017). Although higher temperatures further encourage carrier trapping, the simulations show that the deterioration is driven mainly by the increase in defect density rather than by temperature itself. Similar trends have been reported in previous numerical and experimental studies, where trap-assisted recombination has been identified as a dominant limitation to stable perovskite solar-cell operation (Abdulsalam & Lariski, 2026; Song et al., 2016).

The operational boundaries established in the reliability phase diagram carry profound implications for practical device deployment and integration into multi-junction tandem architectures. In a monolithic tandem configuration (such as silicon/perovskite or perovskite/perovskite double-junction cells), the sub-cells are electrically connected in series, meaning that overall module current is strictly constrained by the lowest-performing layer. If bulk defect densities within the FASnI₃ absorber exceed $1 \times 10^{14} \text{ cm}^{-3}$, the resulting reduction in carrier lifetime not only degrades single-junction output but also induces severe current mismatch across the tandem stack. Furthermore, operating within the Critical or Failure regimes under real-world field conditions—where elevated thermal cycles accelerate defect proliferation—can create localized hot spots, leading to irreversible localized thermal breakdown. Consequently, maintaining the FASnI₃ absorber strictly within the robust regime ($N_t \leq 1 \times 10^{13} \text{ cm}^{-3}$) serves as a non-negotiable threshold for ensuring both long-term stability and high energy yield in tandem solar deployments.

The sensitivity analysis leads to the same conclusion. The defect sensitivity coefficient ($S_N = -2.41\% \text{ per decade increase in defect density}$) is substantially larger than the

corresponding temperature sensitivity, confirming that material quality exerts the strongest influence on long-term device performance. Consequently, strategies aimed at suppressing defect formation or passivating existing defects are likely to produce greater improvements in operational stability than moderate reductions in operating temperature. This observation has practical significance for photovoltaic systems operating in tropical environments, where elevated module temperatures are unavoidable but defect densities remain controllable through material selection and fabrication processes (Ozurumba et al., 2024).

The importance of reliability extends beyond improving electrical performance. Photovoltaic technologies are expected to operate for many years under changing environmental conditions, and their environmental benefit depends not only on conversion efficiency but also on operational lifetime (Besseau et al., 2023). A device that maintains stable performance for a longer period delivers more energy from the same quantity of materials and manufacturing effort, improving overall lifecycle efficiency. By identifying defect-density limits associated with reliable operation, the present framework offers guidance that could assist the design of longer-lasting lead-free perovskite solar cells.

Greater durability also has implications for resource use and waste generation. Although lead-free FASnI₃ removes concerns related to lead contamination, large-scale deployment will still require careful management of materials throughout the product lifecycle (Goetz et al., 2021). Extending service life reduces the frequency with which modules must be replaced, lowering demand for raw materials, manufacturing energy, transportation, and disposal. From this perspective, improving reliability is closely linked to reducing the environmental footprint of future photovoltaic technologies rather than simply increasing device efficiency.

These considerations are especially relevant in tropical and subtropical regions, where solar modules routinely operate at elevated temperatures reaching 340–350 K under high insolation, significantly exceeding the reference simulation temperature of 300 K (Diouf et al., 2022; Nobre et al., 2012). As demonstrated by our simulation results, operating in the 340–350 K range slightly enhances carrier extraction and initial efficiency when bulk defect density remains low ($N_t \leq 1 \times 10^{13} \text{ cm}^{-3}$). However, thermal stress drastically lowers the threshold for acceptable defect tolerance once trap density exceeds $\sim 1 \times 10^{14} \text{ cm}^{-3}$. Under such demanding operational climates in Sub-Saharan Africa or Brazil, controlling bulk defect formation during fabrication becomes the decisive factor in preventing accelerated

thermal degradation and maintaining long-term energy yield. The reliability phase diagram therefore provides more than a graphical summary of simulation results. At the lowest defect density ($1 \times 10^{10} \text{ cm}^{-3}$), the PCE increased from 23.85% at 300 K to 24.29% at 350 K, representing an increase of approximately 1.85%, before decreasing slightly to 24.01% at 400 K. It offers practical guidance for selecting manufacturing tolerances and operating conditions that are compatible with long-term field deployment in demanding climates.

Reliable lead-free perovskite solar cells can also contribute to wider sustainability objectives. Increasing operational lifetime improves lifetime energy yield, lowers maintenance costs, and enhances the economic attractiveness of photovoltaic systems in both developed and developing regions (Peters & Sinha, 2021). These benefits support ongoing efforts to expand renewable-energy use while reducing unnecessary resource consumption and greenhouse-gas emissions, thereby contributing to Sustainable Development Goals 7, 12, and 13 (Tian et al., 2025). In this context, the proposed reliability framework should be viewed not simply as a modelling exercise but as a decision-support approach that links device design with the broader goals of environmentally sustainable and climate-resilient energy systems.

Although the proposed reliability framework provides useful engineering guidance, it is based on steady-state SCAPS-1D simulations and considers only the combined effects of operating temperature and bulk defect density. Other degradation mechanisms, including moisture exposure, ultraviolet irradiation, mechanical stress, ion migration, and long-term ageing, were not explicitly considered. Consequently, the identified reliability boundaries should be regarded as practical design guidelines rather than universal operating limits. Future studies combining accelerated ageing experiments with numerical modelling would further strengthen the predictive capability of the proposed approach.

CONCLUSION

This study evaluated the combined impact of operating temperature (300–400 K) and bulk defect density (1×10^{10} – $1 \times 10^{17} \text{ cm}^{-3}$) on the photovoltaic performance and operational reliability of a Front contact/SnO₂/FASnI₃/CuI/Back contact lead-free perovskite solar cell using SCAPS-1D simulations. The results demonstrate that the optimized device maintains thermal stability across the investigated temperature range at low bulk defect densities (1×10^{10} – $1 \times 10^{13} \text{ cm}^{-3}$). However, once the defect density exceeds $\sim 1 \times 10^{14}$ – $1 \times 10^{15} \text{ cm}^{-3}$, power conversion efficiency declines

rapidly due to enhanced Shockley–Read–Hall trap-assisted recombination. Sensitivity analysis further confirmed that bulk defect density ($S_n = -2.41\%$ per decade) exerts a significantly stronger influence on performance degradation than operating temperature ($S_t = 1.68 \times 10^{-3} \% K^{-1}$).

The introduction of the defect–temperature reliability phase diagram provides a practical framework for mapping operational boundaries into Robust, Reliable, Critical, and Failure regimes based on normalized efficiency thresholds. Practically, these findings indicate that defect mitigation and control during synthesis and fabrication are critical for achieving long-term stability, particularly for photovoltaic systems deployed in high-temperature or tropical climates where elevated thermal conditions are unavoidable. Defining these safe operating limits supports quality control, enhances module service life, and promotes sustainable deployment of lead-free perovskite technologies.

To advance the predictive scope of this framework, future research should integrate additional real-world stress factors into the modeling environment, such as moisture exposure, ultraviolet radiation, mechanical stress, ion migration, and long-term chemical degradation. Furthermore, combining numerical simulations with empirical accelerated ageing experiments will be essential to validate the theoretical reliability boundaries under field-relevant conditions.

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