

Sensitivity-Based Performance Optimisation of a Lead-Free Formamidinium Tin Iodide (Fasni₃) Perovskite Solar Cell Using Scaps-1d Simulation

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ABSTRACT

This work presents a design and simulation framework for the multi-parameter optimization of a lead-free Perovskite Solar Cell (PSC) with an FTO/CeO₂/FASnI₃/CuI structure. It focuses on the device parameters that influence operational stability. Using the Solar Cell Capacitance Simulator One-Dimension (SCAPS-1D) (version 3.3.12), the study first verified the baseline performance of the device. Six parameters, previously optimized for efficiency, were re-evaluated and categorized into fixed design parameters set during fabrication and those susceptible to drift through known FASnI₃ degradation pathways. Normalized sensitivity coefficients were then calculated from the simulation sweeps. The results showed a baseline Power Conversion Efficiency (PCE) of 22.04%, an open-circuit voltage (Voc) of 0.9843V, a short-circuit current density (Jsc) of 26.01 mA/cm², and a fill factor (FF) of 86.12%. Following multi-parameter optimisation of bandgap, absorber thickness, and back-contact work function, the device achieved an optimised PCE of 24.85%, with a Voc of 0.9307 V, a Jsc of 30.65 mA/cm², and an FF of 87.10%. Sensitivity analysis revealed that electron affinity is the most influential factor on PCE, with roughly 19 percentage points per eV, followed by acceptor density (about 0.57 percentage points per decade) and defect density (around 0.20 percentage points per decade). The study highlights interfacial electron affinity control as a priority for enhancing device stability, since among the parameters examined PCE proved most sensitive to drift in electron affinity; defect density, however, remains the parameter most likely to drift in practice through the known Sn²⁺ oxidation pathway. This evidence-based approach provides researchers and engineers a clear pathway toward designing more durable, lead-free perovskite solar cells.

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INTRODUCTION

Solar Photovoltaic (PV) has become the centre for renewable energy research due to its promise in reducing the dependence on fossil fuels and the broader transition from greenhouse energy sources (IEA, 2025). Among the emerging PV technologies, halide perovskites, existing in ABX₃ crystal structure with A as a large organic or inorganic cation, B as a smaller metal cation and X as a halide anion, have recently attracted the attention of the PV community due to their high absorption coefficients, long carrier diffusion lengths, and flexible and ultra-thin device formats (Nordin et al., 2021; Roy et al., 2020). Certified efficiencies for lead-based Perovskite Solar Cells (PSCs) now approach 25.7%, rivalling silicon PV (Shah et al., 2023). Tin (Sn)-based, lead-free perovskites and Formamidinium (FA)-based compositions have emerged as comparatively stable and less toxic alternatives to lead halides (Shah et al., 2020), Positioning FASnI₃ as one of the more promising lead-free absorber candidates.

Many SCAPS-1D studies in recent years have explored FASnI₃-based device architectures pursuing higher efficiency. For instance, Abdelaziz et al. (2020) successfully optimised and experimentally fabricated FASnI₃-based solar cells with a performance efficiency of 14.03%, an FF of 67.74%, a Jsc of 22.65 mAcm⁻², and a Voc of 0.92V. Similarly, Chabri et al. (2023) reported an optimised PCE of 18.11%, an FF of 74.22%, a Jsc of 26.9 mAcm⁻², and a Voc of 0.907V. Manga et al. (2024) modelled a free-hole-transport-layer FASnI₃ device employing C60 as the ETL, reporting a PCE of 17.38%. Again, Jalaludin et al. (2025) also

reported the following optimised device parameters: a PCE of 19.56%, an FF of 72.62%, a Jsc of 29.74 mAcm⁻², and a Voc of 0.91 V. Before that, a study by Rehman et al. (2024) reported an optimised PCE of 24.87%, an FF of 87.10%, a Jsc of 30.68 mAcm⁻², and a Voc of 0.9308V.

Despite this progress, the widespread adoption and commercialisation of PSCs face two related problems; the inherent toxicity of lead and the operational stability of the commonly used materials (Sanni et al., 2026), a challenge that is conceptually distinct from, and not simply a consequence of, low PCE (Shukla et al., 2021). Many of the highly efficient lead-free designs reported in the literature depend on Spiro-OMeTAD and TiO₂ as HTL and ETL, respectively. However, Spiro-OMeTAD requires lithium and chemicals such as 4-tert-butylpyridine and Li-TFSI dopants to reach maximum usable hole mobility, which are hygroscopic and widely known for rapid degradation behaviour (Khawaja et al., 2025). Similarly, compact TiO₂ requires sintering around 500 °C, which is incompatible with flexible substrates and could cause thermal stress at interfaces (Bhandari et al., 2025). This study addresses this by investigating the transport-layer chemistry that limits long-term stability, which prior studies have not examined: whether their reported parameters also reduce solar cell degradation.

This study addresses the problem by pairing FASnI₃ with CuI and CeO₂ as HTL and ETL, respectively; both are inorganic, dopant-free, can be processed at low temperatures and have been reported to slow moisture ingress at the HTL/Absorber interface, which limits the operational lifetime in perovskite devices (Dong et al., 2023; Khawaja et al., 2025; Rehman et

al., 2024). The choice of transport layers is treated as a stability decision rather than a purely efficiency-driven one. The study also aims to simulate and determine whether a stability-motivated FTO/CeO₂/FASnI₃/CuI architecture can yield a competitive PCE and to identify which device design parameters exert the greatest influence on recombination-related performance loss, via steady-state SCAPS-1D sweeps rather than direct simulation of degradation kinetics.

Background Theory

SCAPS-1D solves the Poisson (1) and continuity equations (2 and 3) for electrons and holes, returning the current-density voltage (J-V) characteristics with the PCE, FF, J_{sc} and Voc, as can be seen below.

$$\frac{d}{dx} \left[\epsilon(x) \frac{d\psi}{dx} \right] = q[p(x) - n(x) + N_D(x) - N_A(x) + P_t(x) - n_t(x)] \quad (1)$$

$$\left(\frac{1}{q} \right) \left(\frac{\partial J_p}{\partial x} \right) + R p(x) - G(x) = 0 \quad (2)$$

$$-\left(\frac{1}{q} \right) \left(\frac{\partial J_n}{\partial x} \right) + R n(x) - G(x) = 0 \quad (3)$$

where $\epsilon(x)$ is the permittivity, ψ is the electrostatic potential, q is the elementary charge, P and n are the free carrier densities, N_D and N_A are ionised donor and acceptor densities, P_t and n_t are the trapped carrier densities, J_p and J_n are the current densities, R is the recombination rate, and $G(x)$ is the optical generation rate (Mehrabian et al., 2024). Recombination mechanisms included are radiative band-to-band, Auger, and SRH trap-assisted recombination. The modified diode equation incorporating parasitic resistances is:

$$J = J_p h - J_o \left[\exp \left(\frac{q(V + J R_s)}{n k T} \right) - 1 \right] - \left(\frac{V + J R_s}{R_{sh}} \right) \quad (4)$$

Where $J_p h$ is the photocurrent density, J_o is the dark saturation current, n is the ideality factor, k is Boltzmann's constant, and T is the temperature (Burgelman et al., 2000).

MATERIALS AND METHODS

The designed architecture follows an n-i-p configuration, of FTO/CeO₂/FASnI₃/CuI, matching the structure of (Rehman et al., 2024). The table below contains the baseline electrical parameters for each layer.

Table 1: Baseline Parameters Used for Each Layer of the FTO/CeO₂/FASnI₃/CuI/Au Device

Parameter	CuI	FASnI ₃	CeO ₂	FTO
Bandgap (eV)	3.1	1.45	3.5	3.5
Thickness (μm)	0.1	0.45	0.45	0.4
Electron Affinity (eV)	2.1	4	4.6	4.3
Electron Mobility (cm ² /Vs)	1.0×10^2	2.2×10^1	1.0×10^2	2.0×10^1
Hole Mobility (cm ² /Vs)	4.39×10^1	2.2×10^1	2.5×10^1	1.0×10^1
Acceptor Density NA (cm ⁻³)	1.0×10^{18}	7.0×10^{16}	0	0
Defect Density Nt (cm ⁻³)	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	—
Dielectric Permittivity (ε)	6.5	8.2	9	9
Electron Thermal Velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Hole Thermal Velocity	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Capture Cross Section for Electrons and Holes	1.0×10^{19}	—	—	—

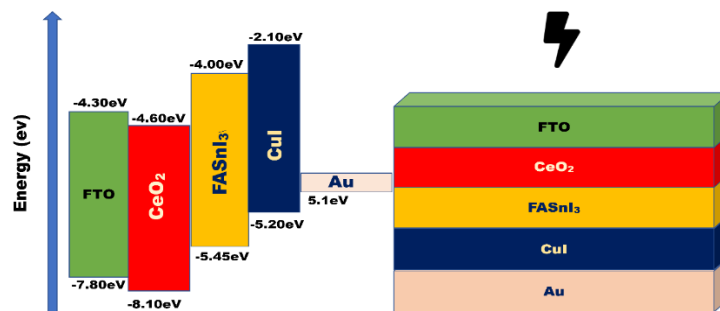


Figure 1: (a) Energy Band Structure and (b) the Solar Cell Structure

The device was modelled using the Solar Cell Capacitance Simulator One-Dimension (SCAPS-1D), a widely used software for thin-film perovskite solar cells, developed by the University of Ghent in Belgium, following the governing equations presented in Section 2. Simulations were conducted under AM 1.5G illumination (100mW/cm² and 300 K); the baseline device performance was first confirmed.

RESULTS AND DISCUSSION

This section presents and discusses the SCAPS-1D simulation results. The following subsections (3.1 to 3.6) examine, one at a time, how the six device parameters, comprising three fixed design parameters (bandgap, thickness, and back contact) and three operationally drifting parameters (electron affinity, acceptor density, and defect density), affect the PCE, Voc, J_{sc}, and FF. Section 3.7 then combines the most favourable settings identified from these sweeps into an

optimised device, whose resulting energy band alignment is examined in Section 3.8. Section 3.9 closes the discussion with a quantitative sensitivity ranking that identifies which parameter most strongly governs the device's long-term stability.

Impact of Perovskite Layer Bandgap (Design Parameter)

The bandgap of the absorber layer was varied from 1.37 to 1.45eV. As the bandgap increases, the PCE rises, then decreases, followed by a small rise, then another steep decline. The FF and the Voc consistently rise with increasing bandgap. The J_{sc} show a consistent drop as the bandgap increases from 1.37 to 1.45eV. This clearly indicates that changing the bandgap affects light absorption and the overall optical performance of the solar cell, as shown in Figure 2 below.

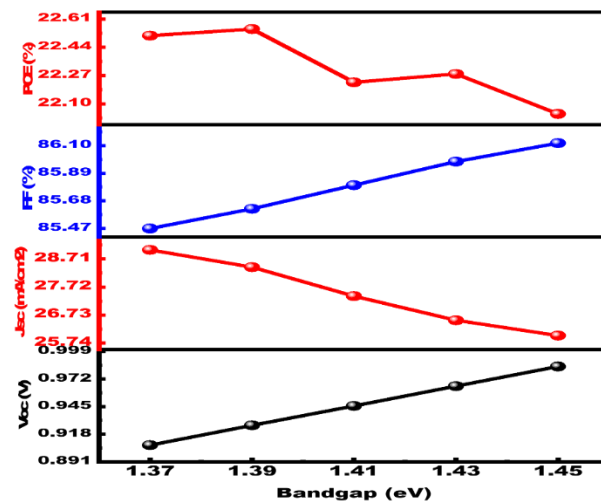


Figure 2: Impact of Perovskite Layer Bandgap on PCE, FF, Jsc, and Voc

At 1.39 eV, the efficiency peaks, with a Voc of 0.9267 V, an FF of 85.62%, and a Jsc of 28.42 mAcm⁻², representing

optimal performance. The remaining points show increased recombination losses.

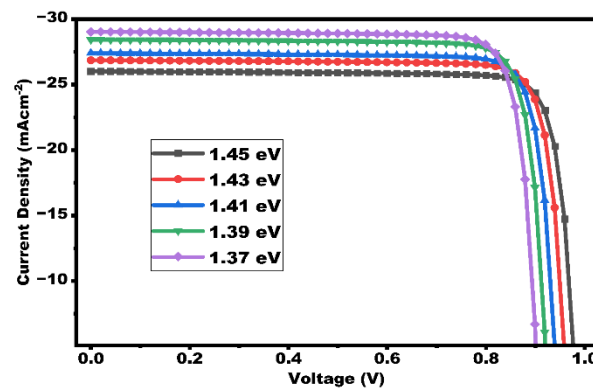


Figure 3: J-V Curves for Perovskite Bandgap Values from 1.37 to 1.45 eV

Impact of Perovskite Layer Electron Affinity (Operational Drift Parameter)

The next parameter varied was the electron affinity, which determines the minimum energy required to lift an electron from the absorber layer's conduction band to the transport layer; it governs the valence band offset at the absorber-transport layer interface. It's varied from 3.6 to 4.0 eV while keeping the remaining parameters fixed. The FF declined from 86.12% to 82.02%; similarly, the open-circuit voltage

decreased from 0.9843 to 0.6684 V, and the PCE fell from 22.04% to 14.45%, while the Jsc increased significantly from 26.01 to 26.36 mAcm⁻².

This clearly shows a stability-signature trend: decreasing the affinity shift alters the energy level alignment at the upper boundary, increasing recombination while decreasing the potential difference for charge separation. The marginal Jsc gain was insignificant relative to the Voc and FF losses, as shown in Figure 4 below.

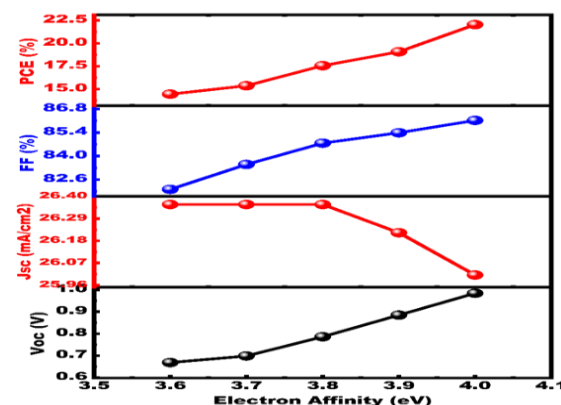


Figure 4: Impact of Perovskite Absorber Electron Affinity on Key Solar Cell Parameters

The current recombination stays low at low bias but rise sharply around 0.7V, which marks the point at which the bias supplies sufficient energy and overcome the degraded interfacial barrier and drive a burst electron-hole recombination, which shows that the lower the electron

affinity values shift onset to progressively the lower the voltages, this clearly means the device become recombination dominance earlier in its operation as can be seen on the figure 5 below.

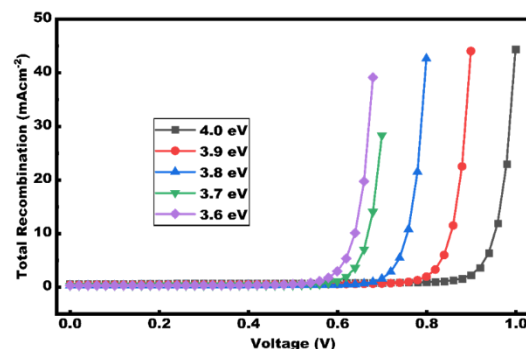


Figure 5: Total Recombination for Different Electron Affinity of the Perovskite Layer

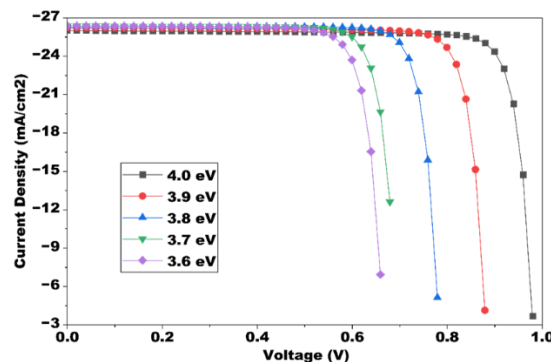


Figure 6: J-V Curves for Different Electron Affinity

The device current density (J_{sc}) at lower voltage showed similar behaviour for each electron affinity value, then dropped sharply past the same recombination onset identified in the figure. With 4.0 eV as the baseline unmodified electron affinity of FASnI₃, all values increase the recombination rate; the highest PCE recorded in this sweep is 22.04% and coincides with the value that minimises interface-driven recombination (Ding et al., 2018). As stated in 3.9, this is the steepest parameter sensitivity found in this study, which suggests and motivates interfacial passivation rather than only bulk defect control as a priority stability target (Mohamad Noh et al., 2026).

Impact of Perovskite Layer Acceptor Density, N_A (Operational Drift Parameter)

Acceptor density, or doping concentration is another parameter prone to operational drift that directly sets the density of ionised dopant available to establish the device's built-in electric field. Because dopant loss through ion migration or dopant deactivation is a documented ageing pathway in halide perovskites, we treat this sweep as a second operationally drift-prone parameter. N_A was varied from 1×10^{16} to $1 \times 10^{17} \text{ cm}^{-3}$. Over this range, PCE fell from 22.04 to 19.79%, V_{oc} from 0.9843 to 0.9708V, FF from 86.12 to 77.11%, while J_{sc} rose only slightly from 26.01 to 26.44 mA cm^{-2} .

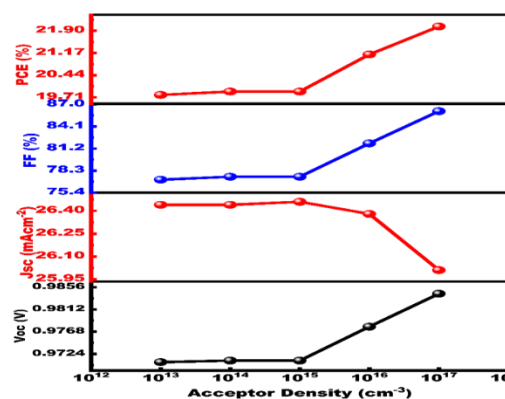


Figure 7: Impact of Perovskite's Layer Acceptor Density on PCE, FF, V_{oc} , and J_{sc} .

The electron affinity was varied as an independent, static parameter in a steady-state sweep, the simulation does not establish the rate or trajectory by which it would actually drift during device operation and the result above should be read as an assessment of PCE sensitivity to impose variation instead of degradation prediction over time.

The Voc trend follows the built-in potential directly; the higher the NA, the higher the density of the ionised dopants spanning the junction, raising the built-in field and Voc, while a lower NA reduce it (Rehman et al., 2024). The FF declines as NA falls; more stable observation: fewer dopants mean

fewer immobile charge centres to screen the field, so a larger share of the recombination that does occur proceeds through trap-assisted channels rather than being suppressed by a strong internal field. The modest Jsc increase at low NA likely reflects fewer dopant-associated recombination centres, but this is not enough to offset the trap-driven FF and Voc losses (Rehman et al., 2024). On this note, NA is $1 \times 10^{16} \text{ cm}^{-3}$ retained as optimal, yielding a PCE of 22.04%, a FF of 86.12%, a Jsc of 26.01 mA cm^{-2} , and a Voc of 0.9843V.

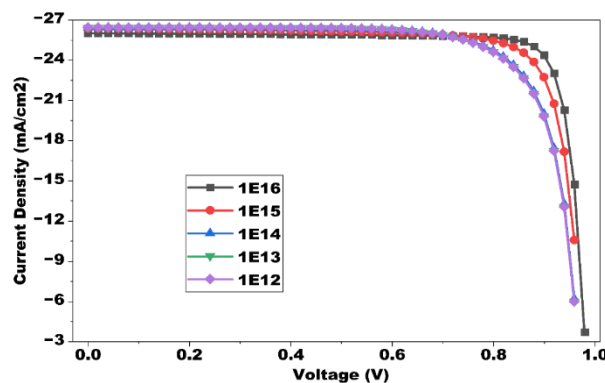


Figure 8: J-V Curves for Perovskite Acceptor Density (NA) from 1×10^{16} to $1 \times 10^{12} \text{ cm}^{-3}$

Like the electron affinity, the acceptor density was swept as a static parameter over a steady-state range, real dopant loss through ion migration or deactivation would occur gradually during operation, a time-dependent process this analysis does not simulate. The sensitivity value reported above therefore indicate show exposed PCE is to acceptor density loss, not the timescale over which such loss would occur.

Impact of Perovskite Layer Thickness (Design Parameter)

Absorber thickness is set once during deposition and, barring gross mechanical or chemical degradation of the absorber, is not expected to change materially during the device's operation; it is treated here as a design parameter. Nonetheless, it affects both light absorption and the physical distance a carrier must travel before recombining or being collected. The thickness was varied from 450 to 650 nm (Kumar et al., 2026). The Voc rose from 0.9843 to 0.9855 V,

the Jsc from 26.01 to 27.56 mA cm^{-2} , and the PCE from 22.04 to 23.34 %, while the FF fell slightly from 86.12 to 85.94 %.

The PCE gain with thickness reflects increased optical absorption, since a thicker film absorbs a larger fraction of incident light and the quarter-wavelength optical interference condition additionally aids light-trapping at some thicknesses; this is distinct from a genuine reduction in recombination losses. Indeed, increasing thickness can also increase bulk recombination, depending on the minority-carrier diffusion length relative to the absorber thickness and on the defect density, so the net PCE gain reported here reflects optical absorption gains outweighing this transport/recombination trade-off over the tested range, rather than thickness itself suppressing recombination (Ayyappa et al., 2026). The FF reduction reflects a small increase in series resistance as the transport path lengthens.

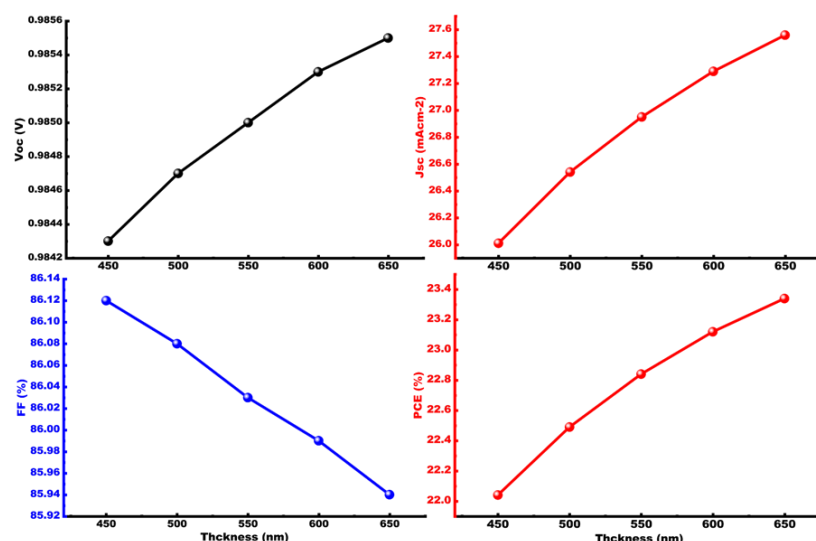


Figure 9: Impact of Perovskite Layer Thickness on the PCE, FF, Jsc, and the Voc

Recombination current stays low and stable for all thicknesses tested up to roughly 0.8 V, after which it rises sharply; thicker films show marginally higher recombination current at the highest voltages, indicating that although thicker absorbers reduce recombination losses overall, they can be more

susceptible to recombination under high-voltage operating conditions specifically (Kadhem et al., 2026). On balance, 650 nm, close to a quarter-wavelength condition for a relevant portion of the solar spectrum, was retained as the optimal thickness.

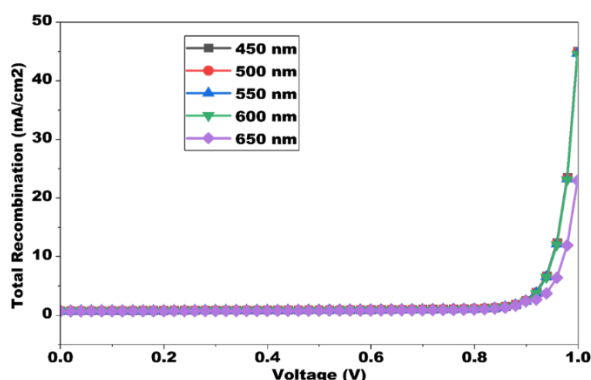


Figure 10: Total Recombination Current for Perovskite Layer Thicknesses from 450 to 650 nm

Impact of Perovskite Layer Defect Density, N_t (Operational Drift Parameter)

Defect density (N_t) is often considered the population of impurities, interstitials, and vacancies within the absorber layer and is often considered the most direct impact parameter tied to trap-assisted recombination and, mechanistically, the clearest single stability lever examined in this study, since N_t is known to increase over time in fabricated FASnI₃ devices

as Sn²⁺ oxidation Sn⁴⁺ (Abdul Karim et al., 2023; Li et al., 2022). Varied from 10¹⁵ to 10¹¹ cm⁻³, positioned 0.6 eV above the valence band edge with all other parameters held fixed. As N_t falls, every headline parameter improves in step. The PCE rises from 22.04 to 22.85 %, the Voc from 0.9843 to 0.9865 V, the FF from 86.12 to 87.62 % and the Jsc from 26.01 to 26.44 mAcm².

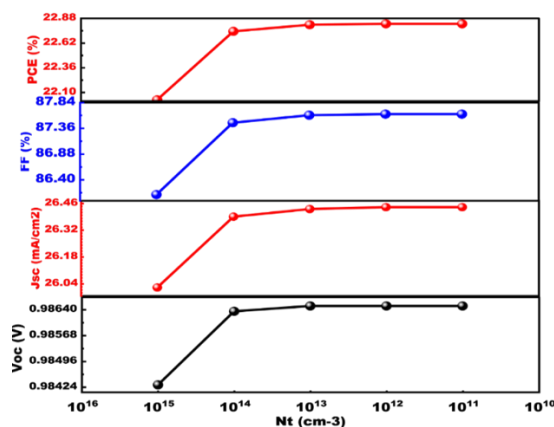


Figure 11: Impact of Varying Defect Density (N_t) on PCE, FF, Jsc, Voc

This is the only sweep in the study where every move is in the favourable direction simultaneously, since N_t has no compensating trade-off comparable to the bandgap/absorption or thickness/series resistance trade-offs seen elsewhere. As quantified in section 4.9, however, the measured PCE sensitivity to N_t over this already-low baseline range (10¹⁵-10¹¹ cm⁻³) is comparatively shallow, a reflection of the fact that the CeO₂/CuI transport layer pair already places the baseline device in a low-defect, well-passivated operating regime, not evidence that N_t is unimportant. In a fabricated device, N_t is not a free parameter but a direct proxy for how well precursor purity, film crystallisation, and interface passivation have been controlled for FASnI₃ specifically; higher defect density is closely tied to Sn²⁺ oxidation, which generates tin vacancies that act as deep recombination centres and can accelerate further decomposition of the absorber (Abdul Karim et al., 2023;

Pesci et al., 2025). This sweep therefore quantifies, in simulation, the performance headroom that experimental antioxidant precursor additives such as SnF₂ or reductive additives are already known to recover by suppressing Sn²⁺ oxidation during film formation (Abdul Karim et al., 2023; Li et al., 2022).

Varying Back Contacts (Design Parameter)

The back-contact metal is a one-time fabrication choice; aside from the interfacial chemical reaction discussed below, it is not expected to change materially during operation and is treated as a design parameter. The back-contact was selected by comparing the work functions of different materials: Gold (Au), Tungsten (W), Copper (Cu), and Silver (Ag), 5.1 to 4.26 eV. While Au, W, and Cu produced comparable Voc, Jsc, FF and PCE, Ag, with the lowest work function, produced degraded performance across every device parameter.

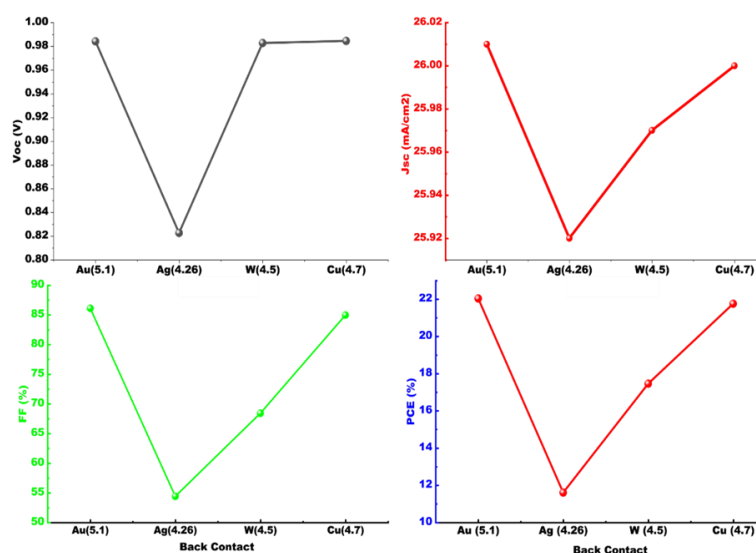


Figure 12: Impact of Different Back-Contact Work Functions (Au, W, Cu, Ag) on PCE, FF, Jsc, and Voc

Higher work function contacts reduce the reverse saturation current through a stronger extraction field, and materials such as Au also improve optical performance by reducing reflection losses at the back interface. The recombination versus voltage behaviour of each contact reinforces this

reading, and high work function contacts maintain low recombination even at high forward bias, while the low work function Ag contact shows an early steep rise in recombination current.

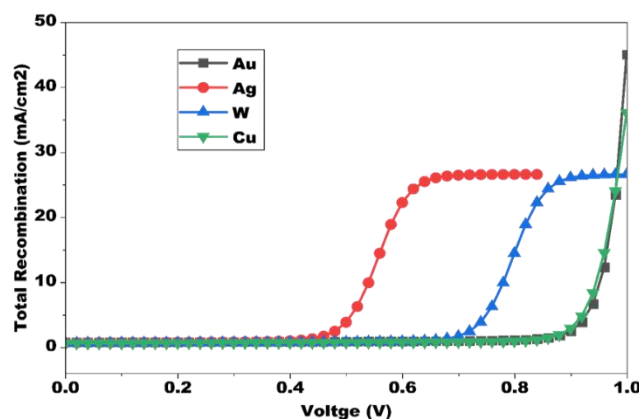


Figure 13: Total Recombination Current for Different Back-Contact Metals (Au, W, Cu, Ag)

A further, specific consideration favours a higher work-function metal contact design choice, with some bearing on stability. Au and similar noble or rare-noble metals do not react with the CuI or perovskite layers beneath them, whereas more reactive lower work function metals carry a greater risk of interfacial chemical degradation over time. On this combined electronic and chemical basis, contacts with a work function exceeding 5.1 eV, Au being identified in this design as the optimal over other high work function candidates.

Device Optimisation

Combining the settings as identified in the preceding sweep, the defect density reduced to $1 \times 10^{12} \text{ cm}^{-3}$, bandgap narrowed to 1.39 eV, and the absorber increased to 650 nm, with the dopant free CeO_2/CuI transport layer pair and an Au back contact held fixed throughout, the optimized device delivered a simulated power conversion efficiency of 24.85%, together with an open-circuit voltage of 0.9307V, a short-

circuit current density of 30.65 mA cm^{-2} , and a fill factor of 87.10%, a marked improvement over the unoptimized baseline of 22.04% PCE, 0.9843V, 26.01 mA cm^{-2} , and 86.12% FF reported earlier in this study. This gain was achieved entirely through informed parameter selection, tightening the defect density, bandgap, and absorber thickness to their identified optima, rather than through the introduction of new materials or additional interfaces, underscoring that the existing dopant-free CeO_2/CuI transport layer pair, once its governing parameters are properly tuned, is capable of markedly stronger performance without added fabrication complexity. Notably, this improvement occurred despite the Voc falling from 0.9843 to 0.9307V (-0.0536V, -5.4%); the net PCE gain was predominantly by a 17.8% relative to rise in Jsc (26.01 to 30.65 mA cm^{-2} , +4.64 mA cm^{-2}), together with a modest FF gain (+0.98 percentage points), which together outweighed the Voc loss.

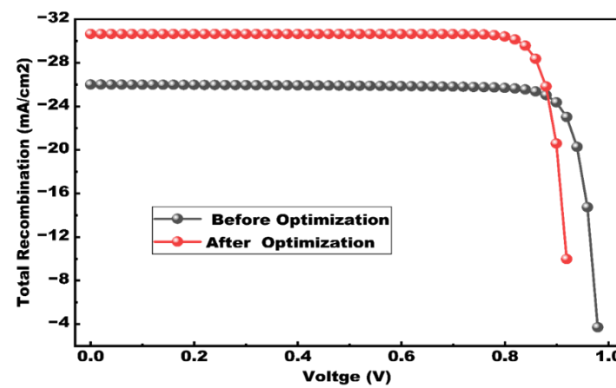


Figure 14: R-V Curves of the Device Before and After Optimisation

Table 4: Simulated Device Performance Before and After Optimisation

Parameter	Before optimization	After optimization
Jsc (mA/cm ²)	26.01	30.65
Voc (V)	0.9843	0.9307
FF (%)	86.12	87.10
PCE (%)	22.04	24.85

Energy Band Alignment Before and After Optimisation

The interface configuration between ETL and absorber and between Absorber and HTL is a direct determinant of interfacial recombination over time, interfacial degradation is discontinuous drop (cliff) in the conduction or valence band

at an interface creates a local trap-like region where carriers accumulate and are more likely to recombine non-radiatively, while small, continuous step (spike) acts as a partial barrier that blocks the unwanted carrier type without materially impeding extraction of the wanted one.

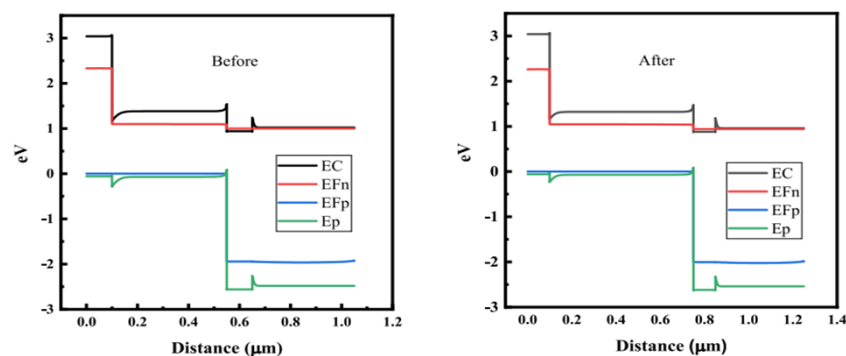


Figure 15: Energy Band Alignment of the Device Before and After Optimisation

Quantitative Sensitivity Ranking and Defect-Tolerance Benchmarking

Sections 3.1-3.6 examined and reported six parameters together; three parameters classified above are exponentially drifting parameters; electron affinity, acceptor density, and defect density are all directly computed by computing the normalised sensitivity coefficient from the sweep data in each

case; for the electron affinity, the sensitivity is expressed as the percentage points of the PCE per eV for both the NA and Nt per concentration. The bandgap, thickness, and back-contact metal are fixed design parameters in this study classification and are not assigned comparable coefficients, since they are not expected to drift after fabrication.

Table 5: Normalised Sensitivity Ranking of the Computed from the Sweep Data

Parameter	Range tested	Δ PCE (pp)	Normalized sensitivity	Degradation link
Electron affinity, χ (eV)	4.0 $\rightarrow$ 3.6	-7.60	≈ 19.0 pp per eV	Interfacial reaction/oxide growth at ETL
Acceptor density, NA (cm ⁻³)	$1 \times 10^{16} \rightarrow \times 10^{12}$	-2.26	≈ 0.57 pp per decade	Dopant loss/ion migration
Defect density, Nt (cm ⁻³)	$10^{15} \rightarrow 10^{11}$	+0.81	≈ 0.20 pp per decade (over this low baseline range)	Sn ²⁺ $\rightarrow$ Sn ⁴⁺ oxidation

Ranked by measured sensitivity alone, electron affinity is by far the steepest lever, with a 0.4 eV shift producing ten times the PCE loss per unit parameter change of the shifts in NA or Nt. Taken at face value, this would suggest that interfacial band-offset control is the single most important stability

target in this device. However, this ranking must be read alongside how readily each parameter actually drifts in a real device. Electron affinity at a well-formed CeO₂/FASnI₃ interface is set largely by the intrinsic properties of the two materials and is not expected to shift rapidly unless a chemical

reaction occurs at that interface; in contrast, N_t is documented to increase specifically and measurably over time in FASnI₃ films through Sn^{2+} oxidation (AbdulKarim et al., 2023.; Pesci et al., 2025), meaning that the device is virtually certain to move along the N_t axis of Fig. 11 as it ages, even though the measured slope that exists is the shallowest of the three at the low N_t baseline tested here.

This reconciles the two readings from the electron affinity, which has the steepest sensitivity but the least established real-world drift mechanism at a chemically stable interface; however, N_t has the shallowest measured sensitivity in this low-defect regime but the best-documented real-world drift mechanism. N_A sits between the two on both axes. The practical implication is that the choice of CeO_2/CuI transport layers, which is reported to slow interfacial chemical reaction relative to $\text{TiO}_2/\text{Spiro-OMeTAD}$ (Bhandari et al., 2025; Dong et al., 2023; Khawaja et al., 2025) is well matched to the parameter this device is most sensitive to (electron affinity), while the well-documented Sn^{2+} oxidation pathway acting on N_t remains the parameter most likely actually to move during real-world ageing and therefore the parameter for which experimental antioxidant strategies (AbdulKarim et al., 2023.; Li et al., 2022) offer the most direct literature-supported route to preserving the simulated performance reported here over time. This sensitivity ranking is derived entirely from steady-state SCAPS-1D sweeps at fixed parameter values; it identifies which parameters would matter most if they were to drift and should not be read as a prediction of an operational lifetime, degradation rate, or time constant, none of which were simulated in this study.

It is worth mentioning that, the optimised PCE obtained as 24.85% is close to the reported 24.87 by Rehman et al. (2024) due to similarity in the structured FASnI₃ device. The present work builds $\text{FTO}/\text{CeO}_2/\text{FASnI}_3/\text{CuI}$ dopant free transport layer architecture matching that of Rehman et al. and a comparable baseline parameter set, a close efficiency is not surprising rather than a novel finding in itself. The contribution of the present study is therefore not the optimised efficiency figure rather, it is twofold. First, it provides a reference designed demonstrating that fully inorganic dopant free CeO_2 and CuI can be paired with FASnI₃ to reach efficiencies competitive with matching architectures reliant on doped or organic contacts such as Spiro-OMeTAD, without added fabrication complexity. Second, and more central, the study layers quantitative sensitivity ranking on top of the efficiency results by classifying the device parameters as fixed design and operationally drift-prone and computing normalised sensitivity coefficients for the latter, it also identifies which parameters require tight fabrication control versus which merely require the device be kept within limited operational drift envelope or post fabrication (acceptor density) whose lower simulated sensitivity does not diminished their practical importance given their well-established real-world degradation pathways. This sensitivity-based framing rather than the efficiency itself as what the present work adds beyond prior FASnI₃ SCAPS-1D optimisation studies.

CONCLUSION

This study successfully examined a stability-motivated $\text{FTO}/\text{CeO}_2/\text{FASnI}_3/\text{CuI}$ architecture, built on the dopant-free, low-temperature processable CuI/CeO_2 transport layer pairing, which delivered competitive PCE. This was achieved by first confirming the baseline device performance, a PCE of 22.04%, a V_{oc} of 0.9843V, a J_{sc} of 26.01 mAcm^{-2} , and a FF of 86.12%, and then tuning fixed design parameters (bandgap, absorber thickness, back-contact work function) to identify

their optima, which raised the simulated PCE to 24.85% alongside a V_{oc} of 0.9307V, a J_{sc} of 30.65 mAcm^{-2} and a FF of 87.10%. This gain was achieved entirely through informed parameter selection, rather than through introducing new materials or additional interfaces. It was possible because the existing dopant-free CeO_2/CuI transport layer pair already placed the device in a favourable operating regime once its governing parameters were properly tuned.

The study also successfully examined which device parameters exert the greatest influence on recombination related performance loss rather than directly simulating degradation kinetics. This was obtained by carefully separating the six device parameters into fixed design parameters and operationally drift-prone parameters tied to documented FASnI₃ degradation chemistry, then computing the normalised sensitivity coefficient for the latter three, electron affinity, acceptor density, and defect density, from the sweep data. Electron affinity exhibited the highest simulated PCE sensitivity among the three assumed drift-prone parameters, at approximately 19 percentage points per eV, well ahead of acceptor density at approximately 0.57 percentage points per decade and defect density at approximately 0.20 percentage points per decade over the tested low defect range. Nevertheless, defect density remains the parameter with better established real-world degradation mechanism through Sn^{2+} oxidation and its lower simulated sensitivity should not be read as evidence that it is the less important variable in practice. This result arose because the CeO_2/CuI transport layer pair already constrains the baseline device to a low-defect, well-passivated regime.

That regime compresses the measured defect-density sensitivity, despite its well-documented Sn^{2+} to Sn^{4+} oxidation pathway, and makes the interfacial band-offset at the $\text{CeO}_2/\text{FASnI}_3$ junction a more consequential performance lever.

This finding was reinforced by examining the energy-band alignment before and after optimisation. The same parameter combination that maximised PCE also reduced the interfacial cliffs at both the ETL/Absorber and Absorber/HTL junctions, consistent with, though not direct proof of, lower interfacial recombination. This was because the tuned defect density, bandgap, and absorber thickness worked together to smooth the band offsets at both the interfaces, rather than any single parameter acting in isolation.

Overall, the study determined that the $\text{FTO}/\text{CeO}_2/\text{FASnI}_3/\text{CuI}$ architecture meets both stated aims. A competitive PCE was achieved without compromising the stability rationale behind the transport layer selection; electron affinity was identified as the parameter offering the greatest leverage over recombination-driven degradation, owing to its steep measured sensitivity relative to acceptor and defect density. Defect density control via antioxidant precursor additives, for instance, SnF_2 , remains the most experimentally tractable complementary route, due to a strong literature basis, even though its simulated sensitivity was comparatively shallow at the low-defect baseline tested here. As these findings were achieved entirely through steady-state SCAPS-1D sweeps rather than a time-domain or experimental ageing study, they should be read as identifying which design parameters matter most for stability, not as a quantitative prediction of device lifetime or degradation rate. Time-resolved degradation studies and experimental validation of the proposed sensitivity ranking are recommended as the natural next step. By identifying interfacial electron affinity control as the priority target, this work offers researchers and device engineers pursuing durable lead-free perovskite solar

cells a concrete, evidence-based roadmap towards achieving that stability.

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