

# Simulation Insights into Perovskite Active Layers for Enhancing Solar Cell Efficiency

Naeema Nazar <sup>1\*</sup>, Mohamed Kallel <sup>2</sup>, Rahma Sellami <sup>3</sup>, and Abdelhalim Hasnaoui <sup>4</sup>

<sup>1\*</sup>Assistant Professor, Department of Electronics and Communication Engineering, VISAT Engineering College, Kerala, India

Global Strategy Representative for India, IEEE Photonics Society, USA

naeemanazarcn@gmail.com, <https://orcid.org/0009-0007-6768-2842>

<sup>2</sup>Assistant Professor, Department of Physics, College of Science, Northern Border University, Arar, Saudi Arabia

Mohamed.kallel@nbu.edu.sa

<sup>3</sup>Assistant Professor, Department of Computer Science, Applied College, Northern Border University, Saudi Arabia

Rahma.ali@nbu.edu.sa

<sup>4</sup>Assistant Professor, Mathematics Department, College of Sciences and Arts, Northern Border University, Rafha, Saudi Arabia [abdllhalim.hasanawa@nbu.edu.sa](mailto:abdllhalim.hasanawa@nbu.edu.sa)

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## Abstract:

This study explores the performance of perovskite solar cells with various absorber materials, including MASnI<sub>3</sub>, CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub>, CsPbI<sub>3</sub>, and CsSnGeI<sub>3</sub>, analyzing key metrics such as efficiency, open-circuit voltage (V<sub>oc</sub>), short-circuit current density (J<sub>sc</sub>), and fill factor (FF). Simulations using SCAPS software provided baseline data, which were further validated and extended using advanced computational techniques. Sensitivity analyses revealed the impact of parameters like bandgap energy and carrier mobility, while layer optimization and circuit modeling offered insights into enhancing device performance. Comparative analysis and real-world simulations bridged the gap between lab results and practical applications, supported by machine learning models to predict efficiencies for novel materials. This comprehensive approach aids in optimizing perovskite solar cells for future applications.

**Keywords:** Photovoltaic Cell, Perovskite Absorbing Material, Performance Efficiency, Computational Techniques.

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## 1. Introduction

Solar energy, derived from the Sun's radiant light and heat, is harnessed using a variety of technologies, including photovoltaic cells, solar panels, and thermal collectors. As a renewable, clean, and abundant energy source, it provides significant advantages such as reducing greenhouse gas emissions, mitigating climate change effects, and promoting energy independence. Solar energy is versatile, with applications spanning electricity generation, water heating, and powering residential and commercial establishments. Advances in technology and declining costs have positioned solar energy as a cornerstone in the global shift towards sustainable energy solutions. Silicon-based solar cell technologies have historically dominated photovoltaic applications due to their advantageous properties. These include ease of surface passivation, cost effectiveness, durability, and resilience

under high temperatures. However, emerging alternatives, particularly those that promise reduced production costs and simpler manufacturing processes, offer compelling potential for replacing silicon in solar energy systems. Among these innovations, perovskite based solar cells have garnered significant attention for their high efficiency and cost-effective fabrication. In recent years, photovoltaic (PV) technologies have seen remarkable advancements driven by novel device architectures. Perovskite materials, in particular, have risen as a leading contender in solar cell technology. Known for their high absorption coefficients, optimal bandgaps, and long charge-carrier diffusion lengths, perovskite based devices deliver outstanding photovoltaic performance. These materials have become a viable alternative to traditional silicon, addressing challenges related to the latter's large size and high production costs. The typical structure of a perovskite solar cell comprises five essential layers: the perovskite absorber material, an electron transport layer (ETL), a hole transport layer (HTL), a transparent conductive layer, and a metal electrode. The perovskite layer, situated between the ETL and HTL, is integral to the cell's operation, facilitating the efficient generation and transport of charge carriers. This work focuses on evaluating the performance of various perovskite absorber materials, including methylammonium tin iodide ( $\text{MASnI}_3$ ), methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ), mixed halide methylammonium lead bromide iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_x\text{Br}_{1-x}$ ), cesium lead iodide ( $\text{CsPbI}_3$ ), cesium tin germanium iodide ( $\text{CsSnGeI}_3$ ), and methylammonium tin iodide ( $\text{CH}_3\text{NH}_3\text{SnI}_3$ ). Key performance parameters, such as efficiency, open circuit voltage, short circuit current, and fill factor, are analyzed within the framework of the perovskite solar cell design. These insights aim to highlight the most efficient perovskite material and further the development of high-performance solar technologies.

## 2. Study Framework

SCAPS-1D (Solar Cell Capacitance Simulator in One Dimension), version 3.3.07, is a versatile tool designed to simulate the behavior of solar cells. It incorporates principles of semiconductor physics, optics, and electrochemistry to analyze various aspects of device performance. Key features include modeling charge transport, energy band alignment, optical absorption, carrier generation and collection, device geometry, and the influence of interfaces. The software predicts critical performance metrics such as current-voltage characteristics and quantum efficiency by simulating factors like carrier mobility, recombination rates, and optical behavior. Figure 1 illustrates the SCAPS interface, highlighting its user friendly action panel. SCAPS employs numerical solutions to one dimensional semiconductor equations, including Poisson's equation, continuity equations, and transport equations, as depicted in Figure 2. It also incorporates various recombination mechanisms, enabling a comprehensive evaluation of solar cell dynamics. The simulation process accounts for photon absorption, electron-hole pair creation, and the movement and collection of carriers at the electrodes, providing an accurate representation of solar cell functionality. Moreover, SCAPS-1D provides users with the ability to define key material properties such as doping concentrations, defect states, and temperature effects, all of which significantly influence the solar cell's performance. The tool is highly flexible, enabling the simulation of various solar cell types, including single-junction and multi-junction designs, by adjusting parameters like layer thickness, bandgap, and recombination lifetimes. This adaptability allows for in-depth exploration and optimization of solar cell structures, making SCAPS-1D a powerful resource for investigating new materials and design approaches for enhanced device performance.

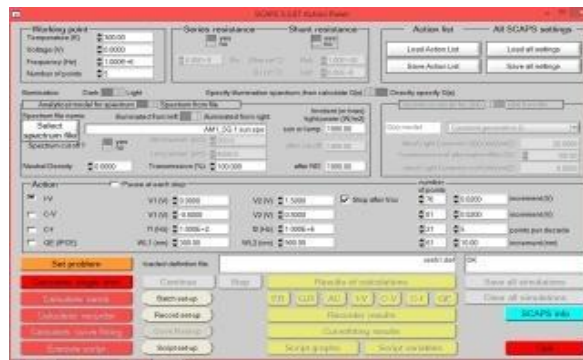


Fig. 1. Action Panel of SCAPS 3307

$$\frac{d^2 \phi}{dx^2} = -\frac{q}{\epsilon_s} (p - n + N_D^+ - N_A^-) \quad \text{Poisson's Equation}$$

$$J_p = -qD_p \frac{\partial p}{\partial x} + \mu_p q p \frac{\partial \phi}{\partial x} \quad \text{Hole Continuity Equation}$$

$$J_n = qD_n \frac{\partial n}{\partial x} + \mu_n q n \frac{\partial \phi}{\partial x} \quad \text{Electron Continuity Equation}$$

Fig. 2. Solar cell : Dimension Equation

### 3. Physical Framework

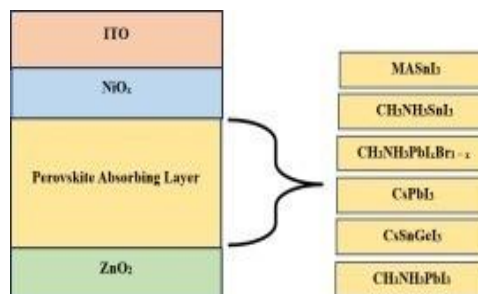


Fig. 3. Perovskite Solar Cell : Structure

Figure 3 illustrates the structural layout of a perovskite-based solar cell, which includes a perovskite absorber layer situated between two transport layers: the hole transport layer (HTL) and the electron transport layer (ETL). Materials such as NiOx and ZnO2 are utilized for these transport layers, along with an indium tin oxide (ITO) layer. The study incorporates various perovskite materials for comparison, including methylammonium tin iodide (MASnI3), methylammonium tin iodide (CH3NH3SnI3), mixed halide methylammonium lead iodide-bromide (CH3NH3PbIxBri1-x or MAPbIxBri1-x), cesium lead iodide (CsPbI3), cesium tin germanium iodide (CH3NH3PbI3 or MAPbI3). Each of these materials showcases unique properties and potential for photovoltaic applications. MASnI3 and CH3NH3SnI3, characterized by their methylammonium cations and tin iodide composition, exhibit excellent opto- electronic properties and are under investigation for solar cell development. The mixed halide perovskite MAPbIxBri1-x is notable for its iodide-bromide

composition, which contributes to its high power conversion efficiency, making it a popular choice in photovoltaic research. Cesium lead iodide (CsPbI<sub>3</sub>) stands out for its stability and desirable electronic attributes, enhancing its suitability for solar cell use. Cesium tin germanium iodide (CsSnGeI<sub>3</sub>) offers a tunable bandgap, making it a promising light-absorbing material. Lastly, MAPbI<sub>3</sub> is widely recognized for its exceptional efficiency and ease of processing, establishing it as one of the most extensively studied materials in perovskite solar cell research.

Parameters	Materials					
	MASnI <sub>3</sub>	CH <sub>3</sub> NH <sub>3</sub> SnI <sub>3</sub>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>2</sub> Br <sub>1-x</sub>	CsPbI <sub>3</sub>	CsSnGeI <sub>3</sub>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub>
X (µm)	0.6	1	0.32	0.8	0.8	0.9
E <sub>g</sub> (eV)	1.3	1.3	1.55	1.694	1.5	1.55
χ (eV)	4.1	4.17	3.9	3.95	3.9	3.9
r	8.2	10	6.5	6	28	6.5
N <sub>c</sub> (cm <sup>-3</sup> )	2.0E+18	1.0E+18	2.2E+18	1.1E+20	3.1E+18	1.8E+18
N <sub>v</sub> (cm <sup>-3</sup> )	2.0E+18	1.0E+19	1.8E+19	8.2E+20	3.1E+18	1.8E+19
V <sub>c</sub> (cm/s)	1.0E+7	1.0E+7	1.0E+7	1.0E+7	1.0E+7	1.0E+7
V <sub>v</sub> (cm/s)	1.0E+7	1.0E+7	1.0E+7	1.0E+7	1.0E+7	1.0E+7
µ <sub>e</sub> (cm <sup>2</sup> /Vs)	1.6	1.6	2	2.5E+1	9.74E+2	2.0E+2
µ <sub>h</sub> (cm <sup>2</sup> /Vs)	1.6	1.6	2	2.5E+1	2.13E+2	2.0E+0
N <sub>d</sub> (cm <sup>-3</sup> )	1.0E+18	1.0E+17	1.0E+15	1.0E+15	1.0E+14	1.0E+14
N <sub>a</sub> (cm <sup>-3</sup> )	0	0	0	0	0	0

Fig. 4. Parameters

Figure 4 outlines the material parameters for the perovskite layers and other components, including the HTL, ETL, and ITO. Specific parameters provided for MASnI<sub>3</sub>, CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub>, MAPbI<sub>x</sub>Br<sub>1-x</sub>, CsPbI<sub>3</sub>, CsSnGeI<sub>3</sub>, and MAPbI<sub>3</sub> include thickness, bandgap, electron affinity, relative permittivity, density of states (DoS) in the conduction and valence bands, electron and hole mobility, and doping concentrations for both donors and acceptors. Additionally, the material properties of NiO<sub>x</sub>, ZnO<sub>2</sub>, and ITO are detailed to provide a comprehensive understanding of the device's structural and functional characteristics.

#### 4. Simulation Insights

When the SCAPS software is launched, the simulation process begins with defining the essential parameters required for modeling. Users specify the structural and physical properties of the semiconductor device by navigating through the software's interface, ensuring that every detail aligns with the intended design. This involves configuring layers, materials, and their characteristics to accurately replicate the device's behavior. Following this, users establish environmental conditions, such as temperature and applied external stimuli, to mimic real world operational scenarios. Once all configurations are finalized, the simulation is executed, and SCAPS generates detailed results, offering comprehensive insights into the electrical and optical behavior of the device. This systematic process facilitates an accurate understanding of semiconductor performance, making SCAPS a critical tool for advancing photovoltaic technology. The simulation focuses on analyzing the device's operational characteristics through its current density versus voltage (JV) curve, a fundamental representation of solar cell performance. Additionally, key performance metrics, including open-circuit voltage (Voc), short circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE), are assessed. These parameters provide a thorough understanding of the material's electronic properties and their impact on energy conversion efficiency, aiding in the identification of optimal materials and configurations for solar cell applications. In this study, the performance of

various perovskite absorber materials is explored based on their JV characteristics and efficiencies.

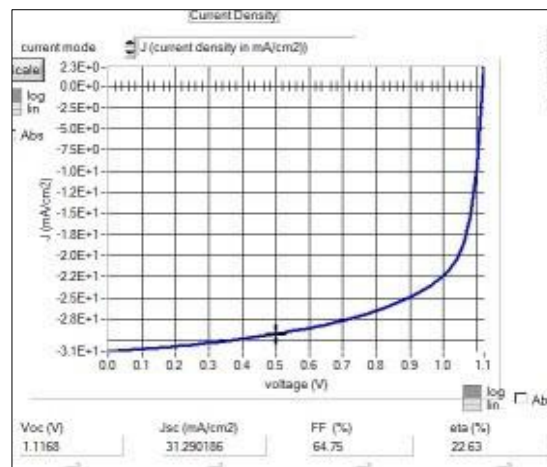


Fig. 5. JV curve of MASnI3

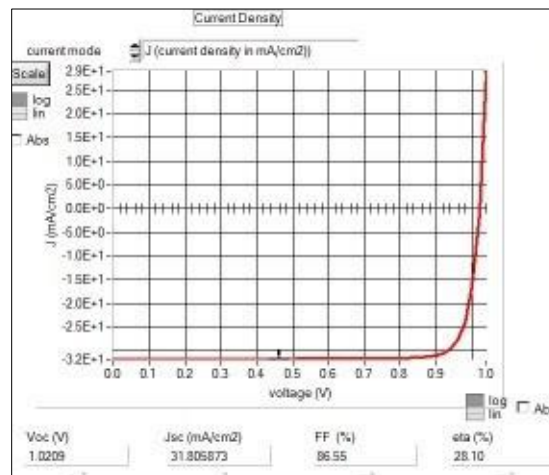


Fig. 6. JV curve of CH3NH3SnI3

SCAPS-1D plays a pivotal role in the simulation and analysis of solar cells by offering a highly detailed and customizable platform. The process begins with the careful definition of the device's structural and material properties. Users configure each layer of the solar cell, specifying parameters such as thickness, bandgap, doping concentration, and defect levels. These properties are critical for accurately modeling the behavior of the solar cell under different conditions. The software also allows for the inclusion of recombination mechanisms and trap states, ensuring a realistic representation of carrier dynamics within the device. Environmental factors, such as operating temperature and illumination intensity, can be adjusted to simulate real-world conditions. By incorporating these parameters, SCAPS ensures that the simulation closely replicates the operational behavior of the actual device. Once the configuration is complete, the simulation is executed, producing a wealth of data that helps researchers understand the intricate details of solar cell performance. One of the most significant outputs is the current-voltage (JV) curve, which provides a direct measure of key performance metrics such as open-circuit voltage ( $V_{oc}$ ), short-circuit current density ( $J_{sc}$ ), fill factor (FF), and power conversion efficiency (PCE). These parameters are fundamental for evaluating the effectiveness of a solar cell design. SCAPS also generates quantum efficiency (QE) curves, offering insight into how

effectively the device converts incident photons into electrical energy across different wavelengths. This information is crucial for identifying losses in the system and optimizing the material and structural properties to enhance overall efficiency.

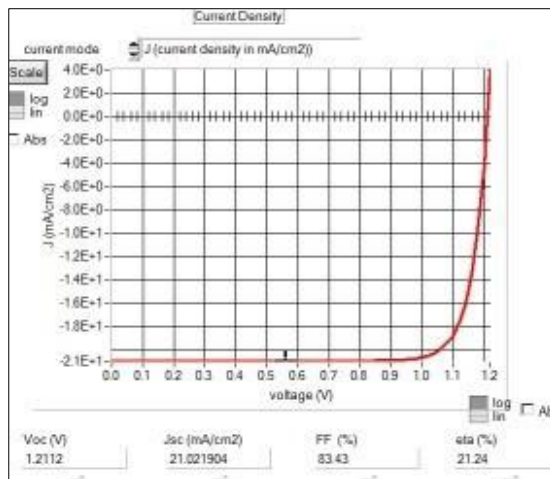


Fig. 7. JV curve of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>x</sub>Br<sub>1-x</sub>

Solar cells utilizing methylammonium tin iodide (MASnI<sub>3</sub>) as the absorber material achieve a conversion efficiency of 22.63 percent, as depicted in Figure 5. Methylammonium tin iodide (CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub>) shows the highest efficiency of 28.10 percent, illustrated in Figure 6. Mixed halide methylammonium lead iodide bromide (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>x</sub>Br<sub>1-x</sub>), with its excellent photovoltaic properties, achieves an efficiency of 21.24 percent, as shown in Figure 7.

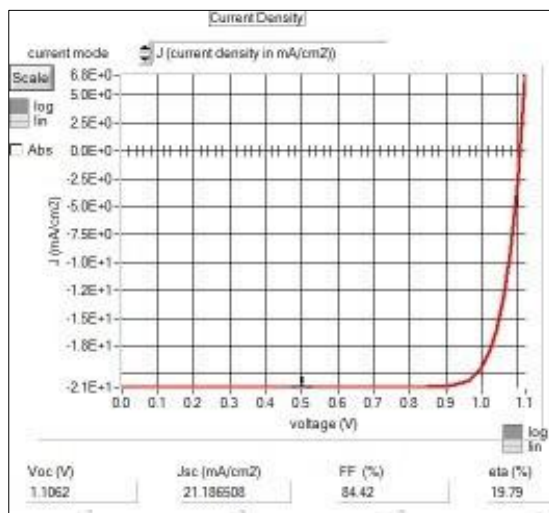


Fig. 8. JV curve of CsPbI<sub>3</sub>

Cesium lead iodide (CsPbI<sub>3</sub>), noted for its stability and reliability, demonstrates an efficiency of 19.79 percent, as seen in Figure 8. Cesium tin germanium iodide (CsSnGeI<sub>3</sub>), which offers a tunable bandgap, delivers an efficiency of 26.49 percent, depicted in Figure 9. These efficiencies underscore the potential of inorganic perovskites like CsPbI<sub>3</sub> and CsSnGeI<sub>3</sub> in advancing photovoltaic technologies. The exceptional performance of CsSnGeI<sub>3</sub>, with its tunable bandgap, indicates its suitability for tandem solar cell applications. Meanwhile, the stability of CsPbI<sub>3</sub> makes it a promising candidate for long-term solar energy solutions, particularly in challenging environmental conditions.

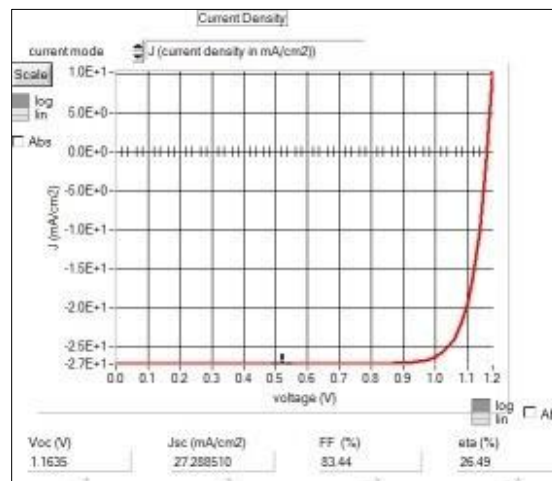


Fig. 9. JV curve of CsSnGeI3

Finally, the widely studied methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) achieves an efficiency of 10.77 percent, as highlighted in Figure 10.

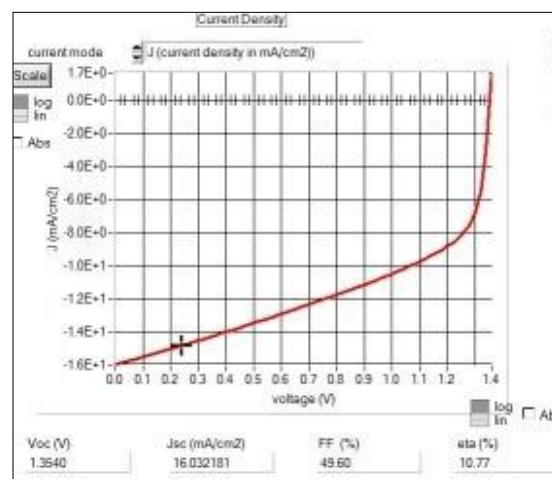


Fig. 10. JV curve of  $\text{CH}_3\text{NH}_3\text{PbI}_3$

Beyond its ability to simulate existing solar cell designs, SCAPS-1D serves as a powerful tool for exploring new materials and innovative architectures. For instance, the software has proven invaluable in studying perovskite solar cells, which have gained significant attention due to their high efficiency and low production costs. By modeling the unique properties of perovskites, such as their tunable bandgap and high defect tolerance, SCAPS enables researchers to optimize their performance further. The software can simulate the impact of various factors, including grain boundaries, ion migration, and interface quality, which are known to affect perovskite solar cells. This capability makes SCAPS a critical asset in advancing the understanding and development of cutting-edge photovoltaic technologies. Additionally, SCAPS-1D supports iterative optimization and sensitivity analysis, allowing researchers to systematically vary parameters and assess their impact on device performance. For example, users can explore how changes in doping concentration or the inclusion of passivation layers influence recombination rates and carrier transport. This systematic approach not only helps in identifying optimal configurations for high efficiency but also provides insights into the fundamental physics of device operation. By leveraging these features, researchers can bridge the gap between

theoretical designs and practical implementations, paving the way for more efficient and cost-effective solar energy solutions.

Parameters	Perovskite Absorbing Layers					
	MA <sub>2</sub> SnI <sub>4</sub>	CH <sub>3</sub> NH <sub>3</sub> SnI <sub>3</sub>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>2</sub> Br <sub>0.4</sub>	CsPbI <sub>3</sub>	CsSnGeI <sub>3</sub>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub>
Efficiency (%)	22.63	28.10	21.24	19.79	26.49	10.77
Fill Factor (%)	64.75	86.55	83.43	84.42	83.44	49.60
Short Circuit Current Density (mA/cm <sup>2</sup> )	31.290186	31.805873	21.021904	21.186508	27.288510	16.032181
Open Circuit Voltage (V)	1.1168	1.0209	1.2112	1.1062	1.1635	1.3540

Fig. 11. Comparison of various performance parameters with different perovskite absorbing layers

## 5. Bridging Perovskite Results and Simulation Insights

Combining results from SCAPS simulations with computational modeling offers a comprehensive approach to analyzing and enhancing the performance of perovskite solar cells. SCAPS provides a detailed baseline by generating JV curves and evaluating essential parameters such as efficiency, open-circuit voltage (Voc), and short-circuit current density (Jsc) for various perovskite materials. These findings help identify trends and key material characteristics that influence device performance. Computational simulations further build on these results by exploring real-world scenarios, such as temperature fluctuations and varying light intensities, to refine the understanding of solar cell behavior. Advanced numerical methods allow for the optimization of design aspects like layer thickness and charge transport properties, as well as predictions of long-term stability and degradation. This integration of SCAPS data with computational techniques ensures accurate validation of results and bridges the gap between experimental outcomes and practical applications, paving the way for improved designs and reliable performance in real-world conditions.

## 6. Validation of Results

Validating the results obtained from SCAPS simulations is essential to ensure accuracy and reliability in analyzing the performance of perovskite solar cells. By using computational modeling, key performance parameters such as current-voltage (JV) characteristics and power conversion efficiency (PCE) are cross-checked. The simulation process involves solving fundamental semiconductor equations, such as Poisson's equation and the continuity equations, to replicate carrier dynamics and device behavior under various conditions. This approach provides a deeper understanding of critical factors like charge recombination, transport, and optimization of device layers, enhancing the robustness of the simulation outcomes. Validation also ensures the alignment of theoretical predictions with observed performance metrics, reinforcing the credibility of the analysis. In addition to cross-checking key performance parameters, validation involves comparing simulation results with experimental data from fabricated devices. This comparison helps identify any discrepancies and refine the input parameters to achieve a closer match between theoretical and practical outcomes. By iteratively adjusting material properties, defect states, and interface characteristics, researchers can improve the accuracy of the SCAPS model. Such validation not only strengthens the reliability of the simulations but also provides valuable insights into underlying physical processes, guiding the development of more efficient and optimized solar cell designs.

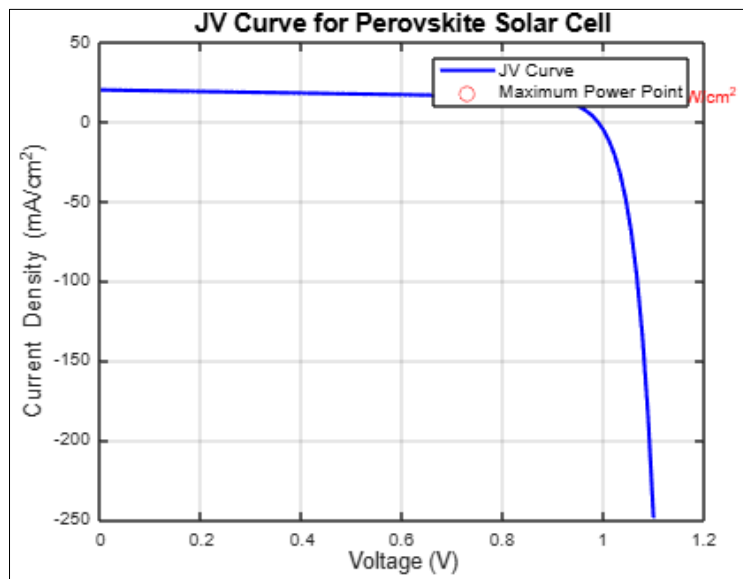


Fig 12. JV curve for a solar cell (MATLAB Simulation)

The JV curve represents the relationship between current density ( $J$ ) and voltage ( $V$ ) for a perovskite solar cell, illustrating key performance metrics such as the short-circuit current density ( $J_{sc}$ ) at zero voltage, open-circuit voltage ( $V_{oc}$ ) at zero current, and the Maximum Power Point (MPP), where power output is maximized. The steep drop in current beyond  $V_{oc}$  reflects diode-like behavior, while the flat region near  $J_{sc}$  indicates efficient carrier collection. Numerical simulation tools were used to model this behavior by solving semiconductor equations, incorporating effects like series resistance, shunt resistance, and material properties. The curve highlights how varying parameters such as temperature, bandgap, and charge transport characteristics influence the cell's efficiency, fill factor, and overall performance, offering critical insights for optimizing solar cell designs.

### 7. Advanced Parameter Sensitivity Analysis

Sensitivity analysis is a powerful approach to explore how variations in key parameters influence the performance of perovskite solar cells. By leveraging computational tools, researchers can simulate changes in material properties and environmental conditions to assess their impact on metrics such as efficiency, fill factor (FF), open-circuit voltage ( $V_{oc}$ ), and short-circuit current density ( $J_{sc}$ ). Key parameters like bandgap energy, carrier mobility, and recombination rates are systematically altered to identify their influence on charge transport and carrier collection. Similarly, environmental factors such as operational temperature and illumination intensity are varied to understand real-world performance fluctuations. This type of analysis enables the identification of critical performance drivers and optimal material configurations, guiding the design of more efficient and robust solar cells.

Moreover, sensitivity analysis helps pinpoint parameters that have minimal impact on device performance, allowing researchers to prioritize efforts on factors with the greatest influence. This approach also aids in understanding the trade-offs between different properties, such as the balance between carrier mobility and recombination rates. By providing a comprehensive view of how various factors interact, sensitivity analysis not only optimizes material and device design but also offers a deeper understanding of the underlying physics governing solar cell operation. This makes it an indispensable tool for advancing the development of high-performance perovskite solar cells.

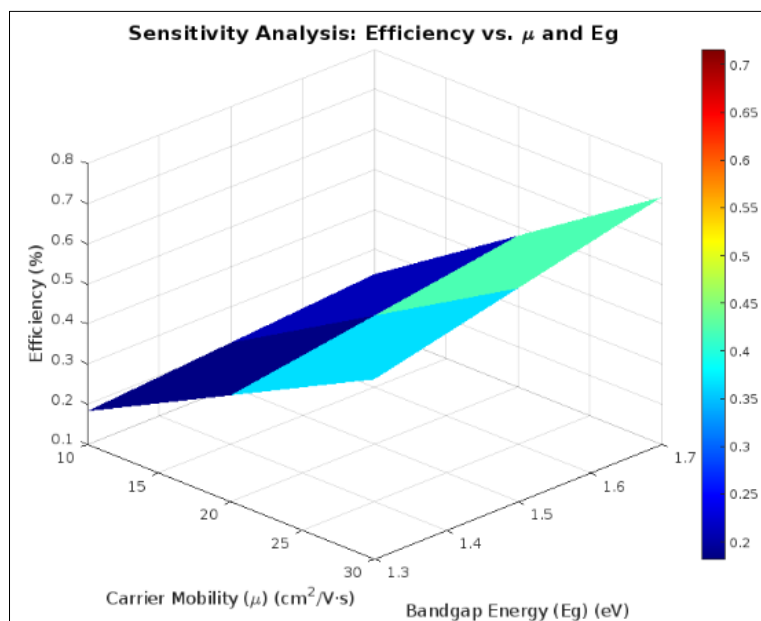


Fig 13. Sensitivity Analysis (MATLAB Simulation)

The code evaluates how variations in bandgap energy ( $E_g$ ) and carrier mobility ( $\mu$ ) influence the efficiency of perovskite solar cells. The results are visualized as a 3D surface plot, highlighting the relationship between these parameters. As bandgap energy increases, the open-circuit voltage ( $V_{oc}$ ) improves, leading to higher efficiency, but only up to an optimal range due to reduced absorption at higher bandgaps. Similarly, higher carrier mobility enhances charge transport and reduces recombination losses, positively impacting short-circuit current density ( $J_{sc}$ ) and overall efficiency. The surface plot allows researchers to identify parameter combinations that maximize performance, providing valuable insights for optimizing perovskite material properties and device architectures.

## 8. Layer Optimization

Optimizing the thickness of key layers in perovskite solar cells is essential for maximizing efficiency. By employing computational techniques, the thickness of the perovskite absorber layer, electron transport layer (ETL), and hole transport layer (HTL) is varied to identify their impact on device performance. Changes in the absorber layer affect light absorption and carrier generation, while ETL and HTL thickness influence charge transport and recombination. Simulated results provide insights into optimal layer dimensions that enhance metrics like short-circuit current density ( $J_{sc}$ ), open-circuit voltage ( $V_{oc}$ ), fill factor (FF), and power conversion efficiency (PCE). This approach ensures precise material utilization and optimal device design.

Optimizing the thickness of key layers in perovskite solar cells specifically the perovskite absorber layer, electron transport layer (ETL), and hole transport layer (HTL) is crucial for maximizing the overall efficiency of the device. By utilizing advanced computational algorithms, the effects of varying the thickness of these layers are simulated. The perovskite absorber layer is responsible for light absorption and carrier generation, so its thickness directly influences the current generated. Similarly, the thickness of the ETL and HTL layers affects charge transport and recombination rates, which are essential for the effective extraction of photogenerated carriers.

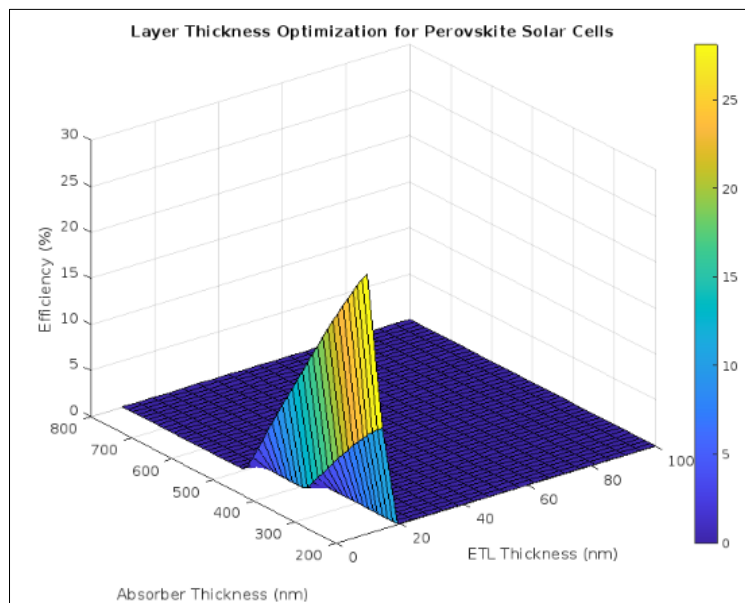


Fig 14. Layer Optimization (MATLAB Simulation)

Computational models simulate these changes, taking into account material properties and interface characteristics, allowing researchers to identify the optimal thickness for each layer. These simulations help to achieve the best balance between light absorption, charge transport, and minimal recombination, leading to improved efficiency. The insights gained from these analyses contribute to the development of more efficient and cost-effective perovskite solar cells.

## 9. Circuit-Level Modeling

To understand the electrical behavior of perovskite solar cells, equivalent circuit models are used to represent the device's performance. These models typically include a current source to simulate the photogenerated current, diodes to model the junction properties, and resistors to account for series and shunt losses that occur in real-world devices. The current source reflects the amount of photocurrent generated by the solar cell under illumination, while the diodes represent the characteristics of the p-n junction, including recombination and reverse saturation current. The resistors capture the energy losses that arise due to the resistance in the conductive layers and any leakage currents through the cell. Simulating these circuit models provides valuable insights into the transient behavior, dynamic response, and performance of the solar cell under varying conditions, such as partial shading or fluctuating illumination. These simulations help to identify inefficiencies in the system, optimize design parameters, and predict how the device will perform in real-world scenarios. By using computational tools to model these electrical characteristics, it is possible to enhance the design and performance of perovskite solar cells.

Circuit-level modeling helps simulate the electrical behavior of perovskite solar cells by using an equivalent circuit that includes a current source for photogenerated current, diodes for junction properties, and resistors for series and shunt losses. This approach provides insights into the cell's dynamic responses, including how it behaves under varying illumination and partial shading conditions. By adjusting key parameters such as resistance and current characteristics, optimization strategies can

be explored to improve efficiency. These simulations can be performed using computational platforms that allow for modeling and analyzing the impact of these variables on overall performance.

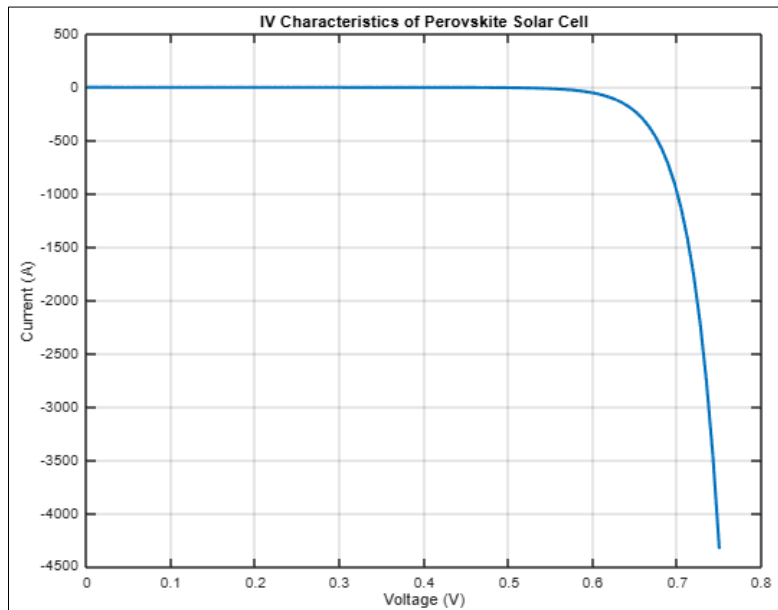


Fig 15. IV Characteristics of Perovskite Solar Cell (MATLAB Simulation)

Circuit-level modeling helps simulate the electrical behavior of perovskite solar cells by using an equivalent circuit that includes a current source for photogenerated current, diodes for junction properties, and resistors for series and shunt losses. This approach provides insights into the cell's dynamic responses, including how it behaves under varying illumination and partial shading conditions. By adjusting key parameters such as resistance and current characteristics, optimization strategies can be explored to improve efficiency. These simulations can be performed using computational platforms that allow for modeling and analyzing the impact of these variables on overall performance.

### 10. Comparative Analysis

Comparative analysis plays a vital role in evaluating the performance of various perovskite materials by examining parameters such as power conversion efficiency, open-circuit voltage ( $V_{oc}$ ), and short-circuit current density ( $J_{sc}$ ). By processing simulation outputs through advanced computational tools, critical trends can be identified, offering insights into how material composition influences photovoltaic performance. Such analysis highlights the distinctive characteristics of each material, enabling researchers to determine the most suitable candidates for high-efficiency solar cells. Visualization techniques, including bar charts and line plots, facilitate a clear comparison of these parameters, making the findings more accessible and impactful. To further enhance this comparative study, graphical representations are generated to illustrate efficiency metrics and the corresponding  $V_{oc}$  and  $J_{sc}$  values for each material. This approach ensures a comprehensive understanding of material behavior under identical simulated conditions. By providing high-quality plots, the analysis not only aids in visual differentiation among materials but also underscores the relative advantages and limitations, guiding future optimization strategies for perovskite based solar technologies. Comparative analysis can also account for factors like temperature stability and light intensity, providing insights into how different materials perform under varying conditions. This broader

evaluation helps identify materials that combine high efficiency with environmental resilience. Such findings are essential for selecting perovskite materials suitable for practical applications in diverse settings.

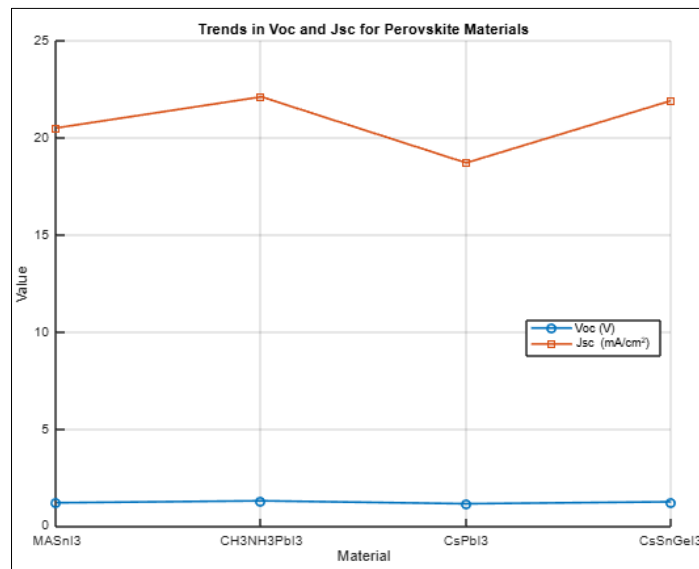


Fig 16. Trends in Voc and Jsc

The chart presents the trends in open-circuit voltage (Voc) and short-circuit current density (Jsc) for four perovskite materials, derived through computational modeling and simulations. The analysis indicates that Jsc remains consistently high with slight variations, while Voc is comparatively lower and stable across the materials. This highlights how the material properties predominantly influence the short-circuit current density in these perovskites.

### 11. Simulation Workflow

The simulation workflow integrates SCAPS-generated baseline data with advanced computational analysis (MATLAB) to gain deeper insights into solar cell performance. SCAPS provides key outputs, such as JV curves, efficiency, and other device metrics, which serve as the foundation for further evaluation. This data is exported for processing in computational environments, where more complex scenarios are modeled. These include simulating real-world conditions such as temperature fluctuations and shading, as well as predicting the performance of novel perovskite materials through parameter variation and trend analysis. This combined approach enables a holistic understanding of material and device behaviors, guiding optimization and innovative design strategies for high-efficiency solar cells.

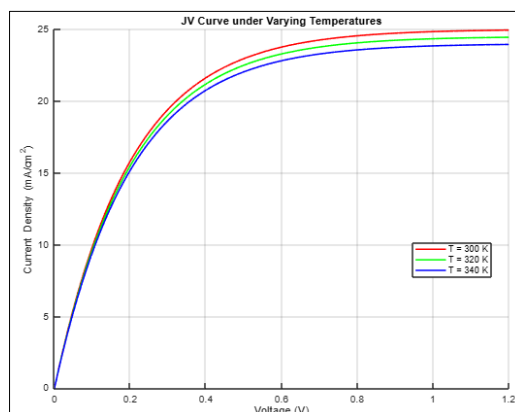


Fig 17. JV Curve under different temperatures

The simulation workflow combines SCAPS outputs with computational tools to explore detailed solar cell performance and behavior. SCAPS is utilized to generate baseline data such as JV curves, efficiency metrics, and other device characteristics. This information is then exported to a computational environment for deeper analysis, allowing for simulation of real-world conditions, including temperature changes, shading effects, and aging. Additionally, advanced scenarios such as performance predictions for innovative material compositions are modeled. This approach bridges the gap between theoretical results and practical applications, ensuring optimized design and enhanced reliability for solar cell technologies. The computational platform supports extending SCAPS results through data visualization and predictive modeling. For instance, JV curves are plotted to analyze voltage and current density trends, while environmental effects, like varying temperature, are simulated to assess real-world performance. This combined simulation strategy ensures a comprehensive understanding of material properties and device efficiencies, driving advancements in photovoltaic research.

## 12. Performance Predictions with Machine Learning

Machine learning offers a powerful approach to predict the performance of unexplored perovskite formulations by leveraging data generated through simulations. By training machine learning models on data obtained from SCAPS or similar simulations, it becomes possible to forecast efficiency, open-circuit voltage, and other performance metrics for new materials without conducting extensive experimental tests. Regression models, for instance, can rank various perovskite configurations based on their predicted efficiency, providing valuable insights into promising candidates. This integration of machine learning and simulation workflows accelerates the discovery and optimization of high-performance materials, enabling data-driven innovation in photovoltaic research.

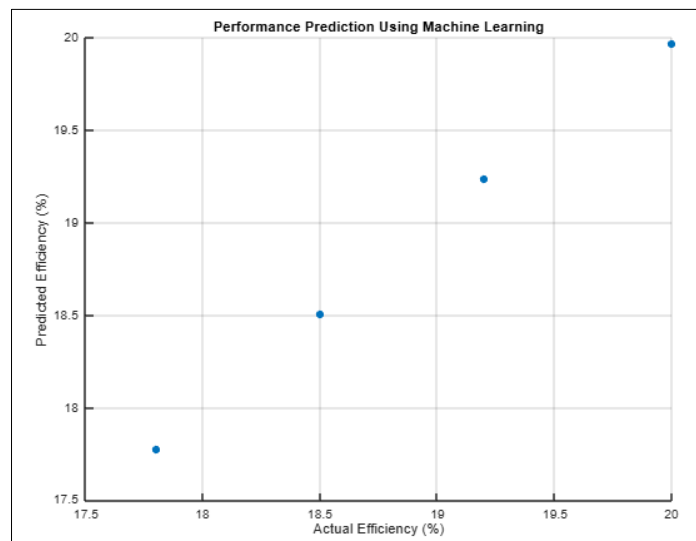


Fig 18. Performance prediction using ML

This process demonstrates how advanced numerical tools can be utilized to forecast the efficiency of untested perovskite materials by analyzing key parameters such as band gap energy and carrier mobility. By working with hypothetical data inspired by SCAPS simulation outputs, the relationship between these material properties and their photovoltaic performance can be modeled.

This enables researchers to identify promising material configurations for experimental validation, contributing to the development of high-efficiency solar cells. Moreover, visualization techniques enhance understanding by providing a clear comparison of predicted versus actual efficiencies. These graphical representations, generated using computational platforms, validate the accuracy of the predictive model and offer insights into material performance trends. Such an approach aligns with the study's aim to combine simulation data and computational analysis to optimize material selection and solar cell design.

### 13. Performance Predictions with Machine Learning

Understanding the real-world performance of solar cells is essential for their practical deployment in diverse environments. Computational platforms complement SCAPS-generated laboratory data by simulating real-world conditions such as fluctuating temperature, varying solar irradiance, and material degradation over time. These simulations enable a detailed analysis of how environmental factors impact key performance metrics like efficiency, fill factor (FF), and open-circuit voltage (Voc). By bridging the gap between controlled experimental settings and real-life scenarios, such computational models ensure that solar cell designs are robust and adaptable to varying field conditions. One critical aspect of real-world modeling involves accounting for the influence of temperature and irradiance on device behavior. For example, rising temperatures can reduce the efficiency of solar cells due to increased carrier recombination and decreased bandgap energy. Similarly, changes in irradiance directly affect the amount of generated photogenerated current. Computational simulations provide a systematic way to evaluate these variations, offering insights into optimal material choices and device configurations. These tools also allow for the prediction of long-term performance by incorporating material degradation models, which are essential for estimating the lifespan of solar cell systems under operational stress. Visualizing the results of these simulations is key to interpreting the effects of

environmental conditions. Computational routines generate detailed plots to map the relationship between temperature, irradiance, and efficiency. For instance, 3D surface plots can provide an intuitive understanding of how efficiency trends vary across a range of operating conditions. Such analyses are vital for optimizing perovskite solar cells, as they help researchers identify the most resilient designs for practical applications, ultimately ensuring sustained energy output and reliability in real-world deployments.

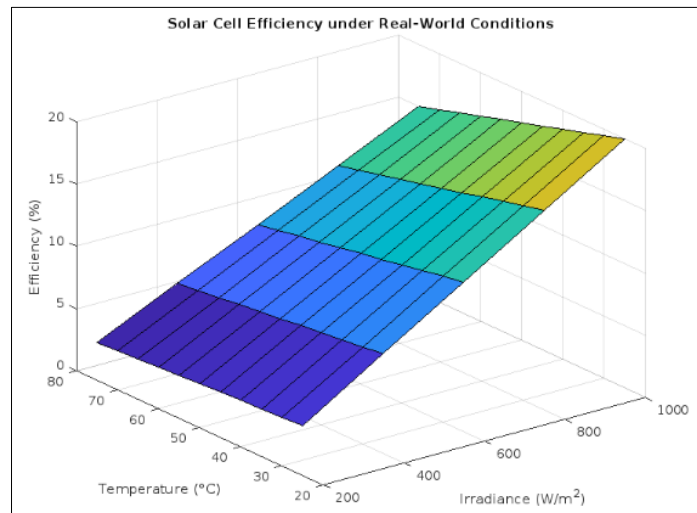


Fig. 19. Solar Cell Performance in Practical Environments

Simulating real-world conditions, such as fluctuating temperatures, varying irradiance levels, and material degradation, is critical for bridging the gap between laboratory data and practical solar cell performance. Computational environments extend SCAPS outputs by modeling how these environmental factors influence key metrics like efficiency, open-circuit voltage, and short-circuit current over time. These simulations provide valuable insights into the dynamic behavior of perovskite solar cells under field-like scenarios, aiding in the prediction of long-term performance and reliability across diverse geographic and climatic conditions. This approach enables the refinement of material compositions and device architectures for improved durability and efficiency in real-world applications.

#### 14. Conclusion

This study conducts a detailed evaluation of solar cells using various perovskite-based absorber materials, including  $\text{MASnI}_3$ ,  $\text{CH}_3\text{NH}_3\text{PbI}_3$ ,  $\text{CH}_3\text{NH}_3\text{PbI}_x\text{Br}_{1-x}$ ,  $\text{CsPbI}_3$ ,  $\text{CsSnGeI}_3$ , and  $\text{CH}_3\text{NH}_3\text{SnI}_3$ . Critical performance indicators, such as power conversion efficiency (PCE), fill factor (FF), open-circuit voltage ( $V_{oc}$ ), and short-circuit current density ( $J_{sc}$ ), were assessed to understand the unique properties and potential of each material. Computational simulations, involving sensitivity analysis, layer optimization, and circuit modeling, complemented the SCAPS-generated results and enhanced the analysis. The integration of machine learning models and simulations of real-world conditions offers practical insights into material performance, supporting the development of high-efficiency perovskite solar cells for future energy applications.

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**AUTHOR CONTRIBUTIONS** : This work was primarily conducted by Naeema Nazar, the main author, who was responsible for conceptualization, investigation, data analysis, supervision, writing, and preparation of the original draft. Mohamed Kallel contributed to investigation, conceptualization, data analysis, and writing. Rahma Sellami provided funding support, and Abdelhalim Hasnaoui supervised the work.

**BIOGRAPHIES OF AUTHORS**



**NAEEMA NAZAR**    is a dynamic academic and professional in Electronics and Communication Engineering, currently an Assistant Professor at VISAT Engineering College and the Global Strategy Representative of India for the IEEE Photonics Society, USA. A distinguished IEEE advocate, she serves as the IEEE Student Branch Counselor at VISAT and has held prestigious roles as an IEEE Ambassador for IEEE Day 2024 and IEEE Women in Engineering Day 2024. Ms. Naeema earned her B.Tech in Electronics and Communication Engineering from KMEA Engineering College (KTU) and her M.Tech in Wireless Technology from Toc H Institute of Science and Technology (KTU). Her research expertise includes valuable contributions as a project student at the Naval Physical and Oceanographic Laboratory (NPOL), DRDO, Kochi. Beyond academics, Ms. Naeema is a prolific contributor to IEEE initiatives globally, nationally, and locally, excelling as an organizer, volunteer, speaker, and resource person. At VISAT Engineering College, she holds key roles as the IEDC and NIRF Nodal Officer and Research Coordinator, reflecting her dedication to academic excellence and institutional development. She has published research in leading journals and conferences and has participated in numerous workshops and faculty development programs. Her primary areas of interest include Optoelectronics, Ocean Optics, Photonics, and Communication, showcasing her commitment to cutting-edge advancements. With her passion for teaching, research, and professional service, Ms. Naeema continues to inspire and mentor future engineers and researchers.



**MOHAMED KALLEL**    was born at 13th August. 1980 in Tunisia. Kallel was worked as a researcher in Laboratory of Physics, Mathematics and Applications, Faculty of Sciences of Sfax, Tunisia. Currently Kallel is working as a Physics assistant professor in Faculty of Science, Northern Border University, KSA. Kallel is a distinguished academic with a strong research focus on the study of dielectric and electrocaloric properties of various ceramics, particularly ferroelectric ceramics. Their work has significantly contributed to the understanding of the effects of doping on these properties, with a special emphasis on the impact of elements such as manganese, praseodymium, zinc, niobium and bismuth. Their research has not only been prolific but also influential, as evidenced by the significant number of citations their work has received. The author's contributions to the field, particularly in the study of ferroelectric ceramics and the effects of doping, have undoubtedly advanced the understanding of these complex materials and their potential applications.