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RESEARCH ARTICLE

Numerical Optimization of HTL-Free Perovskite Solar Cells: A Pathway to Enhanced Efficiency

Manisha Kumari[1], **Manpreet Kaur**[1] **and Ankush Kumar Tangra**[2,*]

[1] Department of Physics, Sant Baba Bhag Singh University, Jalandhar, India
[2] Department of Physics, Research & Incubation Center, Rayat Bahra University, Punjab, India

Abstract

Perovskite solar cells (PSCs) have appeared as an encouraging photovoltaic technology due to their high efficacy and low fabrication cost. However, their stability and scalability are hampered by charge recombination and intricate multilayer architectures. Using HTL-free design, this work explores reduced PSCs designs with the goal of reducing recombination losses and enhancing the overall device performance. Optimized ETL-only and HTL-free topologies may substantially decline the interfacial recombination and progress in charge extraction, according to numerical simulations conducted with SCAPS-1D. The FTO/α-Fe_2O_3/$CH_3NH_3PbI_3$/Au device achieves a high power conversion efficiency (PCE) of 20.99 % with an open-circuit voltage (Voc) of 1.066 V, a short-circuit current density (Jsc) of 25.05 mA/cm^2, and a fill factor (FF) of 78.59 %. The essential of preserving thermal stability into account in HTL-free topologies is shown by temperature-dependent analysis, which reveals a tolerant decrease in PCE with increasing temperature. These effects show how enhanced HTL-free PSCs may lower manufacturing costs without sacrificing high photovoltaic performance.

Keywords: SCAPS-1D, perovskite solar cell, HTL-free, efficiency.

1 Introduction

Due to ongoing advances in solar device performance, environmentally friendly operation, high manufacture scalability, and lower developed costs when compared to traditional fossil fuel-based sources, solar cell technology has become a major competitor in the global shift toward sustainable energy systems. Due to their PCEs and long-term operating stability, silicon-based solar cells - including both mono-crystalline and polycrystalline variants - have dominated the commercial market among other photovoltaic technologies. However, complicated and expensive fabrication processes like high-temperature diffusion, photolithography, and vacuum deposition techniques continue to impede the large-scale production of these cells, limiting their scalability and cost-effectiveness, particularly for emerging cost-cutting looking for affordable energy solutions [1]. As next-generation photovoltaic absorbers, hybrid inorganic and organic perovskite materials have

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***Corresponding author:**
✉ Ankush Kumar Tangra
aktangra@gmail.com

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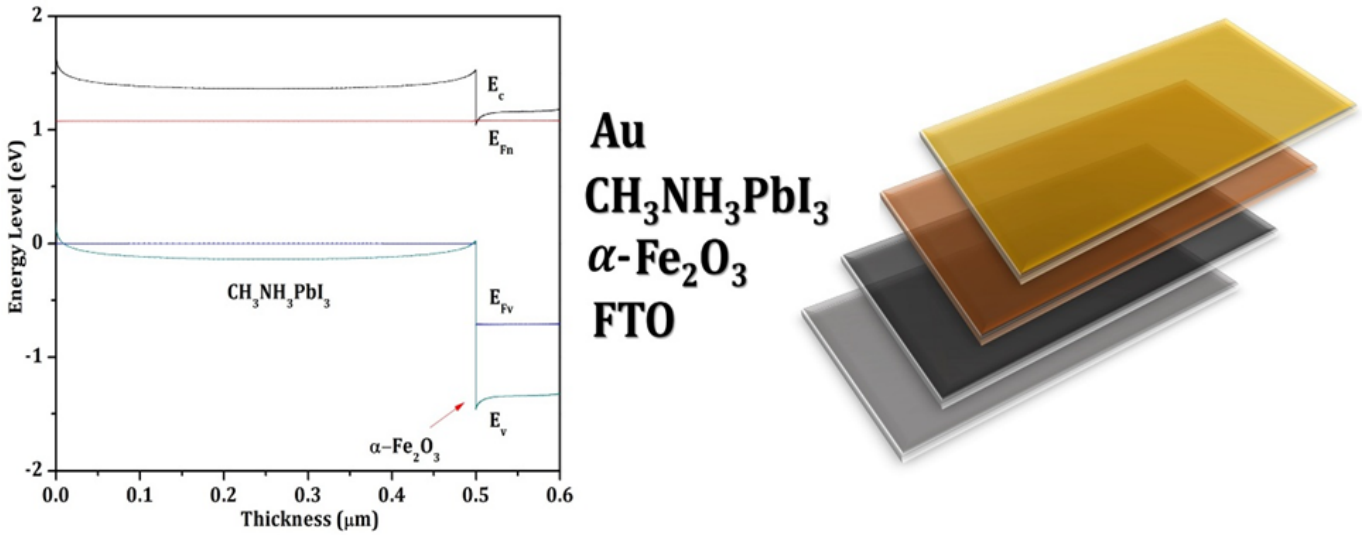

Figure 1. Illustrates the energy band alignment and schematic architecture of the simulated perovskite solar cell (PSC), highlighting the layered configuration of the device and the corresponding electronic energy levels across the thickness of the structure.

drawn a lot of attention and are quickly becoming competitive alternatives to traditional silicon-based solar cells. Since their initial incorporation into solar energy systems in 2009, using a methylammonium lead halide ($MAPbI_3$) absorber to achieve a low PCE of 3.8% [2–5] PSCs have experienced an extraordinary rise in performance due to breakthroughs in material composition, defect passivation, and interface engineering [2–6]. With recent advancements pushing verified PCEs to 25.73% and reported values as high as 26.08% [6], This remarkable development demonstrates PSCs' potential to provide scalable solar systems with low-cost, high-efficiency, and solution-processable alternatives [7].

Recent advances in photovoltaic technologies have been driven by innovations in both device architectures and material systems. In thin-film solar cells, optimized material combinations and interfacial engineering approaches have demonstrated significant efficiency improvements [8, 9]. Similarly, breakthroughs in silicon heterojunction technologies through novel device designs have achieved remarkable performance enhancements [10, 13, 14]. Among these developments, perovskite solar cells (PSCs) have emerged as particularly promising, with their rapid development attributable to several unique advantages.

The exceptional rise of PSCs stems from their remarkable performance metrics, including certified power conversion efficiencies now exceeding 25% [20], combined with their tunable optoelectronic properties. The ability to adjust bandgaps through compositional engineering enables optimal light harvesting across the solar spectrum [22, 23], while solution-processable fabrication methods offer cost advantages over conventional photovoltaic technologies [24]. These characteristics, along with their inexpensive production potential, have propelled PSCs to the forefront of emerging PV research [25].

The excellent photovoltaic performance of PSCs, particularly those based on $CH_3NH_3PbI_3$, arises from several fundamental material properties. A direct bandgap (1.5 eV) enables efficient light absorption [26], while a high absorption coefficient ($>10^4\,cm^{-1}$) allows for thin active layers. Furthermore, long carrier diffusion lengths ($>1\,\mu m$) contribute to outstanding charge collection efficiencies [27]. These intrinsic advantages have motivated extensive research focused on optimizing material quality, interface engineering, and device architectures to further improve PSC performance.

In conventional PSC designs, inorganic electron transport layers (IETLs) and hole transport layers (HTLs) play critical roles as energy-selective contacts. Recent studies on charge transport mechanisms have demonstrated how these layers function as energy barriers to prevent charge backflow while enabling directional charge extraction [11, 12, 15]. However, manufacturing challenges persist in achieving high-quality multilayered structures with sufficiently low defect densities. As stability analyses have shown [21], interfacial mismatches at both IETL/perovskite and HTL/perovskite junctions often lead to increased recombination rates over time,

ultimately compromising device stability.

To address these limitations, the photovoltaic community has increasingly explored HTL-free device architectures as an alternative approach. This design strategy, supported by computational studies [16, 17] and experimental validations [18, 19], offers multiple benefits: (1) reduced interfacial recombination through simplified device structures; (2) lower manufacturing costs by eliminating the HTL deposition step; and (3) improved scalability through more straightforward fabrication processes. These advantages make HTL-free configurations particularly attractive for developing stable and cost-effective PSCs.

In this context, hematite (α-Fe_2O_3) emerges as a promising IETL candidate for HTL-free PSC designs. Its optical properties are especially noteworthy, with high visible-range transparency (70-85%) in the 600-1000 nm spectral region [21] - crucial for perovskite light absorption. Combined with its optimal bandgap (2.1 eV) [26], this ensures minimal parasitic absorption while maintaining effective charge transport capabilities. Material availability studies have further confirmed hematite's potential for large-scale PV deployment due to its earth abundance, cost-effectiveness, and exceptional chemical stability [27].

The charge transport properties of hematite make it particularly suitable for PSC applications. As a charge-selective contact, it effectively extracts photogenerated electrons from the perovskite absorber while blocking hole recombination, thereby enhancing current collection and reducing losses. Numerical simulation has proven invaluable in evaluating such novel material systems, with computational tools enabling detailed analysis of charge dynamics, recombination processes, and energy band alignment prior to device fabrication [21, 26]. These simulation approaches, particularly when combined with experimental data [27], significantly reduce development time and costs by minimizing trial-and-error in the optimization of new device architectures.

2 Simulation Methods

SCAPS-1D, a one-dimensional solar cell simulation program, was used to simulate and analyze the performance of the suggested solar cell configuration. A popular tool for simulating heterojunction and multilayer thin-film photovoltaic systems, SCAPS-1D was created by the Department of Electronics and Information Systems (ELIS) at Ghent University in Belgium. To ascertain important electrical properties of the device under illumination, the program numerically solves a collection of equations, such as Poisson's equation and the continuity equations for electrons and holes. By taking into consideration the spatial distribution of charge carrier densities and electrostatic potential, these equations allow for precise predictions of how material characteristics, interface features, and layer thicknesses will affect device behavior. Therefore, SCAPS-1D offers a dependable platform for solar cell design optimization prior to experimental execution. Figure 1 shows the architecture of the suggested perovskite solar cell (PSC), which is made up of FTO/α-Fe_2O_3/$CH_3NH_3PbI_3$/Au and has a simplified HTL-free design. In order to minimize interfacial recombination losses and manufacturing complexity, this arrangement purposefully removes the hole transport layer.

3 Results and Discussion

The energy band gap and device structure for the simulated device without HTL are shown in Figure 1. The energy band diagram of a perovskite solar cell construction with α-Fe_2O_3 (hematite) as the IETL and $CH_3NH_3PbI_3$ as the absorber is shown in Figure 1(a). The valence band (Ev), conduction band (Ec), and Fermi level (Ef) are plotted throughout the device thickness in the diagram. The comparatively flat band edges within the perovskite area suggest dominating carrier diffusion and good material quality due to the low internal electric fields. While a significant valence band offset substantially reduces recombination losses by creating a barrier to hole injection, a favorable conduction band offset at the interface with α-Fe_2O_3 enables efficient electron transmission from the perovskite to the IETL. A high Voc is maintained and electron extraction is improved by this selective charge transfer. With a broad bandgap (2.1 eV), apparent transparency, and compatibility with perovskite layers that support both optical and electrical performance in HTL-free perovskite solar cells, the energy alignment validates α-Fe_2O_3's promise as a stable and affordable ETL.

In order to begin the simulation, a planar PSCs architecture was constructed without the use of a HTL. FTO is the transparent conducting front contact, α-Fe_2O_3 is the IETL, $CH_3NH_3PbI_3$ is the perovskite absorber, and gold (Au), which has a work function

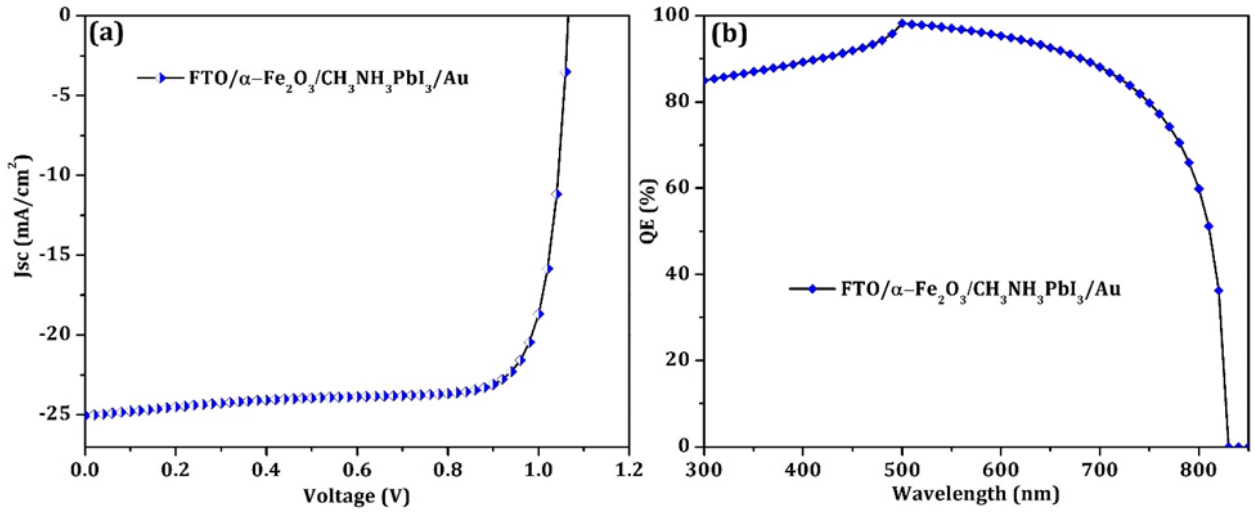

Figure 2. (a) Depicts the current density–voltage (J-V) characteristics of the simulated device, and (b) illustrates its quantum efficiency curve.

Table 1. Material and simulation parameters used for the HTL-free perovskite solar cell with device structure FTO/α-Fe_2O_3/$CH_3NH_3PbI_3$/Au.

Parametrs	α-Fe_2O_3	$CH_3NH_3PbI_3$
Thickness (m)	0.200	0.600
Band gap (eV)	2.1	1.53
Electron affinity (eV)	3.90	3.60
Dielectric Permittivity	10.00	30
CB effective density of states ($1/cm^3$)	2.200E+18	1.000E+18
VB effective density of states ($1/cm^3$)	1.800E+19	1.000E+18
Electron thermal velocity (cm/s)	1.000E+7	1.000E+7
Hole thermal velocity (cm/s)	1.000E+7	1.000E+7
Electron mobility (cm^2/Vs)		

of 5.3 eV, is used as the rear electrode in the suggested device structure.

Table 1 provides a summary of the material and structural characteristics utilized in the simulation. Figure 2 (a) displays the external quantum efficiency (EQE) spectrum and JV characteristics. These show promising photovoltaic performance with an Voc of 1.066 V, Jsc of 25.05 mA/cm^2, FF of 78.59%, and a PCE or η of 20.99%. JMPP = 22.55 mA/cm^2 and VMPP = 0.931 V were the maximum power point (MPP) values, respectively. A high fill factor is a result of effective charge extraction and minimal internal resistance, as seen by the curve's noticeable knee close to the maximum power point. These findings imply that incoming photons are efficiently transformed into useful electrical energy by the device. Additionally, Figure 2 (b) displays the EQE spectrum, which illustrates the device's photoresponse throughout the visible spectrum. The absorber-IETL configuration's effective light absorption and carrier collecting capabilities are highlighted by a peak EQE reaching 90% between 400 and 700 nm. This confirms the feasibility of HTL-free device operation employing α-Fe_2O_3 as an economical and effective electron transport material [28, 29].

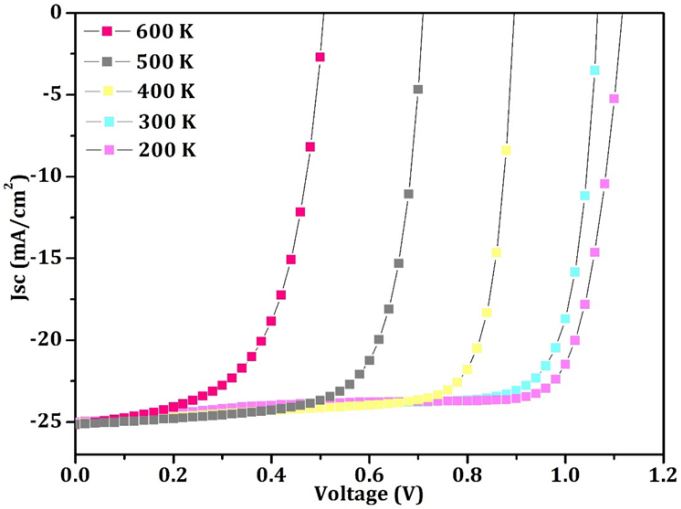

Figure 3. Demonstrates the temperature-dependent behavior of the simulated device.

Table 2. Variation of Photovoltaic Parameters with Temperature in the Range of 200 K to 600.

Temperature	Voc (V)	Jsc (mA/cm^2)	FF (%)	PCE (%)
200 K	1.116560	25·01427648	78.8626	22.0263
300 K	1.066405	25.04552896	78.5909	20.9906
400 K	0·896305	25.09678551	78.2767	17.6079
500 K	0.710368	25.13616693	71.8232	12.8211
600 K	0.507770	25.16558807	59.6956	7.6281

The bandgap of $CH_3NH_3PbI_3$, which restricts absorption of longer-wavelength photons, is shown by the drop-off beyond 750 nm. Strong light-harvesting and carrier-collecting capabilities are confirmed by this broad and effective spectrum response, suggesting that α-Fe_2O_3 is a suitable and affordable IETL for high-performance, HTL-free perovskite solar cells. This study used numerical modeling to examine how operational temperature affects a PSCs performance. In order to evaluate the impact of the temperature on important photovoltaic parameters, such as PCEs, Voc, Jsc, and FF, the device was first simulated at a standard temperature of 300 K. The temperature was then gradually increased from 200 K to 600 K. In order to isolate the thermal effects, these simulations were run with a set buffer layer thickness and perfect absorber conditions. The Jsc is comparatively constant across the temperature range, as shown in Figure 3, indicating that temperature changes do not substantially impair the photogeneration of charge carriers. However, when temperature rises, Voc and PCE noticeably decrease, mostly as a result of increased recombination losses and decreased built-in potential as shown in Table 2. Additionally, the fill factor is trending negative, which suggests a rise in resistive and non-radiative losses. These findings highlight how crucial thermal stability is for solar cell materials and device design, especially for situations where ambient temperatures are high or fluctuate.

Over a temperature range of 200 K to 600 K, the graph illustrates how temperature change affects a perovskite solar cell's J–V properties. Voc decreases noticeably with increasing operational temperature, mainly because of increased thermally induced carrier recombination and reduced quasi-Fermi level splitting in the absorber material. However, there is little variation in the Jsc, suggesting that photon absorption and exciton synthesis are mostly unaffected by temperature changes. Significantly, the device shows improved curve shape and greater Voc at lower temperatures (200 K and 300 K), suggesting better charge extraction and fewer recombination losses. On the other hand, the J-V curve flattens and shifts toward lower voltages at higher temperatures (500 K and 600 K), which is indicative of shortened carrier lifetimes and greater series resistance. The FF and PCEs are impacted by this thermal deterioration, highlighting how important temperature is in determining the durability and dependability of perovskite solar cells.

4 Conclusion

Using SCAPS-1D for numerical modeling, we have successfully constructed and simulated HTL-free PSCs in this work using the device architecture FTO/α-Fe_2O_3/$CH_3NH_3PbI_3$/Au. With an open-circuit voltage (Voc) of 1.066 V, short-circuit current density (Jsc) of 25.05 mA/cm^2, fill factor (FF) of 78.59%, and power conversion efficiency (PCE) of 20.99%, the simulated findings demonstrate encouraging photovoltaic performance. Furthermore, JMPP = 22.55 mA/cm^2 and VMPP = 0.931 V were found to be the maximum power point (MPP) characteristics. The absorber-IETL configuration's outstanding light-harvesting and carrier-collecting capabilities are highlighted by its high external quantum efficiency (EQE), which peaks at 90% in the 400–700 nm spectral region. These results confirm that α-Fe_2O_3 is a low-cost, effective electron transport layer that can be used to create HTL-free PSCs without sacrificing device performance. Additionally, temperature-dependent simulations showed that PCE gradually decreased as the temperature rose, emphasizing the need to optimize devices for thermal sensitivity. All things considered, our findings validate that α-Fe_2O_3-based HTL-free PSCs are a feasible and alluring route for scalable, reasonably priced photovoltaic applications.

Data Availability Statement

Data will be made available on request.

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Conflicts of Interest

The authors declare no conflicts of interest.

Ethical Approval and Consent to Participate

Not applicable.

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Manisha Kumari earned her M.Sc. (Honours) in Physics from DAV University, Jalandhar, in 2017. During her postgraduate studies, she developed a strong interest in nanoscience with a particular focus on energy-related applications such as photocatalysis and solar cell technologies. Her research project provided hands-on experience in the synthesis and characterization of nanomaterials, laying the foundation for her continued interest in harnessing nanotechnology for sustainable energy solutions. Her academic and research pursuits reflect a deep commitment to advancing the fields of photocatalysis and photovoltaic materials. She aspires to contribute to innovative developments in renewable energy through the design and application of advanced functional materials. (Email: manishash286@gmail.com)

Manpreet Kaur completed her M.Sc. (Honours) in Physics from Sant Baba Bhag Singh University, Jalandhar, in 2022. During her postgraduate studies, she developed a strong interest in nanoscience and gained valuable hands-on research experience through her project work in this field. Her academic journey has been driven by a deep passion for scientific research and innovation, with a particular focus on advancing knowledge in physics and nanotechnology. She is enthusiastic about contributing to cutting-edge research and is committed to pursuing impactful work in the areas of nanoscience and materials science. (Email: kaurmann1499@gmail.com)

Ankush Kumar Tangra is currently serving as an Assistant Professor in the Department of Physics and the Research & Incubation Center at Rayat Bahra University, Mohali–140103, Punjab, India. He holds a B.Sc. degree from the University of Jammu, and completed his M.Sc. and Ph.D. in Physics from DAV University, Jalandhar. His doctoral research focused on the multifunctionality of superparamagnetic nanoparticles for biomedical and solar cell applications. Dr. Kumar has published over 15 research papers in high-impact national and international journals. His work spans optoelectronics, perovskite solar cells, and biomedical applications, integrating both experimental and theoretical methodologies. He has also received accolades including Best Oral Presentation Award (2019) and Best Poster Award (2021). Currently, his research is centered on the development of nanomaterials for energy conversion and storage, with a particular focus on superparamagnetic nanomaterials for biomedical, optoelectronic, and photocatalytic applications. (Email: aktangra@gmail.com)