

Effect of Electron Transport Layer Donor Density on the Performance of FASnI₃ Perovskite Solar Cells

Muhammad Sofyan Parlin^{1,2}, Rossyaila Matsna Muslimawati³, Mohammad Kemal Agusta⁴, and Muhammad Haris Mahyudin^{4,*}

¹Master Program of Engineering Physics, Faculty of Industrial Technology, Institut Teknologi Bandung, 40132 Bandung, Indonesia

²PLN Indonesia Power UBP Cilegon, Jl. Raya Bojonegara, 42454 Kab.Serang, Indonesia

³Doctoral Program of Engineering Physics, Faculty of Industrial Technology, Institut Teknologi Bandung, 40132 Bandung, Indonesia

⁴Quantum and Nano Technology Research Group, Faculty of Industrial Technology, Institut Teknologi Bandung, 40132 Bandung, Indonesia

*Email: mahyuddin133@itb.ac.id

Abstract. This study focuses on enhancing the efficiency of FASnI₃-based perovskite solar cells by investigating variations in electron transport layer (ETL) donor density. The solar cell architecture used in this research is FTO/ETL/FASnI₃/PTAA, with ETL materials varied between TiO₂, ZnO, and SnO₂ and donor density varied from 10¹⁶ to 10²² cm⁻³. The results demonstrate that ZnO exhibits the highest power conversion efficiency, reaching 20.23%, making it a promising candidate for improving the performance of perovskite solar cells. This investigation underscores the impact of donor density in ETL materials on enhancing the efficiency of lead-free perovskite solar cells.

Keywords: *electron transport layer; lead-free perovskite solar cell; SCAPS-1D*

1 Introduction

The growing global need for sustainable energy solutions has fueled extensive research in renewable energy technologies, with solar energy being the primary focus. Among different photovoltaic technologies, perovskite solar cells (PSCs) with hybrid organic-inorganic halide elements inside have gained considerable attention from researchers due to their rapid efficiency improvements. Since 2009, when their power conversion efficiency (PCE) was only 3.8% [1], PSCs have now achieved a remarkable efficiency of around 25% [2]. However, the majority of PSCs nowadays contain lead, which raise environmental risks. Ongoing research is therefore focused on replacing the current absorber material with an eco-friendly alternatives [3]. Recently, tin-based perovskites have gained increasing attention as alternatives to lead-based ones, offering a favorable band gap, long carrier diffusion length, and non-toxic characteristics [4] [5].

The structure of hybrid PSCs typically comprises of electron transport layer (ETL), light-absorbing (perovskite) layer, and a hole transport layer, which are all deposited on a glass substrate. The ETL facilitates the transport of electrons generated in the perovskite layer to the cathode, ensuring efficient collection and utilization of electrical charges [6]. Additionally, the ETL acts as a blocking layer preventing direct contact between holes and the front electrode thereby hindering the unwanted electron-hole recombination [7]. Recent studies show that varying donor density in ETL greatly influences performance, Increasing the donor density from 10^{16} to 10^{22} cm^{-3} improves charge extraction and efficiency, with optimal results observed between 10^{19} and 10^{20} cm^{-3} . This range boosts current (J_{sc}) and open-circuit voltage (V_{oc}) while minimizing recombination. However, excessive densities ($> 10^{22} \text{ cm}^{-3}$) lead to higher recombination, reducing overall efficiency [8]. Donor density refers to the concentration of atoms contributing electrons to the conduction band, enhancing material conductivity. While higher donor density boosts charge transport in PSCs, it can also increase recombination rates, which reduces efficiency [7]. Thus, optimizing donor density requires a balance between improved conductivity and managing recombination.

In this study, we utilize a simulation tool to understand the effect of ETL's donor density on the performance of FASnI₃-based PSC (FTO/ETL/FASnI₃/poly(triaryl amine) PTAA). Several semiconductor materials including anatase TiO₂ [9][10][11], ZnO [12] [13] and SnO₂ [13] with variation of donor density are utilized as ETLs. The results show that donor density significantly affects the PCE, where a high PCE can be achieved with a high donor density. These findings potentially assist researchers in developing optimized ETL layers to enhance the performance of perovskite solar cells.

2 Methodology

The device architecture utilized in this study is FTO/ETL/FASnI₃/PTAA, as depicted in Figure 1. In this configuration, the thicknesses of the various layers are carefully defined: the fluorine-doped tin oxide (FTO) layer is set at 200 nm, the ETL at 50 nm, the perovskite layer (FASnI₃) at 500 nm, and the hole transport layer (PTAA) at 20 nm. These specific thicknesses are chosen to optimize the interaction and transport of charge carriers throughout the device.

In this investigation, the donor density within the ETL was varied from 10^{16} to 10^{22} cm^{-3} , allowing for an exploration of how different donor levels influence the overall performance of the solar cell. To analyze the efficiency and behavior of the FASnI₃-based PSCs, numerical simulations were performed using SCAPS 1-D simulation software. This powerful tool, developed at the University of Gent-Zwignarde in Belgium, facilitates the modeling of solar cell structures and enables researchers to predict device performance under various conditions [13].

The physical parameters for all materials incorporated in the simulation—such as band gaps, electron affinities, and mobilities—are detailed in Tables 1 and 2. These parameters are critical for accurately simulating the electronic behavior of the solar cell and understanding how variations in material properties affect overall device performance. All simulation processes were conducted at a temperature of 300 K, a frequency of 1.0×10^6 Hz, and under standard light sources of AM1.5G at 1000 W.m^{-2} .



Figure 1 Device schematic diagram of PSC

Table 1 Material parameters of layers used in the simulation

Parameters	PTAA[14]	FASnI ₃ [15]	FTO[16]
Thickness(nm)	20	500	200
Bandgap (eV)	3.2	1.41	3.6
Electron affinity (eV)	2.13	4.2	4.1
Dielectric permittivity	3	8.2	10
CB effective density of states (cm ⁻³)	2.0×10^{18}	2.2×10^{18}	2.2×10^{18}
VB effective density of states (cm ⁻³)	2.0×10^{18}	1.8×10^{19}	1.8×10^{19}
Electron mobility (cm ² /Vs)	0.001	1.6	100
Hole mobility (cm ² /Vs)	0.001	1.6	25
Electron thermal velocity (cm/s)	10^7	10^7	10^7
Hole thermal velocity (cm/s)	10^7	10^7	10^7
Defect density, Nt [cm ⁻³]	10^{15}	10^{13}	10^{15}
Shallow donor density, ND(cm ⁻³)	-	-	10^{17}
Shallow acceptor density, NA (cm ⁻³)	1.0×10^{22}	1.0×10^{20}	-

Table 2 Material parameters of different ETL layers

Parameters	TiO ₂ [17]	ZnO[15]	SnO ₂ [15]
Thickness(nm)	50	50	50
Bandgap (eV)	3.2	3.3	3.6
Electron affinity (eV)	4.1	4	4
Dielectric permittivity	55	8.656	9
CB effective density of states (cm ⁻³)	1.0×10^{21}	2.2×10^{18}	2.0×10^{19}
VB effective density of states (cm ⁻³)	2.0×10^{20}	1.8×10^{19}	4.0×10^{20}
Electron mobility (cm ² /Vs)	0.006	100	100
Hole mobility (cm ² /Vs)	0.006	25	25
Electron thermal velocity (cm/s)	10^7	10^7	10^7
Hole thermal velocity (cm/s)	10^7	10^7	10^7
Defect density, Nt [cm ⁻³]	10^{15}	10^{15}	10^{15}
Shallow donor density, ND(cm ⁻³)	$10^{16} - 10^{22}$	$10^{16} - 10^{22}$	$10^{16} - 10^{22}$
Shallow acceptor density, NA (cm ⁻³)	-	-	-

3 Results and discussion

3.1 Effect of donor density on device's performance

The donor density of ETL material plays a crucial role in optimizing the performance of perovskite solar cells. By adjusting the type and concentration of donor used, researchers can significantly enhance the efficiency of these devices. In this study, the donor density of the ETL layer was systematically varied, ranging from 10^{16} to 10^{22} cm⁻³. This variation allowed for a comprehensive analysis of how changes in donor density impact the initial performance parameters of the solar cells.

The results show that ZnO achieves the highest solar cell efficiency, peaking at 20.23% with a donor density of 10^{22} cm⁻³. At lower densities (10^{16} to 10^{19} cm⁻³), the PCE remains below 10%, but rapidly increases at higher densities, with Jsc jumping from 5.7 mA/cm² to over 20 mA/cm². This demonstrates that higher donor densities significantly enhance current generation and charge extraction, though Voc slightly declines to 1.10 V which might reflect trade-offs between enhanced conductivity and increased recombination at these levels. Comparatively, TiO₂ achieves a PCE of 18.54%, with Voc of 1.02 V, Jsc of 20.67 mA/cm², and FF of 87.87%. SnO₂ performs with a PCE of 20.18%, Voc of 1.10 V, Jsc of 20.75 mA/cm², and FF of 88.70%. Among these ETLs, ZnO shows the best overall efficiency as illustrated in Figure 2.

QE (Quantum Efficiency) at a wavelength of 400 nm reaches 80% for higher donor density (10^{21} to 10^{22} cm⁻³), meaning that 80% of the incoming photons at that wavelength are successfully converted into electrons within the device. This suggests that the material or system being tested performs very well in converting light into electrical signals at 400 nm.

Considering these findings and the complexities involved in the fabrication process, a donor density of 10^{22} cm⁻³ was determined to be the optimal choice for the ETL layer. This optimal donor density not only maximizes efficiency but also aligns with the practical considerations necessary for successful device manufacturing.

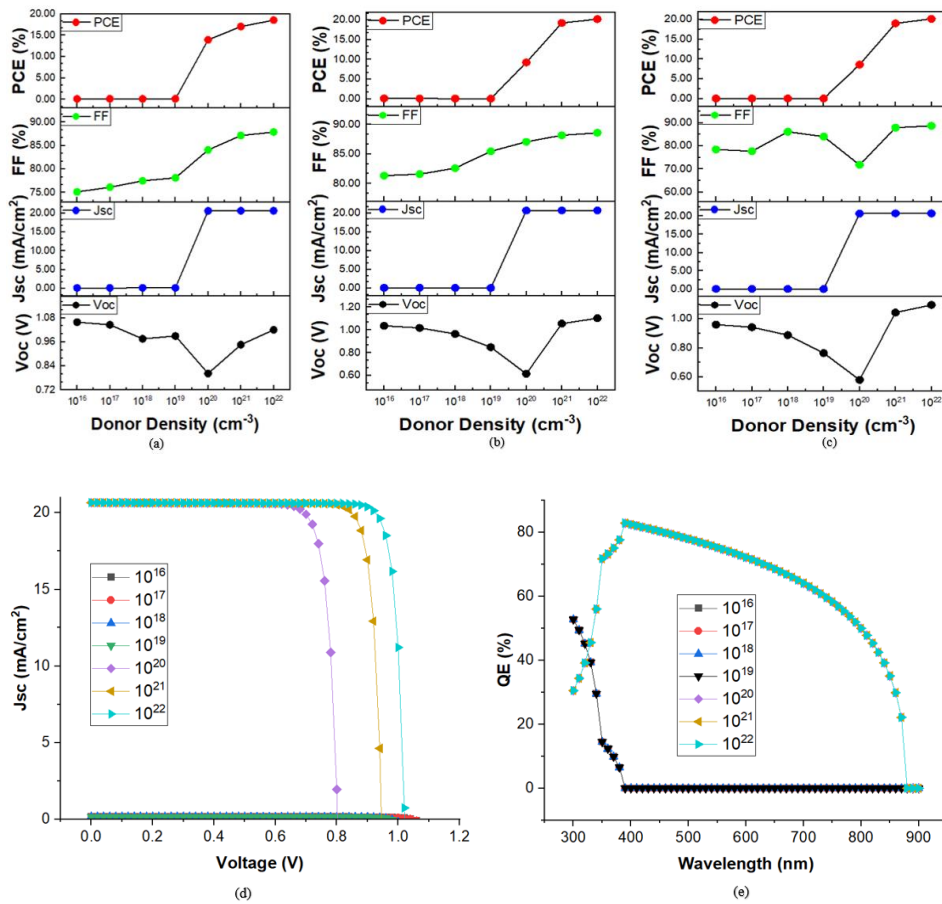


Figure 2 The impact of the ETL's donor density (a) TiO₂, (b) ZnO, (c) SnO₂ (d) J-V curve, and (e) QE characteristic

3.2 Band Alignment Analysis

The band alignment diagram for various ETLs is presented in Figure 3, providing a detailed view of how these layers interact within the solar cell architecture. In this schematic, FTO is depicted as the front contact, which plays a crucial role in facilitating electron flow. Directly beneath the FTO, the band alignment of the different ETL materials is clearly illustrated, showcasing their energy levels in relation to the perovskite layer, specifically FASnI₃.

The lowest unoccupied molecular orbital (LUMO) levels of the perovskite layer and the ETL (ZnO) are recorded at approximately -4.2 eV and -4.0 eV, respectively. This close alignment of LUMO levels establishes a highly efficient pathway for electron transport from the perovskite to the ZnO nanolayer, promoting better charge collection and reducing energy losses.

On the other hand, the highest occupied molecular orbital (HOMO) level of FASnI₃ is situated at -5.61 eV, which is notably lower than the HOMO level of the hole transport material (HTL), PTAA at -5.33 eV. This energy gap creates a significant driving force for the extraction of holes from the perovskite layer, enhancing the transfer of these positive charge carriers into the HTL. Such efficient hole extraction is critical for improving the overall performance and efficiency of the solar cell.

Proper band alignment with the absorber layer is a vital characteristic of an effective ETL. Ideally, the LUMO level of the ETL should be lower than that of the perovskite, while the HOMO level should be higher. This arrangement ensures that both electrons and holes can be effectively extracted and transported through their respective layers. Moreover, it is essential for the ETL to exhibit high transmittance in the ultraviolet (UV) spectrum, allowing energetic photons to pass through and be absorbed by the perovskite layer. This ability to transmit UV light maximizes the absorption of solar energy, further enhancing the device's efficiency [13].

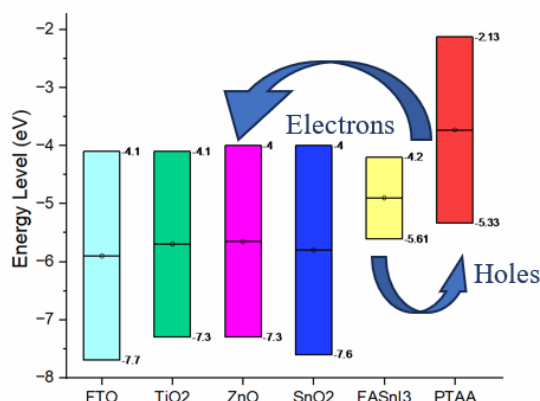


Figure 3 Band energy diagram of FTO/ETL/FASnI₃/PTAA

4 Conclusion

The simulated perovskite solar cell with different ETLs and donor density was analyzed. It was found that the donor density should be kept at around 10^{20} - 10^{22} cm⁻³ to achieve a high PCE. This confirms that fine-tuning donor density, particularly in ETLs like ZnO and SnO₂, is essential for optimizing solar cell efficiency. By adjusting ETL donor density, efficiency can exceed 20%, especially in lead-free perovskite cells. The simulations not only reinforced the understanding from the results but also provided broader insights into selecting ETL materials.

5 References

- [1] A. Kojima, K. Teshima, Y. Shirai, and T. Miyasaka, Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells, *Journal of the American Chemical Society*, 131(17), pp. 6050–6051, May 2009.
- [2] R. Ghosh, A. Singh, and P. Agarwal, Study on effect of different HTL and ETL materials on the perovskite solar cell performance with TCAD simulator, *Material Today Proceedings*, Jun. 2023.
- [3] G. Schileo and G. Grancini, Lead or no lead? Availability, toxicity, sustainability and environmental impact of lead-free perovskite solar cells, *Royal Society of Chemistry*, Jan. 07, 2021.
- [4] A. Tara, V. Bharti, S. Sharma, and R. Gupta, Device simulation of FASnI₃ based perovskite solar cell with Zn(O_{0.3}, S_{0.7}) as electron transport layer using SCAPS-1D, *Optical Materials (Amsterdam. Online)*, 119, Sep. 2021.
- [5] M. Kumar, A. Raj, A. Kumar, and A. Anshul, An optimized lead-free formamidinium Sn-based perovskite solar cell design for high power

- conversion efficiency by SCAPS simulation, *Optical Materials* (Amsterdam. Online), 108, Oct. 2020.
- [6] M. K. Hossain *et al.*, An extensive study on multiple ETL and HTL layers to design and simulation of high-performance lead-free CsSnCl_3 -based perovskite solar cells, *Scientific Reports*, 13(1), Dec. 2023.
- [7] I. Gulomova, O. Accouche, R. Aliev, Z. Al Barakeh, and V. Abduazimov, Optimizing Geometry and ETL Materials for High-Performance Inverted Perovskite Solar Cells by TCAD Simulation, *Nanomaterials*, 14(15), Aug. 2024.
- [8] A. Mohandes, M. Moradi, and M. Kanani, Numerical analysis of high performance perovskite solar cells with stacked ETLs/C60 using SCAPS-1D device simulator, *Optical and Quantum Electronics*, 55(6), p. 533, Apr. 2023.
- [9] M. K. Hossain *et al.*, Influence of natural dye adsorption on the structural, morphological and optical properties of TiO_2 based photoanode of dye-sensitized solar cell, *Materials Science-Poland*, 36, pp. 93–101, May 2018.
- [10] M. K. Hossain *et al.*, A comparative study on the influence of pure anatase and Degussa-P25 TiO_2 nanomaterials on the structural and optical properties of dye sensitized solar cell (DSSC) photoanode, *Optik*, 171, pp. 507-516, Oct. 2018.
- [11] M. K. Hossain *et al.*, Annealing temperature effect on structural, morphological and optical parameters of mesoporous TiO_2 film photoanode for dye-sensitized solar cell application, *Materials Science-Poland*, 35, pp. 868–877, Mar. 2018.
- [12] M. F. Pervez *et al.*, Influence of total absorbed dose of Gamma Radiation on Optical Bandgap and Structural Properties of Mg-Doped Zinc Oxide, *Optik - International Journal for Light and Electron Optics*, 162, pp. 140–150, Feb. 2018.
- [13] X.-F. Diao *et al.*, Study on the Property of Electron-Transport Layer in the Doped Formamidinium Lead Iodide Perovskite Based on DFT, *ACS Omega*, 40, Nov. 2019.
- [14] S. Ravishankar *et al.*, Multilayer Capacitances: How Selective Contacts Affect Capacitance Measurements of Perovskite Solar Cells, June 2021.
- [15] R. S. Almufarij *et al.*, Improving performance and recombination losses in lead free formamidinium tin based perovskite solar cells, *Materials Chemistry Physics*, 307, Oct. 2023.
- [16] S. Mattaparthi *et al.*, Design of an eco-friendly perovskite $\text{Au/NiO/FASnI}_3/\text{ZnO}_{0.25}\text{S}_{0.75}/\text{FTO}$, device structure for solar cell applications using SCAPS-1D, *Results in Optics*, 12, Jul. 2023.
- [17] A. Hosen, M. S. Mian, and S. R. Al Ahmed, Improving the Performance of Lead-Free FASnI_3 -Based Perovskite Solar Cell with Nb_2O_5 as an Electron Transport Layer, *Advance Theory Simulation*, 6(2), Feb. 2023.

Acknowledgement

This work was supported and funded by PT PLN (Persero) and PT PLN Indonesia Power.