A novel approach on FormamidiniumTinIodide-based Perovskite solar cell for the best replacement materials of HTL and ETL by using Solar cell Capacitance Simulation

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Abstract

Perovskite Solar Cells (PSC) research has increased noticeably in recent years as a result of significant improvements in their performance. Perovskite solar cells are a new development in Photovoltaic technology. Because PSCs are inexpensive, have the ability to tune the bandgap and are a promising future option for meeting cell efficiency limits and strong broad optical absorption. Toxicity is an important factor in the development of organic and inorganic Perovskite solar cells. PSCs based on Sn are a worthy competitor to PSCs based on Lead (Pb). The majority of them used Methylammonium tin iodide ($CH_3NH_3SnI_3$) material as an absorber layer because it has greater absorption but suffers from temperature instability. As a result, in this work, we use Formamidinium tin iodide ($FASnI_3$) absorber, which has higher temperature stability than $CH_3NH_3SnI_3$Methylammonium tin iodide with a band gap of 1.4 eV. Solar cell Capacitance simulation used in this work to create $FASnI_3$-based solar cells. This paper proposes a Power Conversion Efficiency of 24.22% for PSCs. For maximum Power Conversion Efficiency (PCE), the optimized thickness values are 10nm for CuI(Hole transport layer), 850nm for $FASnI_3$, and 20nm for ZnOS (Electron Transport Layer). The best temperature range for device performance is around 340K. SCAPS was used to calculate the current work. In addition, we demonstrated that ZnOS is the most promising ETL as a TiO_2 replacement in this work. The proposed work focuses on paving the way for novel eco-friendly non-toxic PSCs as well as investigating optimisedVoltage output circuit (Voc), Current density(Jsc), Fill factor (FF), and Power conversion Efficiency (PCE) device characteristics.

Keywords: Lead-free, Perovskite solar cell, SCAPS-1D Simulation, Zinc oxysulphide (ZnOS), Copper iodide (CuI), Electron transport layer (ETL), Hole transport layer (HTL)

1. Introduction

Nowadays Perovskite solar cell is the mainstream in PV technology with high PCE and PSCs is the best competitor for Si-wafer based solar cells [1]. Recently in perovskite solar cell, halides-based PSCs has the most promising absorber materials in PSCs [2]. The power conversion efficiency of PSCs which is based upon Pb-PSCs had a dramatic improvement from 3.08% to recently certify the value of 25.5% [3]. However, there are some shortcomings faced on Pb based PSCs. Like toxicity, thermal stability, air stability and non-ecofriendly to the humans. These are some of the disadvantages for Pb-based PSCs [4]. For that reasons pollution free and safety to humans, it is emergently needed to develop a nontoxic or low toxic metal to replace the Pb based ab-layer of PSCs. Therefore, research had to be made to replace Pb with some low and nontoxic materials in PSC_S [5]. Sn, Cu, Bi, and Sb have all been studied as potential replacements for Pb-PSCs [6]. Sn has emerged as the most promising immediate replacement material for Pb-based PSCs among these. Because Sn belongs to the same group as Pb in the periodic table, its electric and optical properties are too similar, making Sn the best replacement material in PSCs [7].

The general formula for organic and inorganic halide perovskite solar cells is ABX_3, where A and B are cations and X is always a halogen. MA, FA, and Cs are the most commonly used cations (A) in PSC [8]. From 4^{th} and 7^{th}, group elements are widely used as a B cation and X halogen respectively [9]. In this work, we use Sn be the replacement of Pb. Sn is not only for the alternative ion to Pb, it is also to enhance ecofriendly of PSCs [10]. Due to temperature instability in $CsSnI_3$ and $MASnI_3$ we use the $FASnI_3$ as the Ab-layer in this simulated work [11]. $FASnI_3$ had a more solid perovskite structure, more stable and also the air stability is high compared with $MASnI_3$. These are the reasons we use $FASnI_3$ having a perovskite layer for this simulated Device. Recently many approaches have been done to improve the $FASnI_3$ based device [12]. $FASnI_3$ has higher carrier mobility than $MASnI_3$ according to Milot et al[13]. Krishna moorthy groups

published the first study on $FASnI_3$-based PSCs in 2015, with an efficiency of 1.41 percent [14]. $FASnI_3$ with Eg (1.4eV) which is wider than $MASnI_3$ and $CsSnI_3$ (1.30eV) respectively and narrow to Pb based PSCs. Also, in $FASnX_3$ can be tuned the Eg with different halides [15]. Recently CuI had attained PCE 17.6% which is based upon spray deposition method [16]. CuI had a high electric conductivity compared with Spiro-MeOTD. For that reason, we use CuI as a HTM in this work. CuI [17].Bansal had investigated $MASnI_3$ based solar cell with different ETL and HTL they achieved the PCE 21.1% in that ZnOS act as ETL [18].Currently, before fabricating a cell or a device, the theoretical studies help more to understand and find the behavior of the cell Devices [19].In recent days, many simulation devices are studied for PSCs with novel materials in SCAPS (1D) [20]. The initial structure is based on an 11.01% working PCE. After several optimizations on the thickness of the ab-layer, HTL and ETL, the simulated devices achieve an efficiency of 24.22%. At this present work, we optimized Novel $FASnI_3$ based Perovskite solar cell with CuI and ZnOS act as a very promising HTL and ETL respectively.Replacement of Spiro-MeOTD and TiO_2 and also $FASnI_3$ material is the best replacement for $MASnI_3$ based solar cell.

2. Methodology and Device Simulation

2.1. Basic Structure of the Device

The device's simulated configuration is FTO / ZnOS / FASnI3 /CuI /Au. To date, three types of PSCs have been investigated: mesoporousplanar, and inverted planar. The inverted planner configuration has been completed in this work and is shown in Fig.1. (a) Device configurations of simulated PSCs, CuI as HTL and ZnOS as ETL. Energy band diagram for this device also shown in Fig (b). In Fig.1(c, d) shown the initial Jsc, Voc, and %PCE- wavelength studies. All the basic parameters are collected from various research papers and tabulated in Table.1 [3, 10, 15, 21, and 22]. Meng and his group report that at low temperature the inverted planar would exceed over 18% of efficiency flexibility with J-V hysteresis [23]. Table.2. Summaries the N_t, $N_{D,}$

$N_{A,}$ for the configuration of the device and the work function of front and back contact as FTO (4eV) and Au (5.1 eV) respectively [24,25].

2.2. Methodology of Simulation

The simulated was performed in SCAPS 1D under AM 1.5G illumination. This simulation carries only inside the SCAPS-1D and mainstream to derive from the following fundamental equations Poisson, hole and electron continuity. All the simulated results were examined in separate sections through graphs for each stage. In initial structure results, values of is PCE 11.01%, after several optimization on the absorber layer, HTL, ETL, and temperature in this device we constructed a novel PSCs with high efficiency.

3. Results and Discussions

3.1. Optimization and Simulation of $FASnI_3$ PSC

3.1.1. Effect of Temperature

The temperature of the solar cell has an effect on its overall performance. In this simulation, we kept the temperature constant at 300K at first and then varied it from 300K to 400K to determine the effect of working temperature on PCE, Voc, Jsc, and FF for the best ab-layer thickness, as shown in fig. In this simulated device, it was discovered that as the temperature increased, the PCE, Voc, Jsc, and FF of the solar cell decreased, because of carrier concentrations, charge carrier mobility and the material's bandgap at high temperatures (mariSoucase, et.al.2016). The efficiency slightly decreased from 24.09 % to 23.64% at (300-400) K. The diffusion length reduces and series resistance increases. The resultant is decreased in PCE and FF (Mandadapu and group at 2017), because of the increase in energy enhanced recombination, electrons become unstable at higher temperatures in a solar cell, resulting in a low PCE (Mandadapu 2017). For that 340k is the working temperature for this simulation work.

3.1.2. The Effect of the Ab-layer Thickness

The ab-layer in PSCs absorbs photons from sunlight whose energy is greater than the bandgap of the ab-layer, which causes excisions. These preciseions are essentially charged electron-hole pairs. To maximize PCE, it is necessary to understand the impact of defect density on PSC performance. Because the Ab-layer is a critical factor in determining the performance of PSCs, its effect on solar cell output parameters has been studied using simulation. The active layer thickness was increased from 100nm to 1050nm in 850nm increments and the effect on performance parameters is shown in Fig (3). The device's performance is excellent at 850nm, and it achieves the maximum efficiency. At 850nm, the device's performance is excellent, with the maximum efficiency of 24.22% achieved by using Voc 6.20 V, Jsc 30.77 mA/cm2, and FF 12.68%.

3.1.3. Thickness optimized on Electron Transport Layer

Figure 4 illustrates the effect of ETL thickness and performance on ab-layer at 850nm. When the ETL thickness is 20nm, we get the best performance on the simulated device with the highest PCE of 24 %, which is increased by 0.02 % efficiency with FF of 12.68 %, Voc of 6.20V, and Jsc of 30.77 mA/cm2.

3.1.4. Thickness optimized in Hole Transport layer

From Fig.5. Shows the impact on the HTL and the device performance at 850nm Ab-layer. When the thickness of the Ab-layer is at 850nm, we reach the maximum PCE 24.22% at 10nm thickness of HTL with FF of 12.68%, Voc of 6.20V, Jsc of 30.77 mA/cm^2.

3.1.5. Effect of Nt of the optimized device

In this simulation, the Nt of ab layered varied between 10^{12} cm^{-3} and 10^{18} cm^{-3} to find the best absorber thickness to find the variation in PCE, as shown in the fig 6,7,8 for the simulated device. PCE at other

parameters of the simulated solar cell decreased as the absorber layer's Nt increased. As the defect density decreased, the efficiency stabilized at a certain point in this work, with the device performing well at 10^{16} cm^3 (Nt) of absorber layer. The device performs best at $10^{18}cm^{-3}$ and $10^{20}cm^{-3}$ for ETL and HTL, respectively.

3.1.6. Effect of Bandgap in the simulation device

Sn-based PSC has a tunable band gap ranging from 1.3eV to 2.15eV. (vedanayakam,mandadapu.,2017). In this simulation, the bandgap of the optimized solar cell ranged from 1.2eV to 2.0eV for the best ab-layer to determine the variation in efficiency and other parameters. As shown in the figure 9, as the bandgap increased, PCE,FF, and Jsc decreased slightly while Voc increased. Jsc decreased as the bandgap increased, owing to less electron generation. After several simulations, the device was tested at 1.4eV. Similarly, we optimised the bandgap of ETL and HTL until we found the best performance of CuI at 2.8 eV and ZnOS at 2.4eV after several attempts.Figure 10 depicts the external quantum efficiency curve for the device's best absorber layer.

4. Conclusion

1D SCAPS was used in this study to investigate the optimized and simulated behaviors of the Sn-based PSC with ETL as ZnOS and HTL as CuI configuration. The working temperature 340k for this simulation study at standard illumination of Air mass at 1.5G, the perovskite layer from150nm to 1050nm and the optimum layer range for HTL and ETL as 10-50nm respectively both layers. The best layer thickness ranges from ZnOSare 20nm and CuI is 10nm respectively. The best defect density is performed at $10^{16}cm\text{-}^3$ for this simulated device. The band gap of ab-layer HTL, ETL were to change from after several simulation 1.4eV, 2.4 eV, 2.8 eV, respectively. The device performed well and good at when Nt of the ab-layer $10^{16}cm^{-3}$ with bandgap 1.4eV. When the optimized input parameter values are considered, the highest efficiency

achieved is 24.22 % (FF of 12.68 %, Voc of 6.20V, Jsc of 30.77 mA/cm^2). When we use CuI as the hole transport layer and ZnOS as the electron transport layer in a $FASnI_3$-based solar cell, we get the best results, and CuI and ZnOS are the best replacements for Spiro-OMeTADand TiO_2. The simulated result stands for only replacement materials for $FAPbI_3$, Spiro-OMeTAD and TiO_2 because Pb based material had high toxicity for that reason we use Sn based ab-layer in this work. Spiro-OMeTAD and TiO_2 are too costly for that reason in this work we used lost cost CuI, ZnOS as HTL and ETL respectively.

Acronyms

PSC-Perovskite solar cell

PV- Photovoltaic technology

SCAPS- Solar cell Capacitance simulation

$FASnI_3$ –Formamidinium tin iodide

$MASnI_3$-Methylammonium tin iodide

ZnOS- Zinc oxysulphide

FA-Formamidinium

Cs- Cesium

MA-Methylammonium

Sn- Tin

Pb-Lead

Cu- Copper

Copper iodide- CuI

ETL- Electron transport layer

HTL- Hole transport layer

TiO_2-Titanium Oxide

Spiro-OMeTAD - 2,2',7,7'-Tetrakis[N,N-di(4-methoxyphenyl)amino]-9

Voc- Voltage output circuit (Voc),

Jsc- Current density

FF- Fill factor

PCE- Power conversion Efficiency

N_t- Donor

N_A- Acceptor

Table.1 [3,10,15,20,21,22]

Material property	ZnOS	$FASnI_3$	CuI
Thickness 't'(nm)	Varied	Varied	Varied
Bandgap 'Eg' (eV)	2.8	1.4	2.6
Electron affinity 'χ' (eV)	3.9	3.52	3.9
Relative Dielectric permittivity 'ε_r'	3	8.2	4
CB effectivite density of state 'N_c' (cm^{-3})	1E+20	1.0E+18	1E+21
VB effective density of state 'N_c' (cm^{-3})	1E+20	1.0E+18	2E+20
Electron mobility 'μ_n' (cm^2/V.s)	1E-4	22	0.01
Hole mobility 'μ_p' (cm^2/V.s)	1E-4	22	0.01
Donor concentration 'N_D'(cm^{-3})	1E+7	0	1E+20
Acceptor concentration 'N_A'(cm^{-3})	1E+7	7.0E+16	_
Defect density 'Nt' (cm^{-3})	-	2.0E+15	_

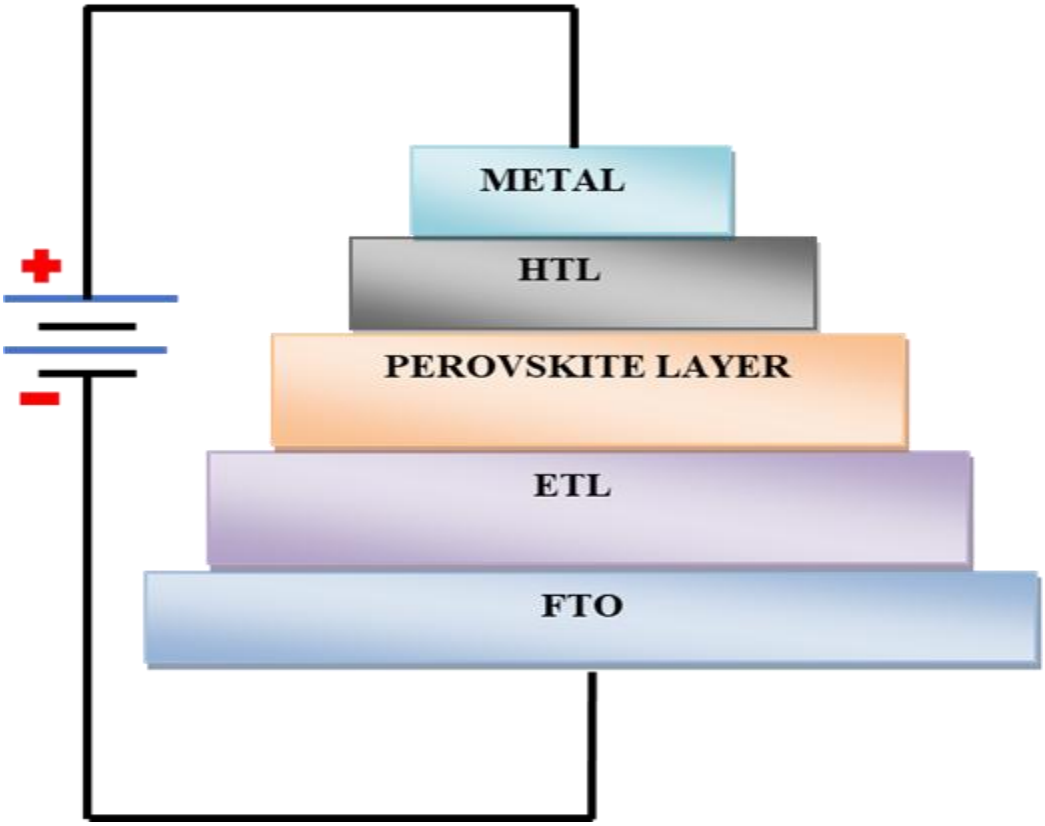


Figure.1 (a). Cell configuration of $FASnI_3$ designed solar ce

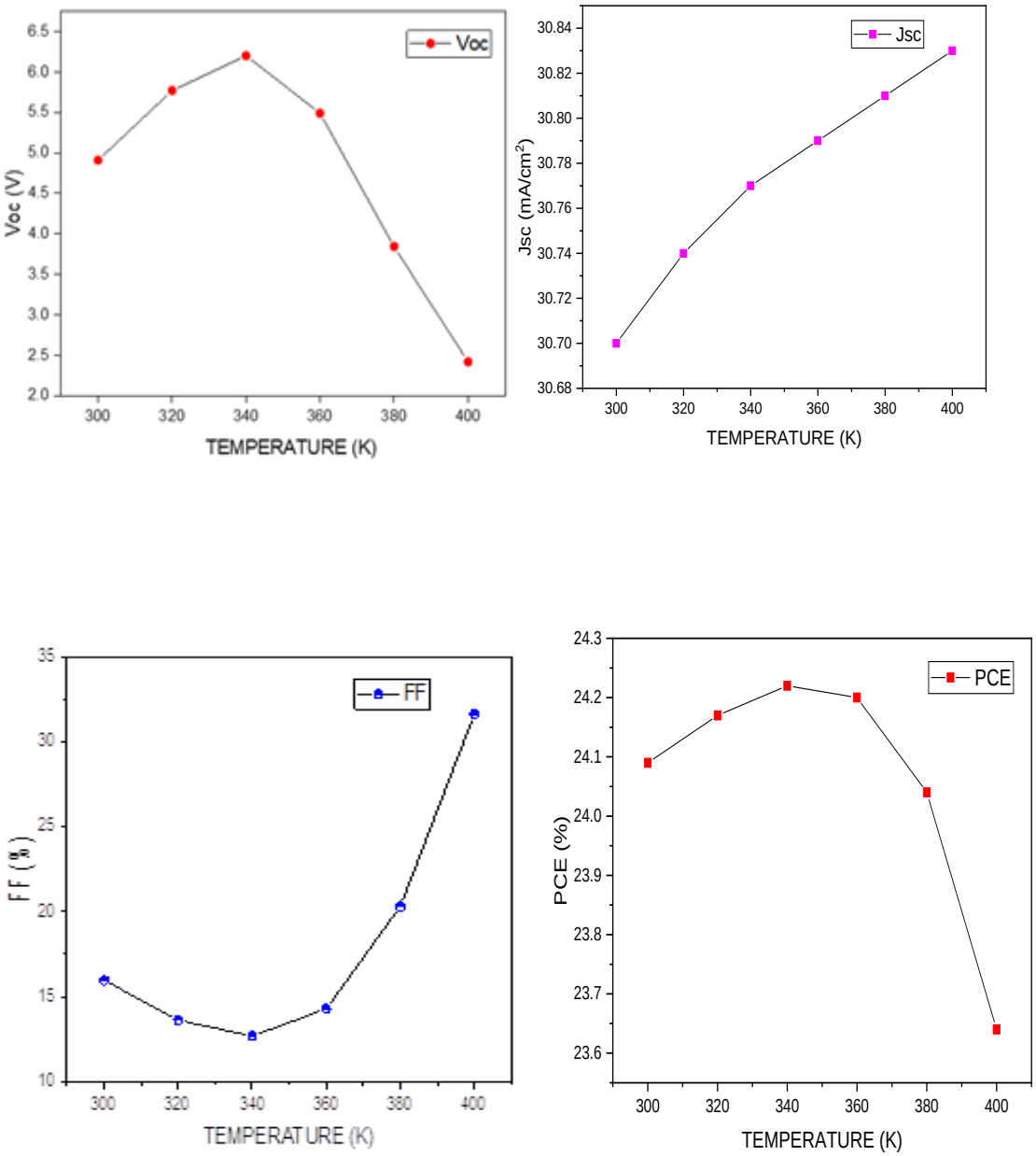


Fig.2. Temperature VS Voc, Jsc, FF, PCE

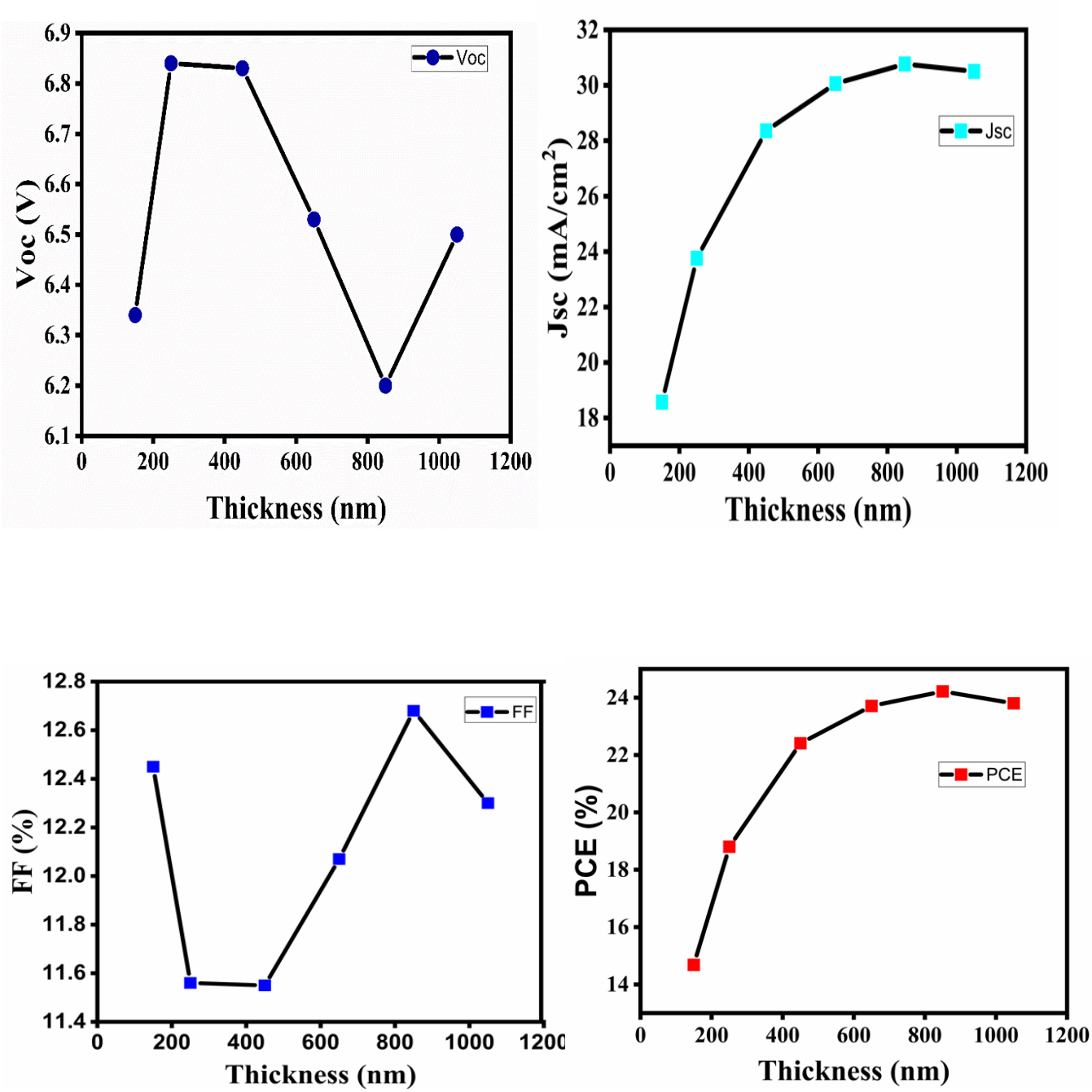


Fig.3. Thickness of active layer Vs Voc, Jsc, FF, PCE

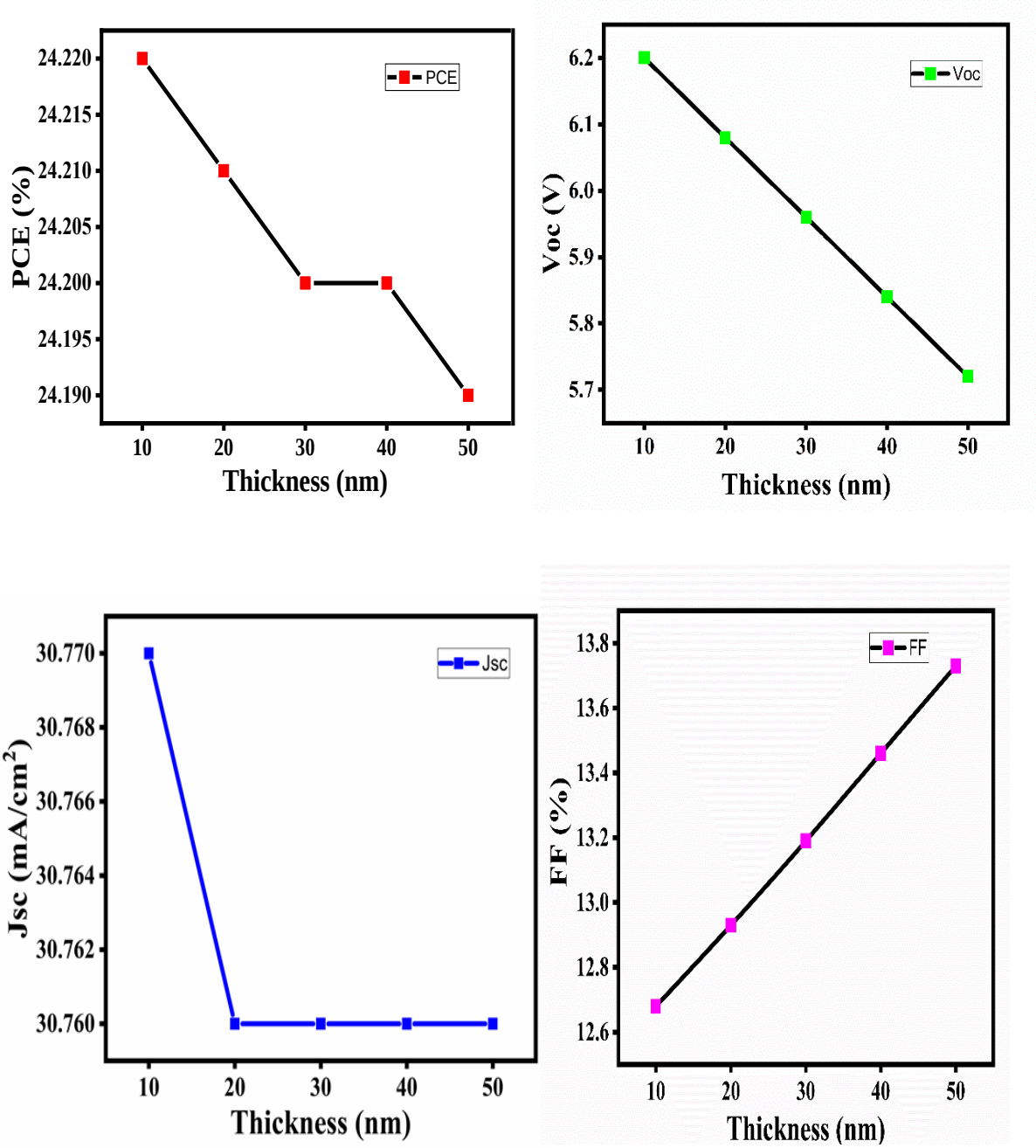


Fig.4. Thickness of CuI Vs Voc, Jsc, FF, PCE

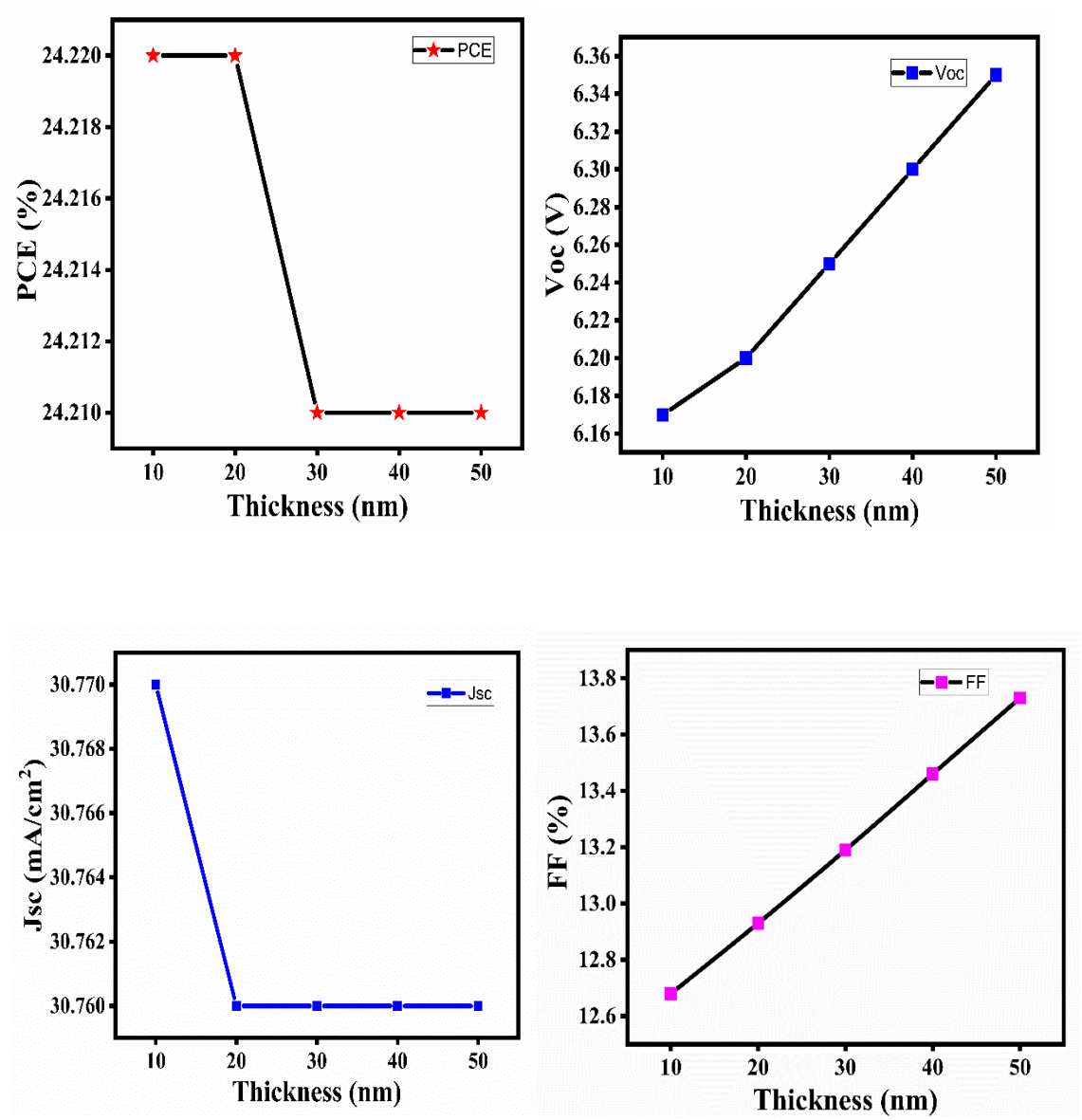


Fig.5. Thickness of ZnOS Vs Voc, Jsc, FF, PCE

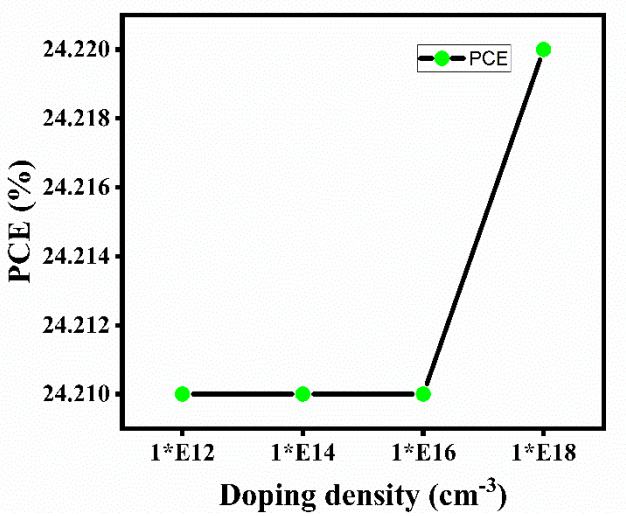


Fig.6.HTL Vs Doping density

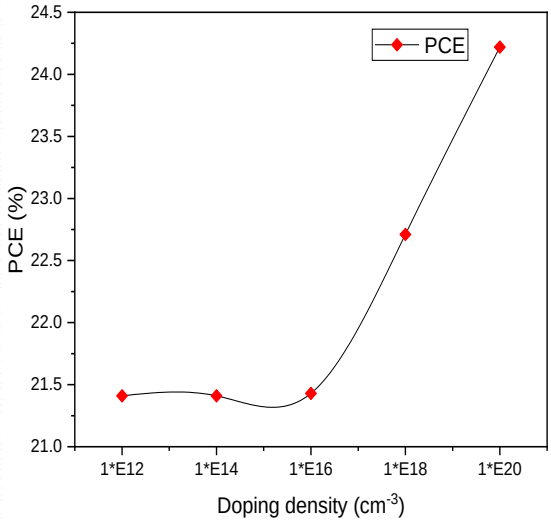


Fig.7. ETL Vs Doping density

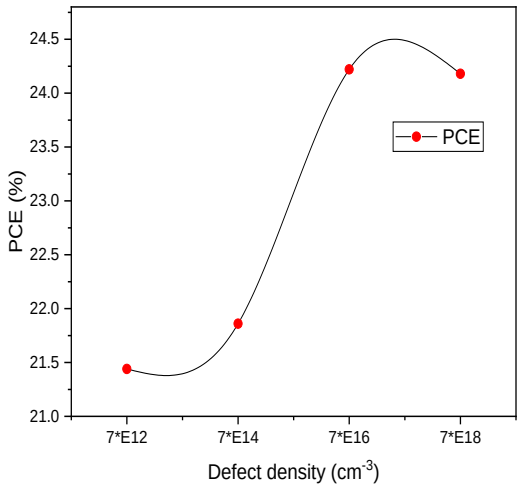
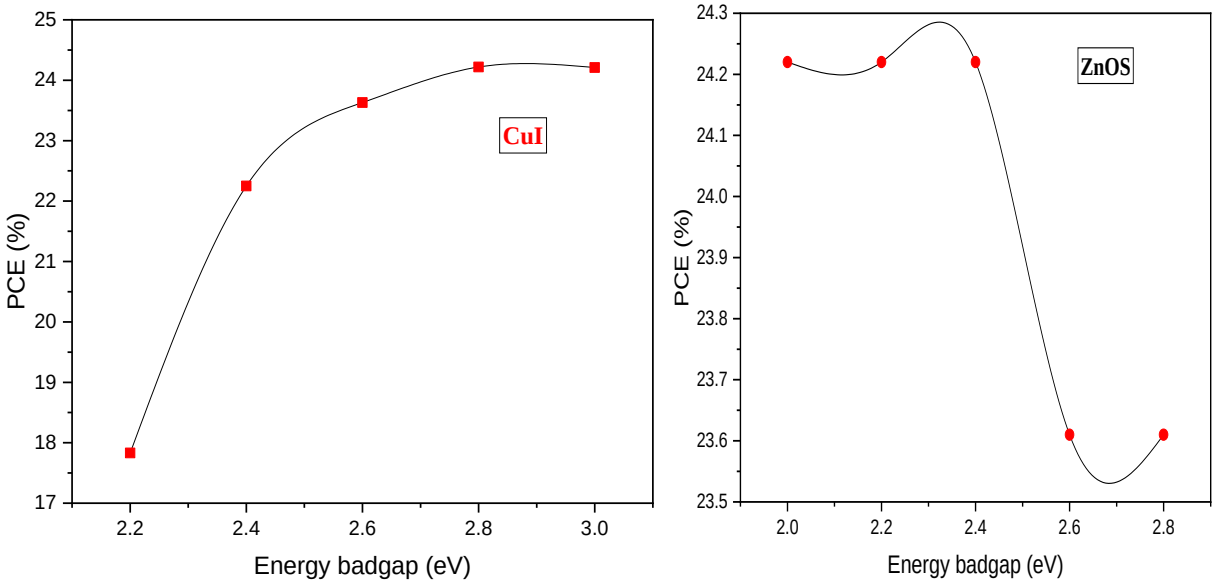


Fig.8. Defect density Vs PCE



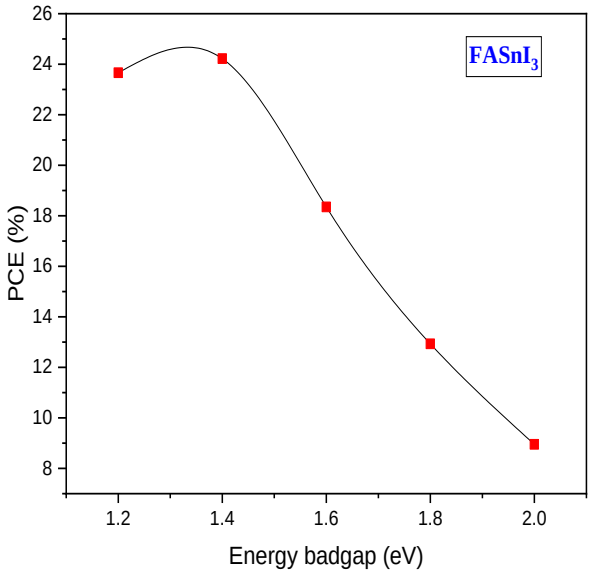


Fig.9. Bandgap for best perovskite layer, HTL and ETL

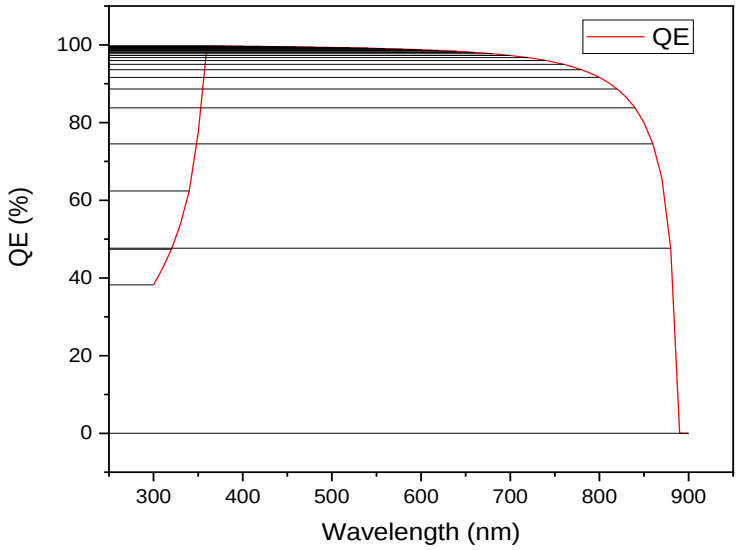


Fig.10. QE vs Wavelength

AUTHORS CONTRIBUTION

First author has involved writing, Analysis and formulating.

Second author has involved Correction, Analysis and formulating.

DECLARATION OF INTEREST STATEMENT

The authors declare that they have no known competing financial interest or personel relationship that could have appeared to influence the work reported in this paper.

HIGHLIGHTS

- Novel approach on $FASnI_3$ based PSC for the best replacement materials of HTL and ETL
- Using low cost materials only as a ETL and HTL layers
- We have designed simulated, compare, and analyzed the high efficiency of FASnI3 and based PSC solar cell with ETL as ZnOS and HTL as CuI.
- Using 1D-SCAPS for numerical analysis.
- Informed simulation results can provide a unique way to improve the efficiency of $FASnI_3$based Perovskite solar cell.
- In this paper we attain 24.22% efficiency of $FASnI_3$ based solar cell
- We also suggesting CuI and ZnOS as an alternative HTL and ETL respectively. Because of its low cost fabrication and excellent mobility.

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