# Analyzing ecofriendly perovskite solar cells

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**Abstract -** *This research paper presents an analysis of highly efficient eco-friendly perovskite solar cells using the SCAPS 1D simulator. Perovskite solar cells(PSCs) have gained a lot of attention as an alternative to conventional silicon –based solar cells due to their high power conversion efficiency (PCE) and low cost fabrication.The study investigates the impact of different –different hole transport layers(HTL) and electron transport layers(ETL) on the performance of the perovskite solar cell.And finding which(HTL/$CH_3NH_3SnI_3$/ETL) combination would be best.The graphs for capacitance-voltage, current density voltage, fill factor and quantum efficiencies are also evaluated. Furthermore,we have used $Cu_2O$,Spiro-MeOTAD and CuO as our best HTL and ZnO , $TiO_2$ and $WS_2$ as our best ETL.The simulation results show that optimizing these parameters can significantly enhance the device efficiency .The study also highlights the potential of perovskite solar cells to be an efficient and cost –effective solution for renewable energy generation.*

***Key Words***: Solar cells - electron transport layer – hole transport layer-SCAPS 1D-PCE

## 1.INTRODUCTION

The world's energy needs have been increasing day by day. The depletion of energy sources and fossil fuels, natural gas, coal, etc. have a negative impact on our societies and the environment [1]. Therefore, the development of alternative energy resources and sustainable energy sources considering economic and environmental aspects is the focus of research worldwide [1]. Perovskite materials are widely used in photovoltaic devices such as solar cells and light-emitting diodes (LEDs) [2]. The energy conversion efficiency of PSCs has improved rapidly in recent years. Lead-based metal halide perovskites have revolutionized photovoltaics in recent years, dramatically increasing the efficiency from 3.8% in 2009 to 25.7% in 2022 [3].But those perovskite are mostly lead based and the use of toxic materials and organic cations in PSCs presents challenges for commercial applications.

In this work, we analyze the solar cells with the help of SCAPS software. There are five layers consisting of ITO/ETL/ $CH_3NH_3SnI_3$ /HTL/Au. ZnO, $TiO_2$ and $WS_2$ was used as electron transporting layer (ETL) and $Cu_2O$, Spiro-MeOTAD and CuO was used as hole transport layer (HTL).ITO and Au are used as they are best suitable[4]. These layers have the advantages of being eco friendly and highly efficient. We analysed the performance of the ETL and HTL layer. We have also shown the influence of absorber and ETL thickness , working temperature, and current-voltage density (J-V) characteristics. We also demonstrated the effect of the layer thickness on PCE and J-Vand I-V characteristics of $CH_3NH_3SnI_3$.

## 2. Device structure and simulation

SCAPS 1D software[5] [6][7][8]solves the poisson equation(a) ,continuity equation of electron(b) and holes(c).[9]

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\psi}{dx}\right) = q[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (a)$$

$$\frac{dp_n}{dt} = G_p - \frac{p_n - p_{n0}}{\tau_p} + p_n\mu_p\frac{d\xi}{dx} + \mu_p\xi\frac{dp_n}{dx} + D_p\frac{d^2p_n}{dx^2} \quad (b)$$

$$\frac{dn_p}{dt} = G_n - \frac{n_p - n_{p0}}{\tau_n} + n_p\mu_n\frac{d\xi}{dx} + \mu_n\xi\frac{dn_p}{dx} + D_n\frac{d^2n_p}{dx^2} \quad (c)$$

where, $G$, $\tau_n$, $\tau_p$, $D$, $q$, $\Psi$, $\mu_n$, $\mu_p$, $n$ $(x)$, $p$ $(x)$, $n_t$ $(x)$, $p_t$ $(x)$, N−A (x) , N+D (x) and $\xi$ denote the generation rate, electron lifespan, diffusion coefficient, electron charge, electrostatic potential, electron mobility, hole mobility, free electrons concentration, free holes concentration, trapped electrons concentration, trapped holes concentration, ionized acceptor concentrations, ionized donor concentrations and electric field.[9]

**Table 1** :Input parameters of the ITOs, ETLs and absorber layer

| Parameters | ITO | $TiO_2$ | ZnO | $WS_2$ | $CH_3NH_3SnI_3$ |
|---|---|---|---|---|---|
| Thickness(nm) | 500 | 30 | 50 | 100 | 500 |
| Band gap,$E_g$(eV) | 3.5 | 3.2 | 3.3 | 1.8 | 1.3 |
| Electron affinity,(eV) | 4 | 4 | 4 | 3.95 | 4.170 |
| Dielectric permittivity(relative), | 9 | 9 | 9 | 13.6 | 6.5 |
| CB effective density of states,$N_c$($1/cm^3$) | 2.20E+18 | 2.0E+18 | 3.7E+18 | 1.0E+18 | 2.2E+19 |
| VB effective density of states,$N_v$($1/cm^3$) | 1.8E+19 | 1.8E+19 | 1.8E+19 | 2.4E+19 | 2.2E+19 |
| Electron mobility,($cm^2/Vs$) | 20 | 20 | 100 | 100 | 1.6 |
| Hole mobility,($cm^2/Vs$) | 10 | 10 | 25 | 100 | 1.6 |
| Shallow uniform acceptor density,$N_A$($1/cm^3$) | -------- | --------- | ---------- | ---------- | 3.2E+15 |
| Defects density,$N_t$($1/cm^3$) | 1.0E+15 | 1.0E+15 | 1.0E+15 | 1.0E+15 | 1.0E+13 |
| References | [4][10][11][12] | [13][10][4] | [8][14][4] | [10][15][4] | [16] |

**Table 2**: Input parameters of the HTLs

| Parameters | $Cu_2O$ | Spiro-MeOTAD | CuO |
|---|---|---|---|
| Thickness(nm) | 50 | 200 | 50 |
| Band gap,$E_g$(eV) | 2.2 | 3 | 1.51 |
| Electron affinity,(eV) | 3.4 | 2.2 | 4.07 |
| Dielectric permittivity(relative), | 7.5 | 3 | 18.1 |
| CB effective density of states,$N_c$(1/cm$^3$) | 2.0E+19 | 2.2E+18 | 2.2E+19 |
| VB effective density of states,$N_v$(1/cm$^3$) | 1.0E+19 | 1.8E+19 | 5.5E+20 |
| Electron mobility,(cm$^2$/Vs) | 200 | 2.1E-3 | 100 |
| Hole mobility,(cm$^2$/Vs) | 8600 | 2.16E-3 | 0.1 |
| Shallow uniform acceptor density,$N_A$(1/cm$^3$) | 1.0E+18 | 1.0E+18 | 1.0E+18 |
| Shallow uniform donor density,$N_D$(1/cm$^3$) | ------- | ---------- | --------- |
| Defects density,$N_t$(1/cm$^3$) | 1.0E+15 | 1.0E+15 | 1.0E+15 |
| References | [13][4] | [4][8] | [4] |

| Interface | Defect type | Capture cross-section:electrons /holes(cm$^3$) | Energetic Distribution | Reference for defect energy level | Total density (cm$^{-2}$) |
|---|---|---|---|---|---|
| ETL/ $CH_3NH_3SnI_3$ | Neutral | 1.000E-15[17] 1.000E-15 | Single | Above the EV maximum | 1.000E+15[17] |
| $CH_3NH_3SnI_3$/HTL | Neutral | 1.000E-15[12] 1.000E-15 | Single | Above the EV maximum | 1.000E+15[12] |

## 3. RESULTS AND DISCUSSIONS

**Table 3**: Results of solar cells with different –different HTL layers

| Optimized device | Voc(V) | Jsc(mA/cm$^2$) | FF(%) | PCE(%) |
|---|---|---|---|---|
| $TiO_2$/ $CH_3NH_3SnI_3$/ $Cu_2O$ | 1.0091 | 31.642 | 81.20 | 25.93 |
| ZnO / $CH_3NH_3SnI_3$/ $Cu_2O$ | 1.0098 | 31.881 | 81.23 | 26.15 |
| $WS_2$/ $CH_3NH_3SnI_3$/ $Cu_2O$ | 0.98 | 19.13 | 81.23 | 15.30 |

**Table 4**: Results of solar cells with different-different ETL layers

| Optimized device | Voc(V) | Jsc(mA/cm$^2$) | FF(%) | PCE(%) |
|---|---|---|---|---|
| ZnO/ $CH_3NH_3SnI_3$/ $Cu_2O$ | 1.01 | 32.53 | 81.22 | 26.70 |
| ZnO/ $CH_3NH_3SnI_3$/ Spiro-MeOTAD | 0.88 | 32.45 | 71.98 | 20.68 |
| ZnO/ $CH_3NH_3SnI_3$/ CuO | 0.98 | 33.41 | 83.13 | 27.28 |

## 3.1 Discussions

### 3.1.1. Effect of thickness –

**FOR HTL:**

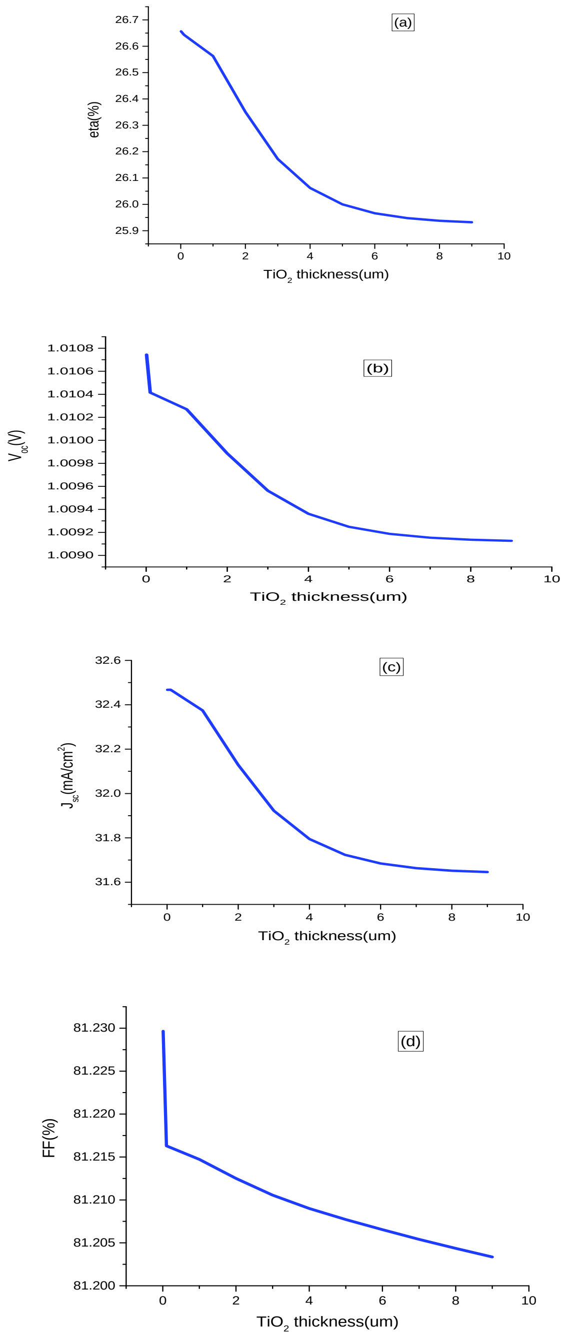


**Fig.1** Dependence of layer thickness of $TiO_2$ on PCE (%), Voc(V), Jsc(mA/cm$^2$), FF (%)

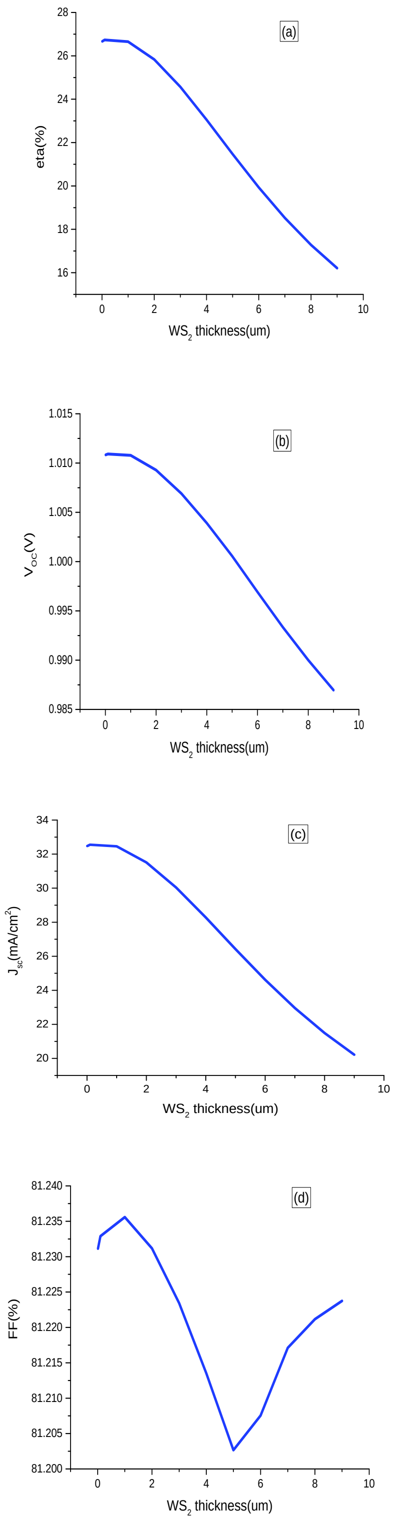


**Fig.2** Dependence of layer thickness of $WS_2$ on PCE (%), Voc(V), Jsc(mA/cm$^2$), FF (%)

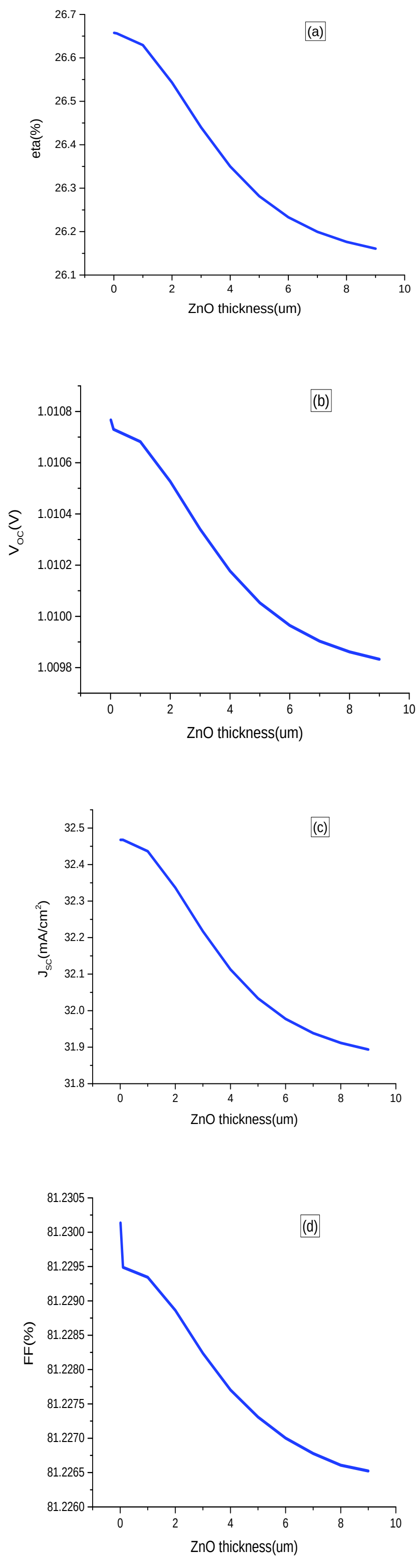


**Fig.3** Dependence of layer thickness of ZnO on PCE (%), Voc (V), Jsc(mA/cm$^2$), FF (%)

**FOR ETL:**

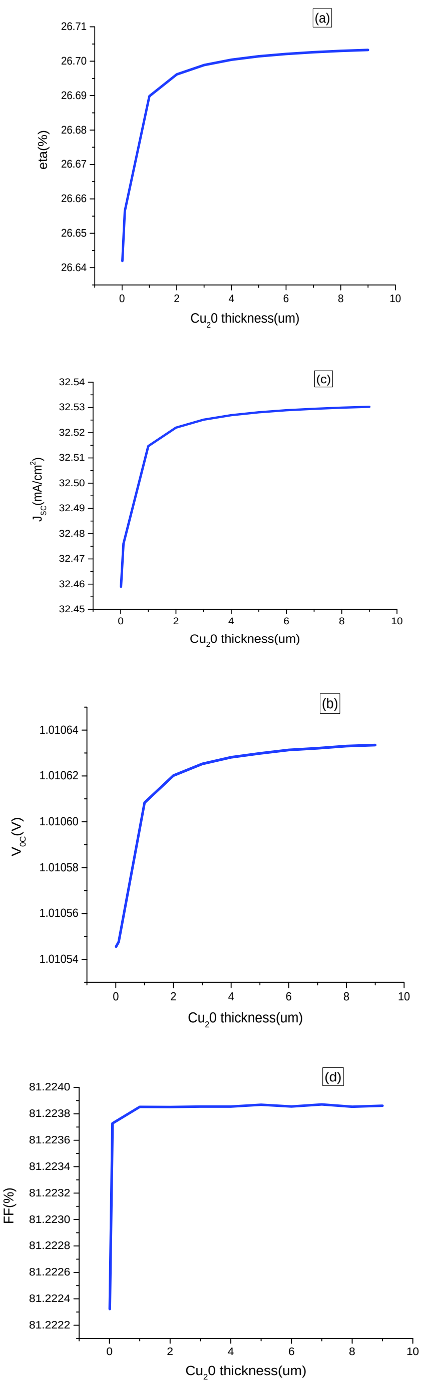


**Fig.4** Dependence of layer thickness of $Cu_2O$ on PCE (%), Voc(V), Jsc(mA/cm$^2$), FF (%)

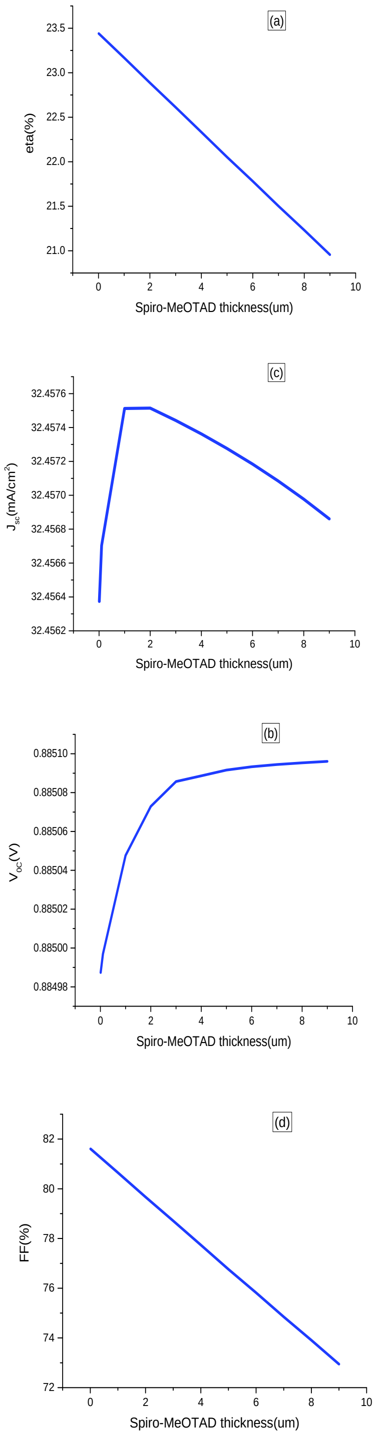


**Fig.5** Dependence of layer thickness of Spiro-MeOTAD on PCE (%), Voc (V), Jsc (mA/cm$^2$), FF (%)

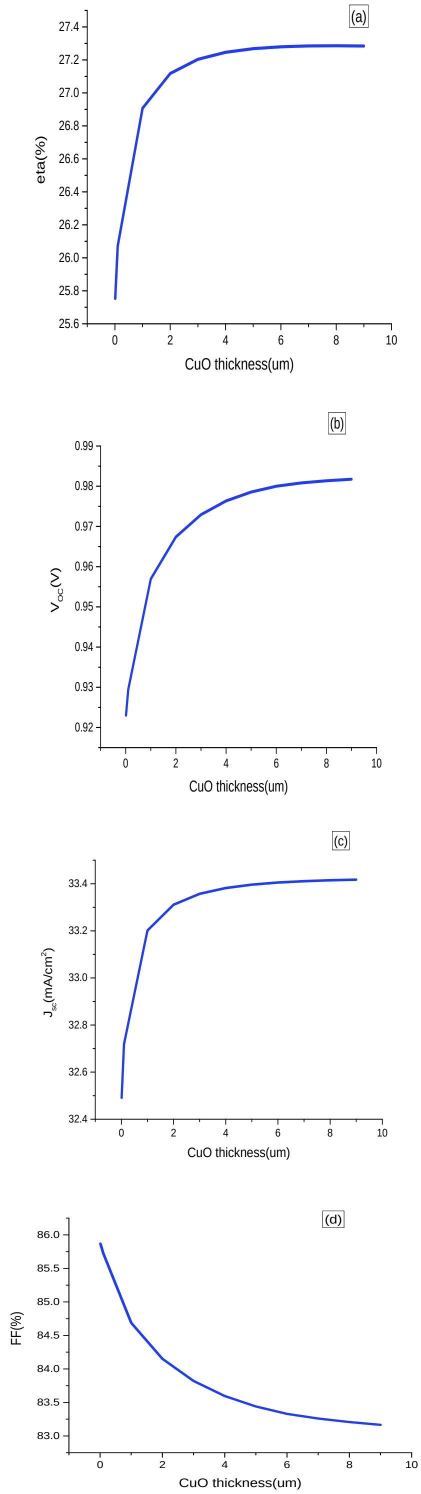


**Fig.6** Dependence of layer thickness of CuO on PCE(%), Voc(V), Jsc(mA/cm$^2$), FF(%)

**FOR PEROVSKITE LAYER($CH_3NH_3SnI_3$):**

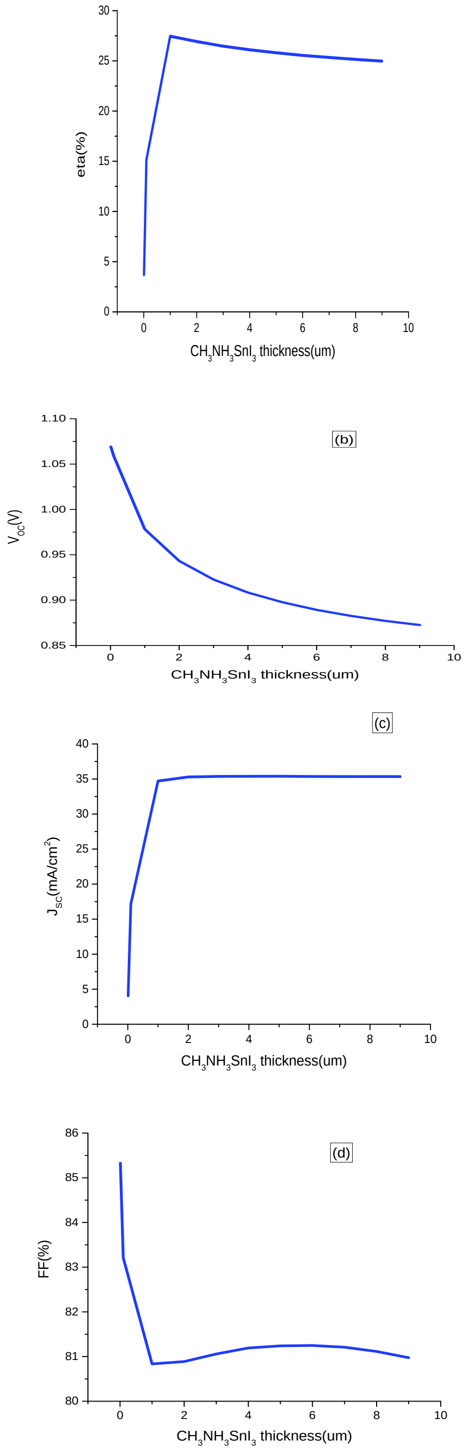


**Fig.7** Dependence of layer thickness of $CH_3NH_3SnI_3$ on PCE(%), Voc(V), Jsc(mA/cm$^2$), FF(%)

## 2-EFFECT OF TEMPERATURE

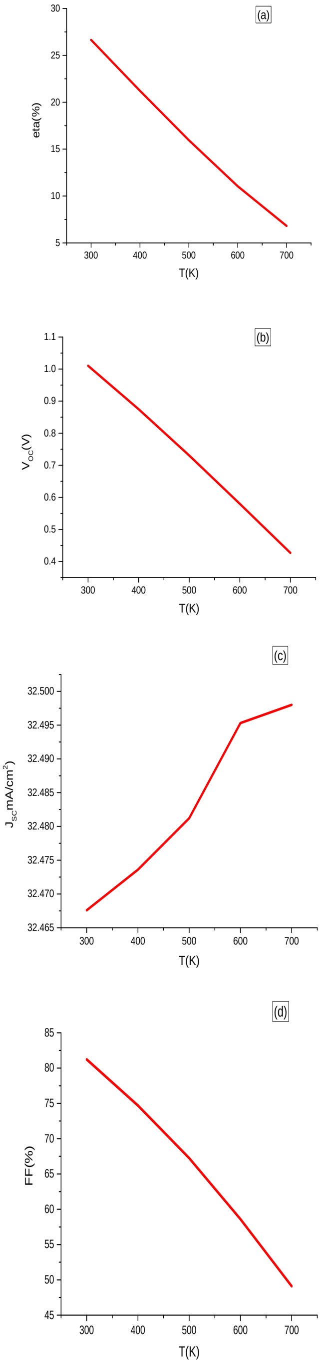


**Fig.8** Effect of temperature on PCE(%), Voc(V), Jsc(mA/cm²), FF(%) of $TiO_2$(variable) $CH_3NH_3SnI_3$/ $Cu_2O$ ; ZnO(variable) / $CH_3NH_3SnI_3$/ $Cu_2O$ ; $WS_2$(variable)/ $CH_3NH_3SnI_3$/ $Cu_2O$ ; ZnO/ $CH_3NH_3SnI_3$/ $Cu_2O$(variable)

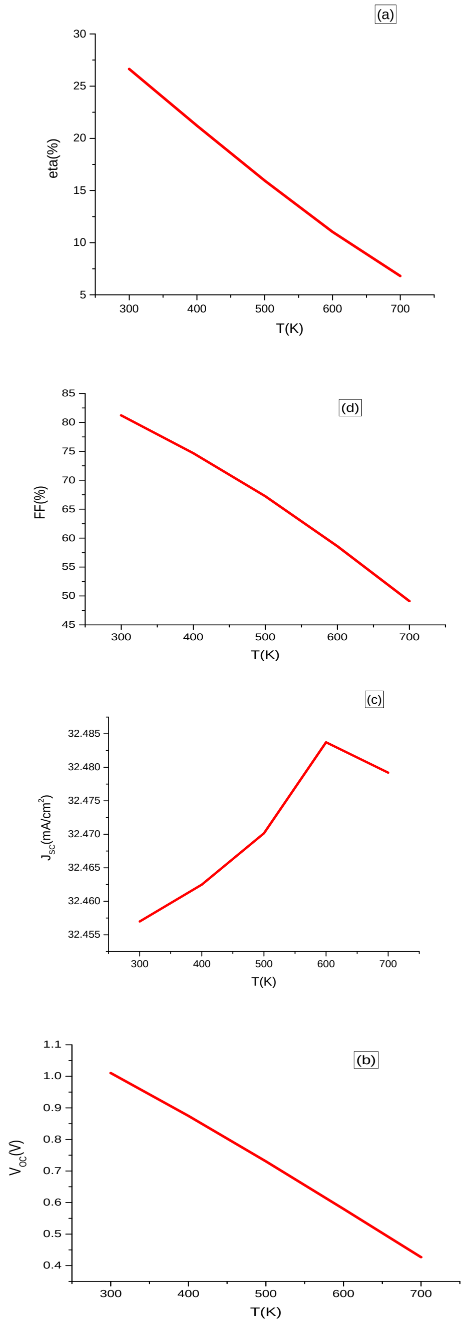


Fig.9 Effect of temperature on PCE(%), Voc(V), Jsc(mA/cm²), FF(%) of ZnO/ $CH_3NH_3SnI_3$/ Spiro-MeOTAD

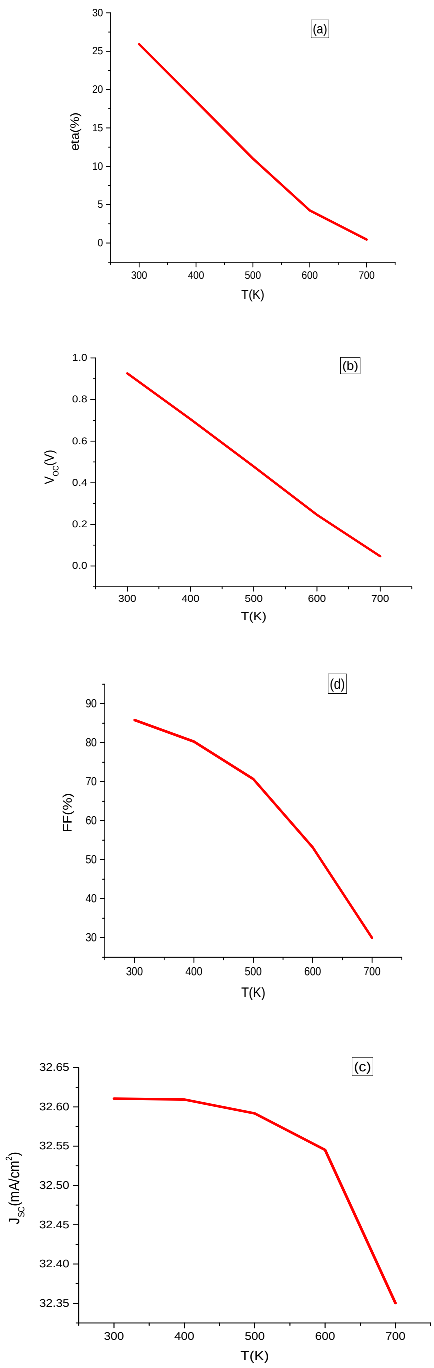


**Fig.10** Effect of temperature on PCE (%), Voc(V), Jsc(mA/cm$^2$), FF(%) of ZnO/ $CH_3NH_3SnI_3$/ CuO

**Table 5**: Comparison between different perovskite parameters with the current study.

| ETL | HTL | Perovskite layer | Jsc(mA/cm$^2$) | $V_{OC}$(V) | FF(%) | eta(%) | Ref |
|---|---|---|---|---|---|---|---|
| $Zn_2SnO_4$ | Spiro-OMeTAD | $CH_3NH_3SnI_3$ | 32.30 | 1.185 | 64 | 24.3 | [18] |
| $TiO_2$ | $CuO_2$ | $MAPbI_2Br$ | 31.4 | 0.89 | 76.7 | 22 | [19] |
| $TiO_2$ | Spiro-OMeTAD | $CH_3NH_3SnI_3$ | 32.76 | 0.82 | 74 | 20.08 | [18] |
| $TiO_2$ | CBTS | $CsPbI_3$ | 21.07 | 0.997 | 85.21 | 17.90 | [4] |
| $TiO_2$ | $CuO_2$ | $CH_3NH_3SnI_3$ | 34 | 0.99 | 71.30 | 24.54 | [16] |
| ZnO | CuO | $CH_3NH_3SnI_3$ | 33.41 | 0.98 | 83.13 | 27.28 | This wor |

## 3. CONCLUSIONS

This study analyses environment friendly perovskite solar cells by focusing on their efficiency. Different – different HTL and ETL has been successfully analyzed with the help of SCAPS 1D. As per the findings, ZnO as HTL and CuO as ETL are best suitable for non-lead based perovskite solar cells. The influence of different HTLs and ETLs thickness on PCE (eta),$V_{OC}$,$J_{SC}$ and FF was studied, similarly influence of temperature is also studied with the help of SCAPS 1D. SCAPS 1D software gives us a fair results about the thickness and temperature of different layers of solar cells to get more efficient perovskite solar cell.

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