Investigation of Effect of Operating Temperature Variation over Performance of Lead Based Perovskite Solar Cell using SCAPS-1D

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Abstract— Perovskite solar cells (PSCs) have become an incredible progress over last decade in the solar energy device area due to high efficiency and low cost photovoltaic technology. PSCs have exhibited their great improvement in performance within a decade with increment in power conversion efficiency (PCE) from 3.2 % to 25.2%. The widely used absorber material in PSCs is methyl ammonium lead trihalide (MAPbX3 where X=Cl, Br, I). Numerical simulation is a fundamental technique in deeply understanding the operational mechanisms of solar cells and structure optimization for different devices. In this paper device modeling for perovskite solar cell based on MAPbI3 has been optimized and report the effect of operating temperature variation (300 -400 K) on performance parameters ,capacitance voltage plot, Mott-Schottky plot and different illumination level in open circuit voltage of MAPbI3 based solar cell . The SCAPS 1D (Solar Cell Capacitance Simulator) has been tool used for numerical simulation of these device.

Key words: Perovskite Solar Cell, SCAPS-1D

I. INTRODUCTION

Perovskite solar cells (PSCs) represents an developing photovoltaic technology due to their efficiency increased extensively from 3.8% efficiency recorded in 2009 [1] to 22.7 % in 2017[2] and about 27.3% in 2018[3] which is still rising with pace. Figure 1 shows the planer structure of perovskite solar cells (PSC). It consists of an ETL (Electron Transporting Layer), an absorber layer and HTL (Hole Transporting Layer). The absorber layer is constitute of perovskite material and as a inorganic HTLs include NiO, Cul,Cu2O and CuSCN whereas organic HTLs are spiro-MeOTAD , P3HT, PTAA, PEDOT: PSS etc. and various ETLs are TiO_2,ZnO,SnO_2,PCBM ,CdZnS,C_{60},IGZO,WS_2 , Cds etc. Solar cell performance is dependent on its layers. G.A.Casas [4] proposed effects of using five different materials as HTL in perovskite solar cells have been analyzed and find out that efficiency in order of 28% has been obtained for Cu_2O/Perovskite/TiO_2 solar cell. According to previous work modeling for different perovskite solar cell has been performed for different ETL layer such as TiO_2,ZnO,SnO_2,PCBM ,CdZnS,C_{60},IGZO,WS_2 and Cds and effect of bandgap upon PCE of device have been examine and find out that ZnO as a ETM layer structure give maximum efficiency up to 21.58%.

In this work an analysis of the impact of operating temperature variation in range 300K -400 K over device performance parameters like open circuit voltage (Voc),short circuit current (Isc) ,fill factor(FF) and power conversion efficiency (PCE) ,Capacitance-voltage plot, Mott-Schottky plot and different illumination level in open circuit voltage of $MAPbI_3$ based solar cell

II. METHODOLOGY

Simulation of the perovskite solar cell was carried out using the SCAPS-1D (Solar Cell Capacitors Simulator) version 3.3.08. The software was developed particularly again for CdTe and $CuInSe_2$ semiconductor families, as well as other semiconductor families. In addition to an operation window, SCAPS- 1D provides a selection of defect, genetic recombination, and grating models from which to choose. To create this software, overall semiconductor physics equations such as the Toxins equation, the drift-diffusion equation, and the continuity equation both for electron-hole pairs are used. Typically, the fundamental calculations are done in one parallel universe in a steady flow environment. It aims to investigate the physics that underlies the prototype, along with the electric fields, cell division profiles, external dc densities, as well as carrier transport mechanism to name a few topics that have been investigated. you can generate up to seven semi-conducting layers upon layer using this software, each of which has a unique material and defect characteristic.

A. Architecture of Device

The design to simulate PSC is divided into different stages, which are as follows:

1) Gold (Au) as metal cathode
2) Hole transport layer (HTL) as Cu_2O
3) Absorber layer methyl ammonium lead trihalide ($MAPbI_3$)
4) An electron transport layer (ETL) as ZnO
5) Transparent Conductive Oxide (TCO) as Fluorine doped Tin Oxide (FTO).

Several different configurations of this device are simulated, including Au/Cu_2O/$MAPbI_3$/Zn_O/TCO. A simplified representation of the device's framework is in Figure 1. The quantity of absorber that is present in interfacial behavior, is characterized by strong electron-hole migration on both corners of the material's axis, making it a superior conductor of electricity to other materials of similar composition. Its capacity to digest incident radiation, which leads to the formation of cations in the external environment, is what distinguishes it from other materials.

Electron transfer layer (ETL) are the functions, whereas the feature of hole transfer and electron transfer is to extract as well as transfer holes while also blocking electrons. In general, electron and hole mobility in ETLs and HTLs is high, whereas electron and hole mobility in HTLs is low. The estimation of the band offset here between ETL/Perovskite/HTL layers is needed to reach high efficiency between the two layers found in figure 2.

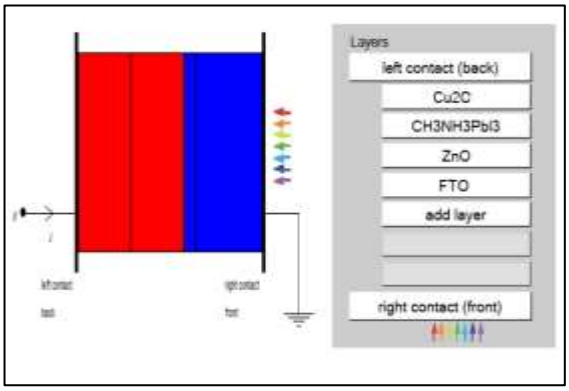

Fig. 1: Schematic of device structure

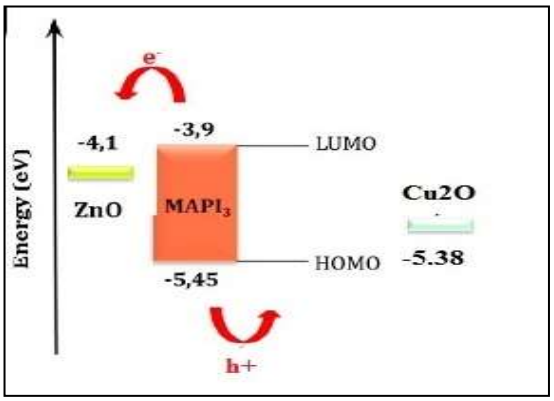

Fig. 2: Energy –band diagram of simulated cell

B. Device Simulation Parameter

The variables that were used in the simulation were derived from previously published information. A brief description of all the variables that were used in the simulation can be found in Table 1.

The data both for front and back connection points can be found in Table 2. Under the conditions of AM 1.5G illumination, the $MAPbI_3$-based photovoltaic panels perform optimally in the simulation.

LAYER		Perovskite [5]	HTL [4]	ETL[5]
Parameters	Symbol(Unit)	$CH_3NH_3PbI_3$	Cu_2O	ZnO
Thickness	W(μm)	0.6	0.4	0.1
Band gap	E_g (eV)	1.55	2.17	3.3
Electron affinity	χ(eV)	3.9	3.2	4.1
Relative dielectric permittivity	ϵ_r	32	6.6	9
effective density of states (DOS) in conduction band	Nc(cm^{-3})	$2.8x10^{18}$	$2.50x10^{20}$	$4x\ 10^{18}$
effective density of states (DOS) in Valence band	Nv(cm^{-3})	$3.9x10^{18}$	$2.50x10^{20}$	$1x\ 10^{19}$
Mobility of electron	μ_e ($cm^2V^{-1}\ s^{-1}$)	11.8	80	100
Mobility of holes	μ_h ($cm^2V^{-1}\ s^{-1}$)	11.8	80	25
Acceptor density	N_A(cm^{-3})	$1x10^{13}$	$3x10^{18}$	$1x\ 10^{16}$
Donor density	N_D(cm^{-3})	$1x10^{13}$	0	0
Defect density	Nt(cm^{-3})	$3x10^{14}$	$1x10^{15}$	$1x\ 10^{14}$

Table 1: List the parameters used in simulation

Parameters	Back contact	Front contact
Surface recombination velocity of electrons (cm/s)	1.00E + 7	1.00E + 5
Surface recombination velocity of holes (cm/s)	1.00E + 5	1.00E + 7
Metal work function(eV)	5.1	4.2552
Majority carrier barrier height relative to Ef(eV)	0.2700	0.1552
Majority carrier barrier height relative to Ev(eV)	0.1554	0.0000

Table 2: Parameters for back and front contact

III. RESULT AND DISCUSSION

A. I-V Characteristics

The PSC with configuration Au/Cu2O/$MAPbI_3$/ ZnO /TCO structure find out PCE of 21.58%, Voc of 1.08V, Jsc of 24.44 mA/cm^2 and FF of 81.70 % using layer thickness of o.4μm for HTL, 0.6 μm for absorber and 0.1 μm for ETL layer. The JV curves of above simulated cell is shown in fig.3

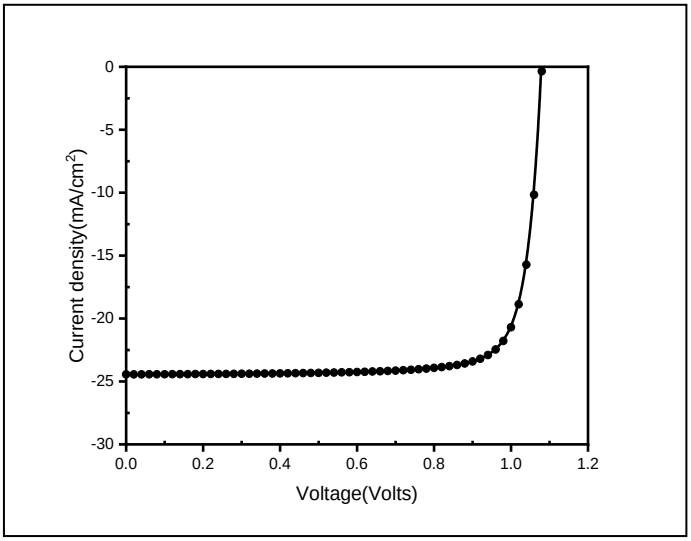

Fig. 3: JV curve of simulated cell with lead based PSC

B. Effect of operating temperature on performance of $MAPbI_3$ based PSCs

Operating temperature has a vital effect on the performance of a solar cell. Normally, the standard operating temperature used for a solar cell is 300 K. However, during the operation of solar cell it will be subjected to even higher temperature. Therefore, in order to examine the thermal stability of the device, the temperature was varied from 300 K to 400 K. Variation in operating temperature has vital effect on absorber layer, ETL and HTL and also play a considerable impact on the performance of PSCs. The transport layers are responsible for collection of the charge carriers towards the charge collective contact. The various materials exhibit variable behavior in temperature fluctuations because all vary in conductivity, specific heat and density. The impact of temperature variation on the performance parameters (Voc, Jsc, FF and PCE) of lead based PSCs is shown in Fig. 4. It is also observed that the Voc decreases (significantly) and Jsc increases also decrease (in less magnitude) with increase in temperature.

In solar cell increasing the temperature reduces the band gap. The parameter most affected by an increase in temperature is the open-circuit voltage

The Voc of a solar cell is given by the equation 1[9]

$$Voc = \frac{KT}{q}\ln\left(\frac{Jsc}{Jo}+1\right) \tag{3.1}$$

Here K is Boltzmann constant, T is temperature and Jo is reverse saturation current.

$$\frac{dVoc}{dT} = -\frac{V_{GO} - V_{OC} + \gamma\frac{kT}{q}}{T} \approx \text{-2.2 mV per °C for si} \tag{3.2}$$

According to this equation open circuit voltage decrease 2.2mV per ˚C

So, open circuit voltage of lead based PSC decrease linearly with increasing in temperature shown in fig.4 (a) the dependence of Voc upon Io is the reason of its decrement with temperature.

The short circuit current increases with increase in temperature

The short-circuit current, I_{sc}, increases slightly with temperature, since the band gap energy, E_G, decreases and more photons have enough energy to create e-h pairs. However, this is a small effect and the temperature dependence of the short-circuit current from a silicon solar cell is [9]

$$\frac{1}{I_{SC}}\frac{dI_{SC}}{dT} \approx 0.0006 \text{ per °C for si} \tag{3.3}$$

According to this equation short circuit current increase 0.06% per °C for silicon.

So, short-circuit current, I_{sc} of lead based PSC increase slightly with increasing in temperature shown in fig.4 (b)

The temperature dependency FF for silicon is approximated by the following equation;[9]

$$\frac{1}{FF}\frac{dFF}{dT} \approx \left(\frac{1}{V_{OC}}\frac{dV_{OC}}{dT} - \frac{1}{T}\right) \approx \text{-0.0015 per °C for si} \tag{3.4}$$

According to this equation fill factor decrease 0.0015 % per °C for silicon.

So, Fill factor of lead based PSC decrease linearly with increasing in temperature shown in fig.4 (c)

The effect of temperature on the power conversion efficiency (PCE) is; The PCE of lead based PSC decrease linearly with increase in temperature shown in fig.4 (d)

Parameters	At 400K	At 300	Change
Voc (Volts)	0.888403	1.0805	-0.1921
Isc (mA/cm^2)	24.44068	24.42831	0.01237
FF (%)	76.5024	81.7015	-5.1991
PCE(%)	16.6027	21.5764	-4.9737

Table 3: Change in the performance parameters at higher temperature (400K) with respect to parameters at room temperature (300 K)

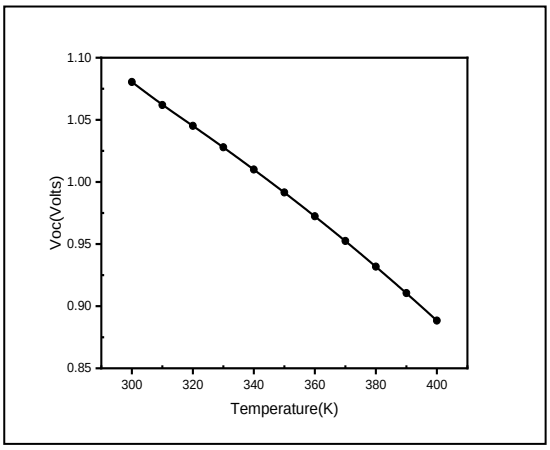

Fig. 4: (a) Open circuit Voltage with increase in temperature (300k-400k) of $MAPbI_3$ based PSC

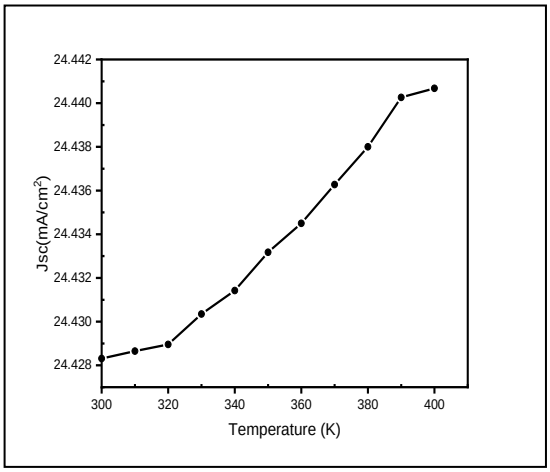

Fig. 4: (b) Short circuit current density with increase in temperature (300k-400k) of $MAPbI_3$ based PSC

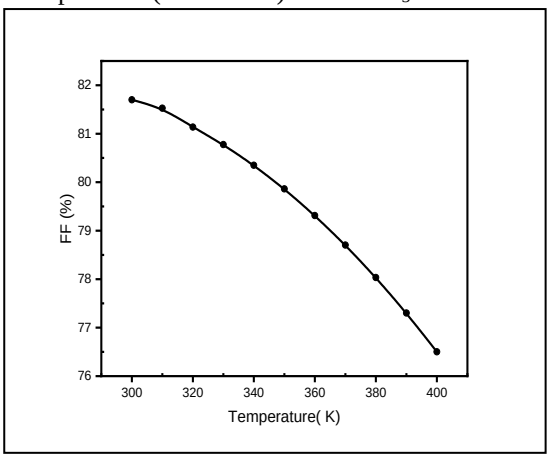

Fig. 4: (c) Fill factor with increase in temperature (300k-400k) of $MAPbI_3$ based PSC

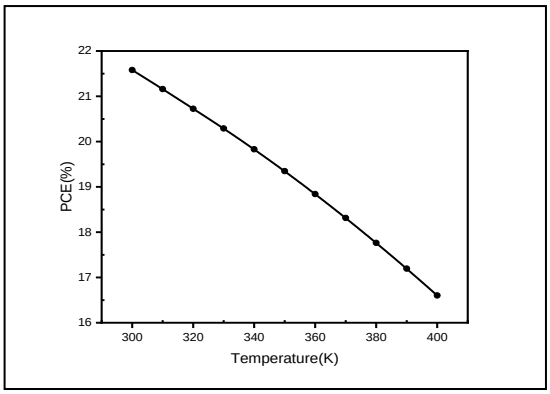

Fig. 4: (d) Power conversion efficiency with increase in temperature (300k-400k) of $MAPbI_3$ based PSC

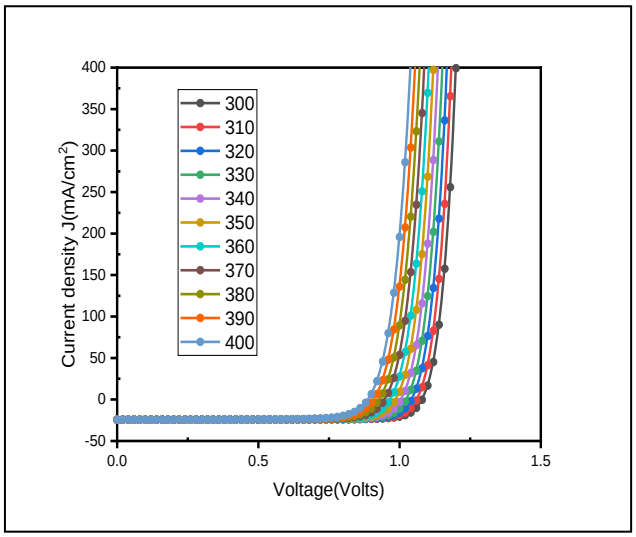

Fig. 5: Impact of temperature variation (300-400K) on the J-V curve of lead based PSC

C. Effect of operating temperature on variations of Capacitance-voltage plots

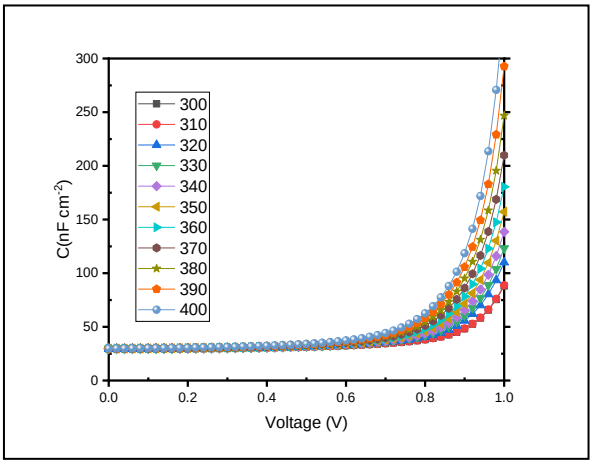

Fig. 6: Variation of capacitance according to the voltage for various use temperature of lead based PSC

The Fig 6 shows us the variation of capacitance according to the voltage for different temperature. For an applied voltage going until 0.3V, the capacitance of the cell changes in small amount to temperature .After 0.3v we note that capacitance increase significantly in same direction but according to different proportions.

Differential capacity of the hetero-junction has as the expression-5 [7]

$$C(V) = \left| \frac{dQ}{dV} \right| \tag{3.5}$$

D. Effect of temperature on Mott Schottky Plot

In Mott schottky analysis performs voltage modulation of depletion layer width that extracting relevant parameters as the absorber defect density and built in potential

C-V measurement can provide important information on nature of semiconductor device

The build in potential Vbi of semiconductor p-n junction can be estimated from the Mott-Schottky (3.7)

$$\frac{1}{C^2_p} = \frac{2}{A^2 q \varepsilon \varepsilon_o N}(V_{bi} - V) \tag{3.6}$$

$$X = \frac{2}{A^2 q \varepsilon \varepsilon_0 N}$$

$$\frac{1}{C^2_p} = (V_{bi} - V)X$$

$$\frac{1}{C^2_p} = XV_{bi} - VX \tag{3.7}$$

By plotting the curve $(1/C^2)=f(V)$ we obtain an affine transformation (on a range of value of voltage) whose intercept makes it possible to calculate the intrinsic bias voltage V_{bi} and whose slope allows to find out defect density of absorber material

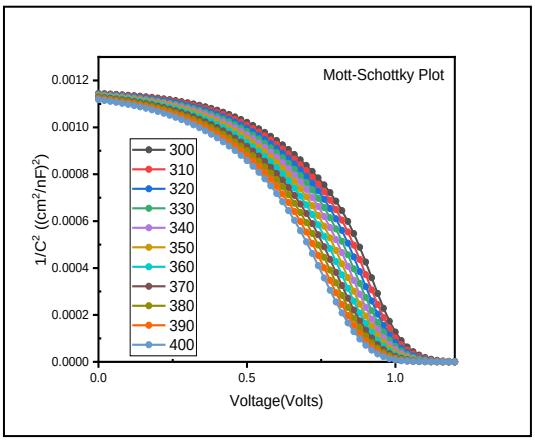

Fig 7: Impact of temperature variation (300-400K) on the Mott Schottky plot of lead based PSC

The fig.7 shows decrease of the reverse of square of capacitance according to voltage for the various use temperatures. Due to this build in potential also decrease according to increase in temperature in fig.8 the build in potential (V_{bi}) is directly affects the performance of the solar cell especially Voc.

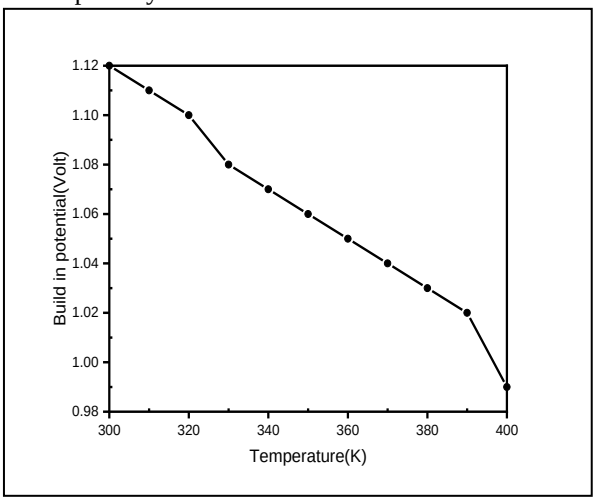

Fig. 8: Effect of operating temperature on build in potential

E. Effect of operating temperature on open circuit voltage (Voc) at different illumination level

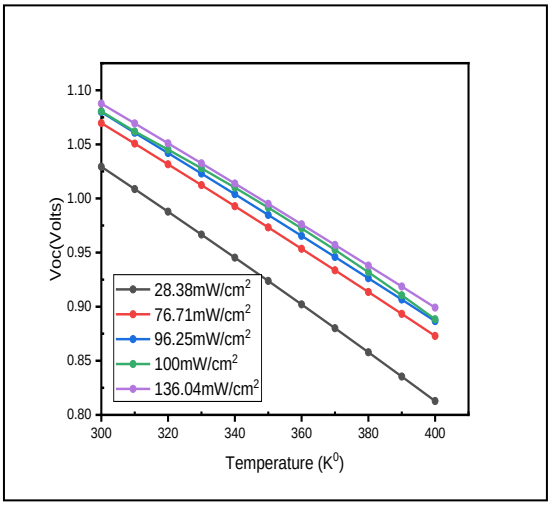

Fig. 9: Effect of operating temperature on open circuit voltage (Voc) at different illumination level

In this figure, the Voc are plotted as a function of the operating temperature for different illumination intensities. The impact of all the voltages is such that the total open circuit voltage decreases with increasing cell temperature. The decrease in the open circuit voltage with increasing operating temperature at low and medium levels of illumination is larger than that at high levels of illumination. According to R.V. Singh et. [8] Due to effect of temperature on intrinsic carrier concentration (n_i). The temperature dependency of carrier concentration is very significant in determining the variation in the open circuit voltage. Its requirement on temperature at high levels of illumination is also related to the energy band gap reduction which comes into play when the carrier concentration develops large.

The maximum reachable efficiency for each solar cell is calculated based on the current density, open circuit voltage and fill factor. The most important observation of this study is that a noticeable decrease in performance occurs in Voc and Jsc to increase with increasing temperature in the perovskite solar cells results in a decrease in the efficiency with increasing temperature. Then effect of increasing in temperature also effect capacitance and Mott-Schottly analysis so due to this built in potential also decrease with increase in temperature so overall performance of perovskite solar cell is degrade due to increase in temperature so this type of cell do not use for real time application design.

IV. CONCLUSION

In this work, we have demonstrated the impact of operating temperature on performance of lead based PSC. Performance parameter like open circuit voltage (Voc) decrease linearly, short circuit current (Isc) increase slightly, Fill factor decrease linearly and PCE also decrease with increasing in temperature. Temperature also affected in capacitance so in C-V plot capacitance is significant for voltages higher than 0.3eV then in the Mott-Schottky curves decrease of the reverse of square of capacitance according to voltage for the different temperatures. Due to this build in potential also decrease according to increase in temperature. Effect of temperature on open circuit voltage (Voc) at different illumination level, with increasing cell

temperature open circuit voltage decreases. In this, decrease in the open circuit voltage with increasing temperature at low and medium levels of illumination is larger than that at high levels of illumination

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