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# Numerical Modeling Baseline for high efficiency ( $Cu_2FeSnS_4$ ) CFTS based Thin Film Kesterite Solar Cell

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## Abstract:

$Cu_2FeSnS_4$  (CFTS) is auspicious nontoxic and earth abundant semiconductor compound having kesterite symmetrical structure. It is an attractive and suitable material for the fabrication of low cost, high efficiency and sustainable thin film photovoltaic cell. CFTS based kesterite photovoltaic cell device modeling was performed in this work. The influence of device parameters such as the thickness, acceptor and donor carrier concentration densities of absorber and electron transport layer (ETL), effect of back contact metal work function and the temperature effect on the performance of CFTS based kesterite photovoltaic cell is analyzed by using one dimensional solar cell capacitance simulator (SCAPS) software. In this work, promising optimized results had been achieved with the conversion efficiency of 19.97%, fill factor (FF) 85.94 %, short-circuit current ( $J_{sc}$ ) 23.37 mA/cm<sup>2</sup> and open circuit voltage ( $V_{oc}$ ) 0.995V. The above results will give imperative baselines and feasible directions for the fabrication of higher efficiency CFTS based photovoltaic cell.

**Keywords:** SCAPS, Photovoltaics,  $Cu_2FeSnS_4$ , CFTS, Kesterite, Solar cell, Numerical Analysis.

## I. INTRODUCTION:

Thin film technology is the one of the most cost effective and efficient technology for the manufacturing of photovoltaic cells and it is an excellent subject of intense research in photovoltaic industry. Thin films are very suitable for low and large scale photovoltaic cell applications. To fulfill the consumer demand and for the generation of electricity, the high-power conversion efficiency solar cell without degradation of materials and economical photovoltaic cells are fabricated [1]. Silicon based photovoltaic cells dominated the market from many years and due to intensification in manufacturing capabilities thin film photovoltaic cells are gaining significance [2]. For the manufacturing and production of silicon based thin film solar cell, different major deposition techniques like sputtering, thermal evaporation, molecular beam epitaxy, e-beam evaporation, close space sublimation, and metal organic chemical vapor deposition techniques are attempted [3]. So, cost of the material, technology and energy consumption used by these sophisticated fabrication techniques makes the solar cell panel costly [4].  $CdTe$ ,  $CIGS$  ( $CuIn_{1-x}Ga_xSe_2$ ) and related alloy based thin-film chalcopyrite photovoltaic cells materials are commercially used for the fabrication of thin film photovoltaic devices because of high conversion efficiency, excellent electrical as well as optical properties [5] and also these types of devices have high absorption coefficient [6],[7]. The toxic materials restrict the further development of these types of cells and the rare materials like Indium and Gallium used for the fabrication of cell also increase the fabrication cost [5]. So, the commercial production of  $CIGS$  based photovoltaic cell is limited.

Non-toxic earth abundant materials having kesterite symmetrical structure like  $CZTS$  ( $Cu_2ZnSnS_4$ ),  $CZTSe$  ( $Cu_2ZnSnSe_4$ ), [8–12]  $CFTS$  ( $Cu_2FeSnS_4$ ),  $CFTSe$  ( $Cu_2FeSnSe_4$ ) and their alloys are emerging as the most auspicious replacement for the chalcopyrite absorbers ( $CIGS$ ,  $CIGSe$ ) [13–15]. The growing attention towards these quaternary compounds for photovoltaic cells production is due to their potential [16–19]. Among these quaternary compounds,  $CFTS$  is one of the most auspicious compound for an effective light absorber material due to its suitable optical band gap of 1.2–1.5eV [20–24] and large absorption coefficient  $\alpha > 10^4 cm^{-1}$  [18,25–29]. Power conversion efficiency of about 0.29% for  $CFTS$  based solar cell is presented in [30]. In [26], the reported conversion efficiency is 2.73%.

Numerical modeling or numerical analysis is an essential tool for the better understanding of device working parameters. Numerical analysis can play a significant role in manufacturing and fabrication of an efficient photovoltaic device. Numerical analysis of the kesterite based  $FTO/TiO_2/CFTS/back\ contact$  photovoltaic cell is proposed in this work. In our simulations, thickness of absorber layer ( $CFTS$ ) varies from  $1\mu m$  to  $4\mu m$  and the bandgap energy is 1.3eV. The band gap of electron transport layer is larger than that of absorber layer; hence, maximum photons are absorbed in  $CFTS$ , which will increase the overall conversion efficiency of photovoltaic cell. The proposed results will give a valuable baseline for the design of high performance  $CFTS$  based kesterite solar cells.

## II. SOLAR CELL DESIGN

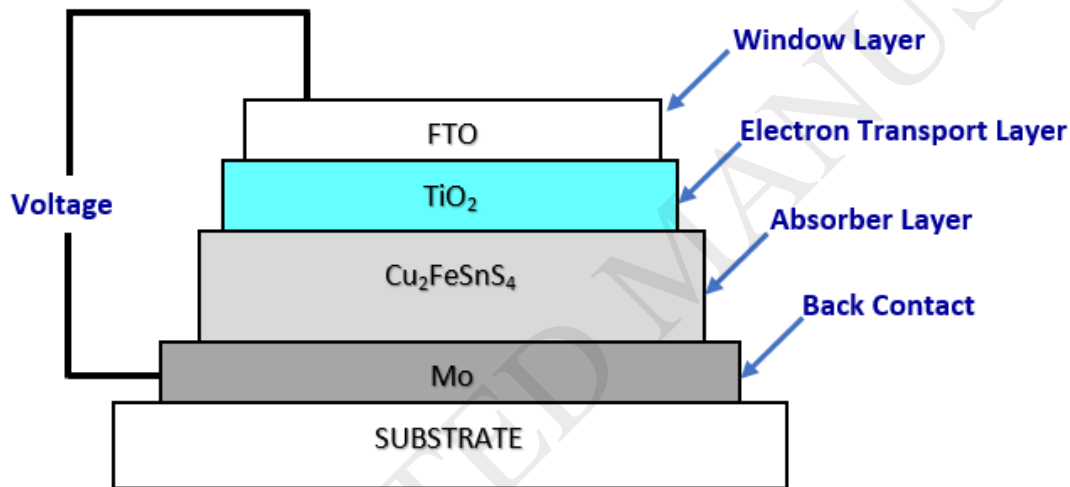


Figure 1. Block diagram of CFTS solar cell

Figure 1 shows our proposed photovoltaic cell structure  $FTO/TiO_2/CFTS/Mo$ , which comprises back contact layer  $Mo$ , absorber layer  $CFTS$ , electron transport layer  $TiO_2$  and window layer  $FTO$ . We have investigated the influence of parameters like temperature variations, absorber layer dopant concentration and thickness, electron transport layer dopant concentration and thickness, as well as compensation ratio and illumination power of the sun, on the performance of our photovoltaic cell model. For optimum values of parameters (absorber layer thickness  $4\mu m$  and acceptor carrier concentration  $3 \times 10^{18} cm^{-3}$ ), we found a conversion efficiency of 19.97%.

## III. NUMERICAL MODELING AND MATERIAL PARAMETERS.

The simulation software that can be used for the numerical modeling of photovoltaic cell must be able to solve the semiconductor basic equations like the continuity equation for holes and electrons and the poisson's equation relating the charge to the electrostatic potential. The charge carrier transport equation and the basic equations are well explained in simya O.K.et al [31]. We have used one dimensional Solar Cell Capacitance Simulator (SCAP-1D) software developed at the University of Gent, Belgium, to simulate our proposed model of photovoltaic cell. That software is designed for simulations and helps for analysis of J-V characteristics curve, ac characteristics (C-V and C-f), spectral response(QE) of a device, power conversion efficiency(PCE), fill factor (FF), short-circuit current ( $J_{sc}$ ), open circuit

voltage ( $V_{oc}$ ) used, energy bands of materials used in solar cell and concentration of different material used by solving the semiconductor basic equations, the hole and electron continuity equation and the Poissons equations.

The measure of a photovoltaic cell quality is Fill Factor ( $FF$ ), which is derived by equating the maximum power ( $P_{max}$ ) to the theoretical power ( $P_t$ ). Where power ( $P_t$ ) would be output at both the short circuit current ( $J_{sc}$ ) and open circuit voltage ( $V_{oc}$ ) as given in equation 1.

$$FF = \frac{P_{max}}{P_t} = \frac{V_{max} I_{max}}{V_{oc} J_{sc}} \quad (1)$$

The product of  $P_t$  and  $FF$ , divided by the energy input from the sun is the power conversion efficiency ( $PCE$ ) mathematically expressed in equation 2.

$$PCE = \frac{V_{oc} J_{sc} FF}{P_{in}} \quad (2)$$

The parameters used in SCAPS software for numerical analysis are absorber layer thickness, electron-hole mobility, intrinsic carrier concentration, electron affinity, band gap and doping density. For buffer and window layer similar parameters are also required which are enlisted in table 1. Where  $p$  is the hole concentration and  $n$  is electron concentration in  $cm^{-3}$ ,  $W$  is the thickness in  $\mu m$ .  $\chi$  is the affinity in  $eV$ ,  $E_g$  is the bandgap in  $eV$ ,  $\mu_e$  is the electron mobility in  $cm^2/Vs$ ,  $\mu_p$  is the hole mobility in  $cm^2/Vs$ ,  $N_V$  is the valence band effective density of state and  $N_C$  is the conduction band effective density of states in  $cm^{-3}$ . All the simulations are performed under AM 1.5 illumination.

Table-I: Baseline parameters for modeling CFTS based solar cells[3,32,33]

Parameters	<i>p</i> -CFTS	<i>n</i> -TiO <sub>2</sub>	<i>n</i> -FTO
Thickness, $W$ ( $\mu m$ )	1~4	0.4	0.5
Band gap, $E_g$ (eV)	1.3	3.2	3.5
Electron affinity, $\chi$ (eV)	3.3	3.86	4
Dielectric permittivity, $\epsilon_r$	9	9	9
Effective Density of states, $N_C$ ( $cm^{-3}$ )	$2.2 \times 10^{18}$	$1.8 \times 10^{19}$	$1 \times 10^{19}$
Effective Density of states, $N_V$ ( $cm^{-3}$ )	$1.8 \times 10^{19}$	$2.4 \times 10^{18}$	$1 \times 10^{18}$
Electron mobility, $\mu_e$ ( $cm^2/Vs$ )	$2.198 \times 10^1$	100	20
Hole mobility, $\mu_p$ ( $cm^2/Vs$ )	$2.198 \times 10^1$	25	10
Electron and hole concentration, $n, p$ ( $cm^{-3}$ )	$3 \times 10^{18}$	$1 \times 10^{15}$	$1 \times 10^{18}$

## IV. RESULTS AND DISCUSSION

### A. Energy Band Diagram

Energy band diagram of a proposed CFTS/TiO<sub>2</sub> device is shown in figure 2 and is taken from SCAPS software. Energy band diagram helps in explaining the properties of solar cell. For incident light photons the band gap value that is optimal for most of light to be absorbed for effective power conversion efficiency is greater or equal to the maximum band gap value of 1.3 eV.

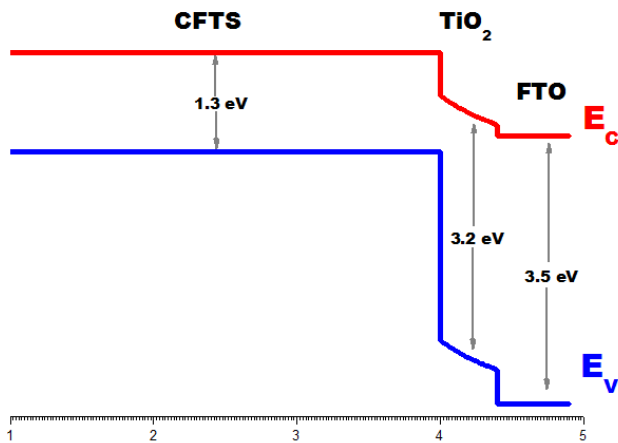


Figure 2. Energy band illustration of CFTS solar cell

### B. $J$ - $V$ characteristics of CFTS/ $\text{TiO}_2$ photovoltaic cell

The main working of a photovoltaic cell is to convert sun light energy into electricity. When there is absence of light, the photovoltaic cell is a large flat diode and gives the exponential curve in  $J - V$  measurements. The cell gives an extreme smallest value of current that is due to minority carriers in dark condition, as illustrated in figure 3.

Photovoltaic cell starts working under light illumination condition. Generation of charge carriers due to absorption of incident photons from sun light in this state is the main reason of the flow of a the current. The  $J$ - $V$  characteristic curve of CFTS/ $\text{TiO}_2$  photovoltaic cell is given in figure 3.

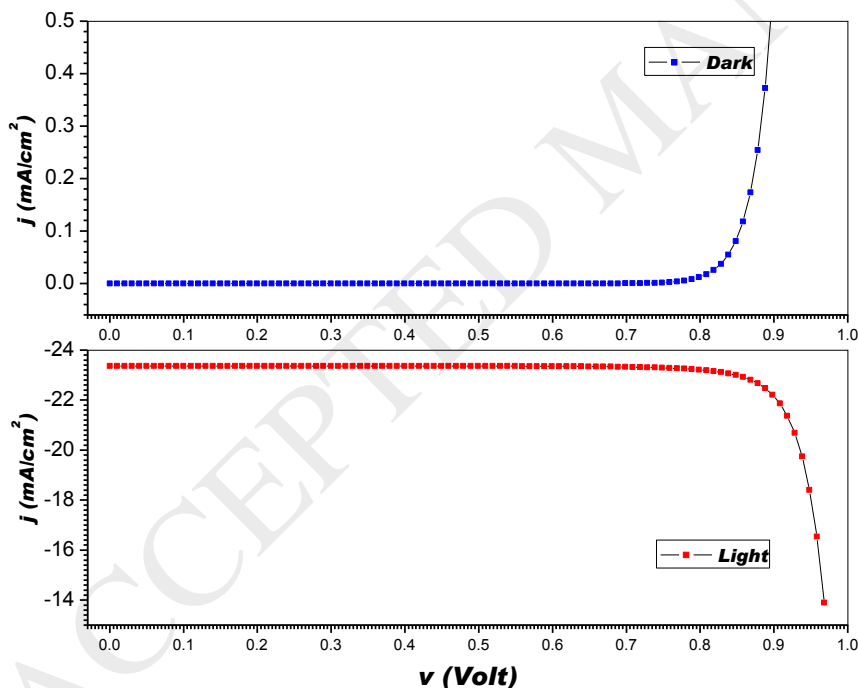


Figure 3: Dark Vs Light  $J - V$  characteristics.

### C. Effect of CFTS absorber layer thickness.

The absorber layer (CFTS) thickness effect on photovoltaic cell performance is shown in figure 4. Effect of the thickness of CFTS absorber layer is analyzed by varying the thickness value from  $1\mu\text{m}$  -  $10\mu\text{m}$ , while all other material parameters of different layers are constant. With increasing the absorber thickness, short circuit current ( $J_{SC}$ ) increases with an increase of open circuit voltage ( $V_{OC}$ ). Fill factor ( $FF$ ) and power conversion efficiency ( $PCE$ ) are also increases up to a point of optimal thickness. After reaching to the optimal absorber thickness values, Fill factor starts to decrease. The increase in  $J_{SC}$  with an increase of  $V_{OC}$  and  $PCE$  up to optimal absorber thickness, is principally due to

more absorption of photons of longer wavelength and this will in turn, affect the ratio of photo-generated carriers. The optimal value for absorber thickness layer is  $4\mu\text{m}$ .

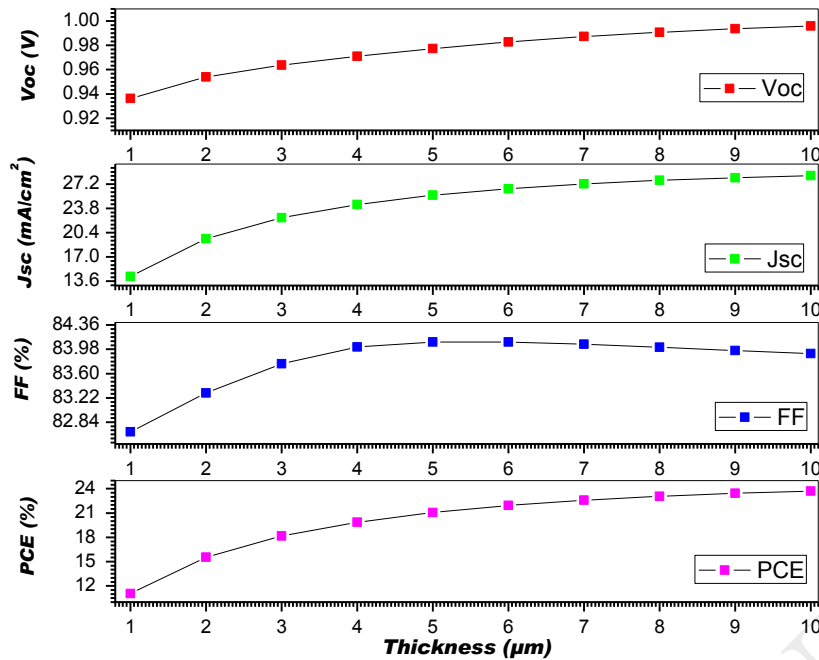


Figure 4: Effect of the absorber layer thickness on CFTS photovoltaic cells

#### D. Effect of absorber layer acceptor concentration densities

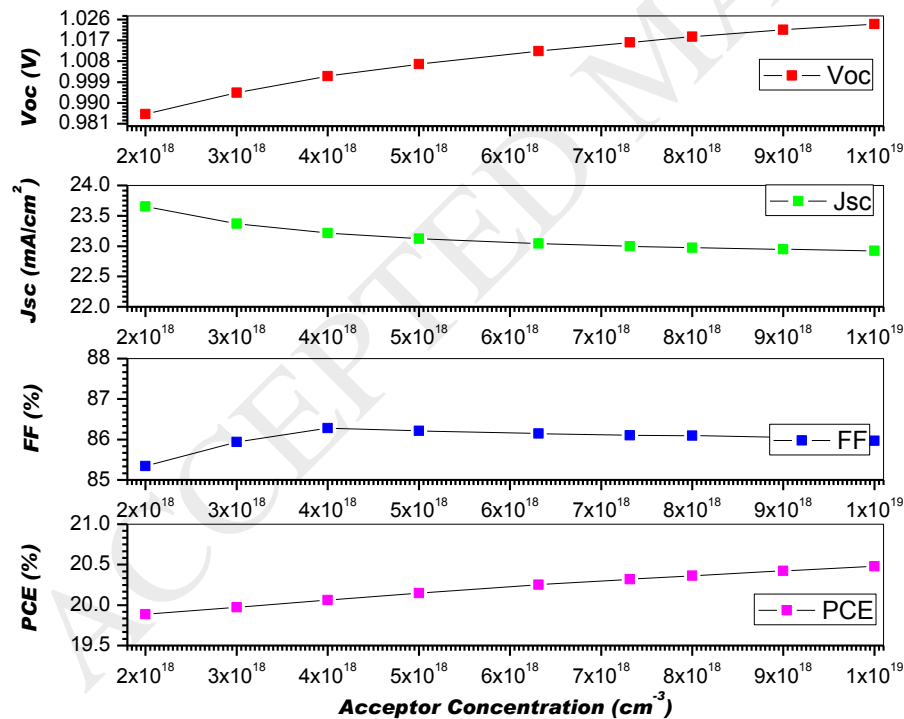


Figure 5: Acceptor concentration in the absorber layer.

Acceptor concentration densities in absorber layer is varied from  $1 \times 10^{18} \text{cm}^{-3}$  to  $1 \times 10^{19} \text{cm}^{-3}$  as shown in figure 5. The figure illustrates that  $V_{oc}$  increases with increase in the doping concentration whereas  $J_{sc}$  decreases with increase in the doping concentration. The main reason is that the saturation current of a device increases with the increase of the carrier concentration density and resultantly the  $V_{oc}$  increases with increasing doping concentration. However, the short-circuit current will decrease with the increasing of carrier densities. This decrease in  $J_{sc}$  with increasing doping concentration is due to the fact that the higher carrier densities will increase the recombination process and lessen the probability of the collection of the photon-generated electrons. So the collected conversion efficiency is more dependent on the influence of the concentration density. From figure 5, it is clear that power conversion efficiency and fill factor increases with increase in the carrier concentration in absorber layer material. The optimal value of the concentration of acceptor density of absorber layer is  $3 \times 10^{18} \text{cm}^{-3}$ .

#### E. Effect of electron transport layer on CFTS/ $\text{TiO}_2$ photovoltaic cell.

$\text{TiO}_2$  electron transport layer (ETL) influence on the performance of a photovoltaic cell is also explored and given in figure 6. The ETL thickness is varied from  $0.1 \mu\text{m}$  to  $1 \mu\text{m}$ . Simulated fallouts illustrate that with an increase in the ETL thickness, there is no change in short-circuit current ( $J_{sc}$ ), open circuit voltage ( $V_{oc}$ ), power conversion efficiency (PCE) and the Fill Factor (FF). So, this result is comprehended that change in thickness of ETL layer did not affect the output of CFTS/ $\text{TiO}_2$  photovoltaic device. For the designing of CFTS/ $\text{TiO}_2$  based kesterite device, optimum thickness taken is  $0.4 \mu\text{m}$ .

The effect of ETL donor concentration on the device performance is analysed by changing the concentration density value varied from  $1 \times 10^{15} \text{cm}^{-3}$  to  $1 \times 10^{17} \text{cm}^{-3}$ . With increase in doping concentration in ETL, there is no major change obtained that affects the performance of device as illustrated in figure 7. So, this result is comprehended that by changing the ETL donor concentration, output of photovoltaic device is not affected.

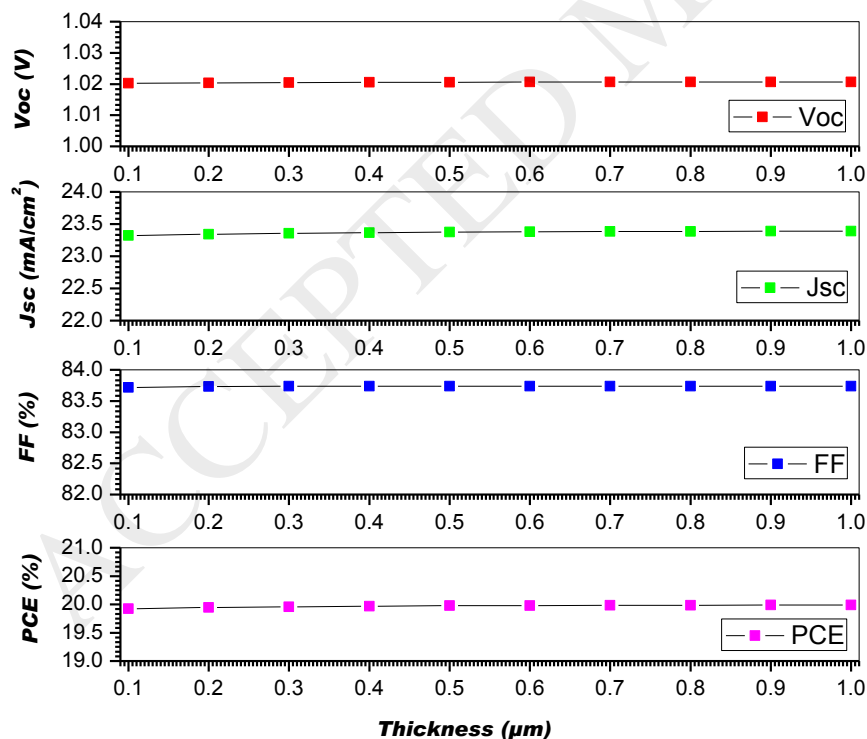


Figure 6: Effect of the Electron Transport Layer thickness on CFTS photovoltaic cells.



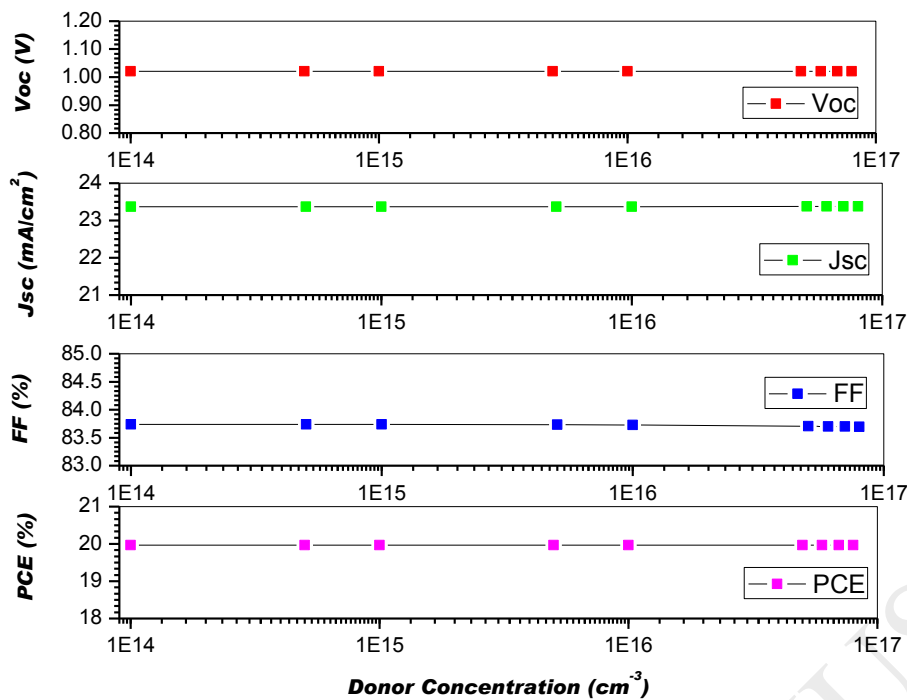


Figure 7: Donor concentration in the Electron Transport Layer.

**F. Effect of back contact metal work function on JV characteristic curve.**

Metal work function of back contact affects the performance of solar cell. The metal work function is well illustrated in figure 8. With increase in the contact metal work function, open circuit voltage increases. Along with open circuit voltage, short circuit current also increases. This can be explained with the aid of energy band diagram shown in figure 9 for metal work function of 4.9 eV. From figure 8, it can be seen that there is a conduction band offset which stops the flow of electrons to the back contact, thus helps in improving the open circuit voltage of solar cell.

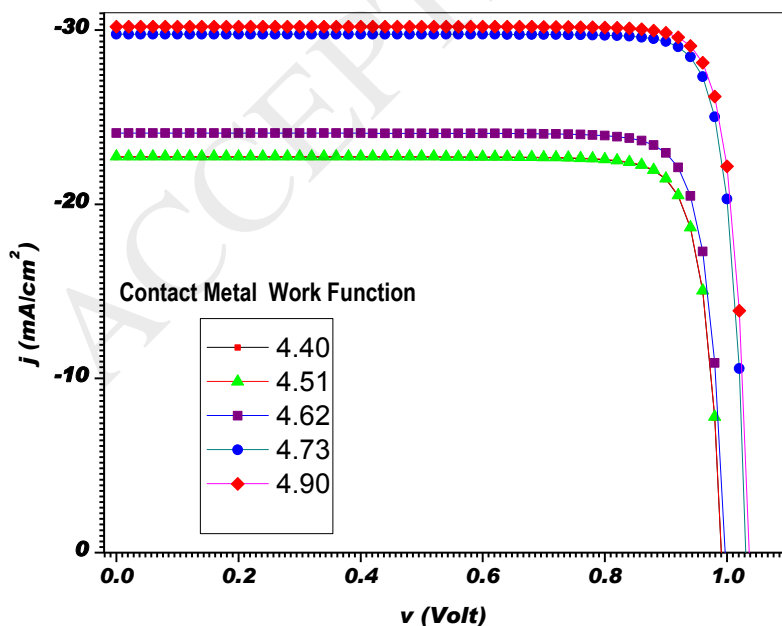


Figure 8: Effect of back contact metal work function on JV characteristic curve.

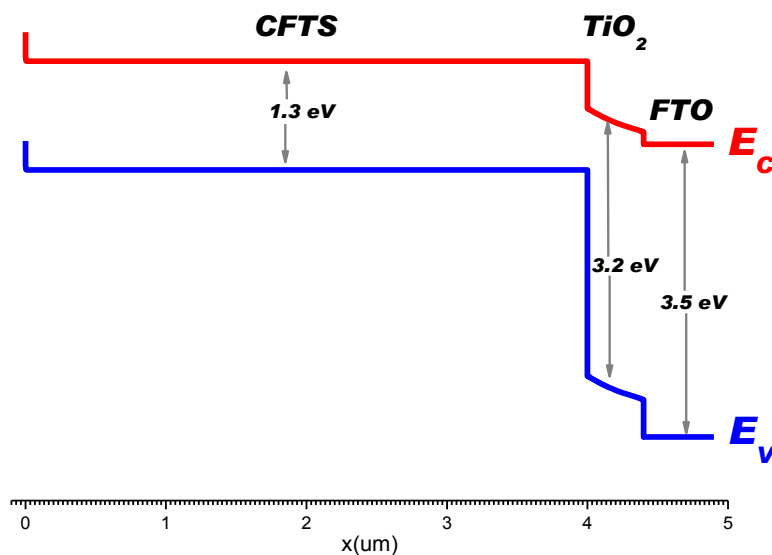


Figure 9: Energy band diagram illustration of back contact metal work function effect

### G. Effect of working temperature on photovoltaic cell performance.

Analysis of device by means of its working temperature is explored to check the performance of photovoltaic cell. The photovoltaic panels are installed in the open sky. So, heating on photovoltaic cell increases due to the sunlight, which directly affects the performance of photovoltaic cells. The panels are operated at temperatures greater than 300K. The influence of the working temperature on the proposed device is also investigated. For inquiring the temperature effect, we take the temperature in a range from 300K to 500K. The simulation results are shown in figure 10.

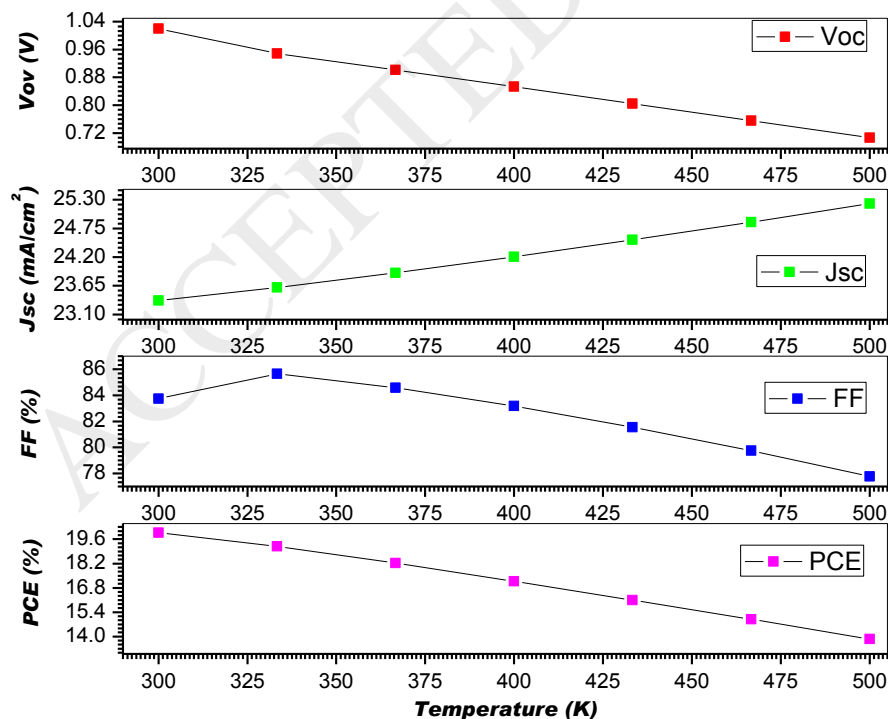


Figure 10: Effect of temperature on CFTS solar cell.

Overall solar cell performance is affected due to increase in temperature as well understood from figure 10. Power conversion efficiency and open circuit voltage decreases with increase in temperature. This decrease in conversion efficiency is due to higher temperature, because carrier concentration, band gaps, electron and hole mobility are directly affected by temperature [23]. Reverse saturation current  $J_0$  depends on the temperature due to this  $V_{oc}$  decreases with increase in temperature as given in equation. 3[34]. Electrons gain more energy from the increased operating temperature. These electrons are unstable due to the higher temperature and are more likely to recombine with the holes before reaching the depletion region. Figure 10 illustrates that conversion efficiency,  $FF$  and  $V_{oc}$  of the device decreases; whereas  $J_{sc}$  increases with increase in temperature.

$$J_e(V) = J_0 \left[ \exp\left(\frac{qV_{oc}}{k_B T}\right) - 1 \right] \quad (3)$$

## V. CONCLUSION:

The base line parameters of kesterite based  $FTO/TiO_2 / CFTS / Mo$  photovoltaic device is proposed in this work. This will be very helpful for designers, researchers and engineers for analyzing and manufacturing of  $CFTS$  based devices. The different parameters which affects the cell performance are described. For the in depth understanding and getting the confidence in the modeling of a photovoltaic cell, different characteristics, as well as different possible conditions, are to be considered for simulation. In this work, promising optimized results have been achieved with the conversion efficiency of 19.97%, fill factor ( $FF$ ) 85.94 %, short-circuit current ( $J_{sc}$ )  $23.37 \text{ mA/cm}^2$  and open circuit voltage ( $V_{oc}$ ) 0.995V. The results will give imperative guidance for the feasible fabrication of higher efficiency  $CFTS$  based photovoltaic cells.

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