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The Impact of Interface Defect Density on the Performance of $CH_3NH_3PbI_3$ Based Solar Cell Using SCAPS-1D

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Abstract

In this work, Solar Cell Capacitance Simulator-1D (SCAPS-1D) was utilized to study the interface defect densities with varying absorber layer thickness of perovskite solar cells. The planar heterojunction n-i-p structure was defined as 2D-$MoTe_2$/$CH_3NH_3PbI_3$/Cu_2O, and its performance was simulated. Power conversion efficiency > 23% was realized at < 10^{14} cm^{-3} defect density at 2D-$MoTe_2$/$CH_3NH_3PbI_3$ and $CH_3NH_3PbI_3$/Cu_2O interfaces and >1.0 µm thickness of absorber layer. The study was carried out at 300k temperature. These results show constraints on numerical simulation for correlation between defect mechanism and performance.

Keywords: Perovskite solar cells, 2D-$MoTe_2$, electron transport layer, interface defects, SCAPS-1D simulation, power conversion efficiency, fill factor, open-circuit voltage, short-circuit current density.

1. Introduction

Perovskite solar cells (PSCs) have garnered significant attention due to their remarkable power conversion efficiency (PCE) and potential for low-cost, scalable photovoltaic technology. The incorporation of two dimensional (2D) transition metal dichalcogenides (TMDCs), such as 2D-$MoTe_2$ as electron transport layers (ETLs) has emerged as a promising strategy to enhance PSC performance. However, interfacial defects between the 2D-$MoTe_2$ ETL and the $CH_3NH_3PbI_3$ (methylammonium lead iodide) perovskite absorber layer can significantly impact charge carrier dynamics, leading to recombination losses and reduced device efficiency.

PSCs have shown remarkable progress in recent years, with power conversion efficiencies (PCEs) exceeding 23% [1]. The planar heterojunction architecture, employing a perovskite absorber layer sandwiched between electron transport (ETL) and hole transport layers (HTL), has become a popular configuration[2].

2D TMDCs, such as $MoTe_2$, have been explored as ETLs due to their, high electron mobility[3], Suitable energy band alignment [4, 5] and Enhanced stability [6]. Interface defects between the ETL and perovskite absorber layer can lead to, Increased recombination losses[7], reduced PCE[8] decreased V_{OC} and FF [9].

SCAPS-1D simulations have been employed to investigate the impact of interface defects on PSC performance [10], optimization of ETL thickness and material properties [11], the effects of doping concentration on the performance of PSC [12]

Perovskite solar cells are commonly synthesized by the method of one-step or two-step spin-on solution-based method [13]. Since the component materials are entirely different in their nature, defects are often found at the interfaces of this heterojunction device. These defects have significant effect on the performance of the cell [14].

While previous studies have investigated the impact of interface defects on PSC performance, the specific effects of defect density on 2D-$MoTe_2$ ETLs in $CH_3NH_3PbI_3$ solar cells remain unexplored.

This study investigates the impact of interface defect density on the performance of 2D- $MoTe_2$ ETLs and Cu_2O HTL in $CH_3NH_3PbI_3$ solar cells using SCAPS-1D simulations. Specifically, we examine the effects of interface defect density on key solar cell performance parameters: power conversion efficiency (PCE), open circuit voltage (V_{oc}), short circuit current density (J_{sc}) and fill factor (FF).

2. Method

The perovskite solar cell structure used in this work is shown in figure 1. Meanwhile the material properties of the design (n-i-p planer) is gotten from literature as indicated in table 1. Using these information, we constructed the basic structure 2D-$MoTe_2$/$CH_3NH_3PbI_3$/Cu_2O, where 2D-$MoTe_2$ serves as the electron transport layer, $CH_3NH_3PbI_3$ (methylammonium lead iodide) the light absorbing layer and Cu_2O the hole transport layer. Fluorine-doped Tin Oxide (FTO) is used as front contact and gold (Au) as back metal contact. The simulation was carried out at temperature (300 k) under Illumination of AM 1.5G (100 mW/cm^2) or 1sun spectra, with V_{oc} highest limit of 1.8 V.

Table 1: Values representing the material properties used in the simulation.

Material property	**Cu_2O[15]**	**$CH_3NH_3PbI_3$ [16, 17]**	**2D-$MoTe_2$ [17]**
Thickness (um)	Varied	Varied	Varied
Band gap (eV)	2.17	1.50	1.01
Electron affinity (eV)	3.2	3.90	3.91
Dielectric permittivity	7.5	6.50	7.20
CB effective density of states (cm^{-3})	$2.0x10^{18}$	$2.2x10^{18}$	$1.8x10^{19}$
VB effective density of states (cm^{-3})	$1.8x10^{18}$	$2.2x10^{18}$	$1.8x10^{19}$
Electron mobility (cm^2 /V.s)	20	20	$1.6x10^4$
Hole mobility (cm^2 /V. s)	80	20	2.1x10
Shallow Acceptor density NA (cm^{-3})	varied	$1.0x10^{15}$	0.0
Shallow donor density ND (cm^{-3})	$1x10^{14}$	0.0	$1.0x10^{15}$

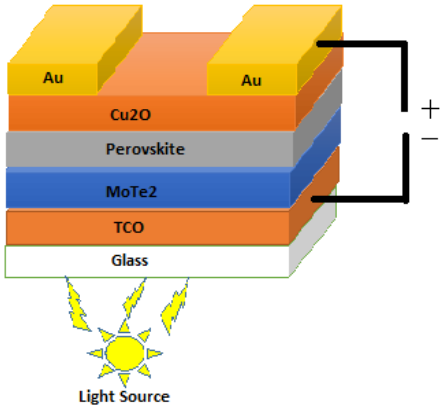

Figure 1: Schematic structure of the simulated PSC

SCAPS-1D version 3.3.10, a software developed at the Department of Electronics and Information Systems (ELIS) of the University of Ghent, Belgium was employed for the simulation [18, 19]. The software works one of the best among its kind [20], it works based on Poisson's equation and the continuity equation of both charge carriers[21], these equations are given as

$$\nabla^2\varphi = \frac{q}{\varepsilon}(n - p + N_A - N_D) \qquad 1$$

Where, N_A is the acceptor concentration, N_D is the donor concentration and φ is the electrostatic potential, q electric charge and the ε dielectric permittivity of the semiconductor.

$$\nabla J_n - q\frac{\partial n}{\partial r} = +qR \qquad 2$$

$$\nabla J_p + q\frac{\partial p}{\partial r} = -qR \qquad 3$$

Here, J_n represents the current density for electrons, J_P represents the current density for holes and R is the rate of carrier recombination

$$J_n = qn\mu_n E + qD_n\nabla_n \qquad 4$$

$$J_p = qp\mu_p E - qD_p\nabla_p \qquad 5$$

Where, D_p is the diffusion coefficient for holes and D_n is the diffusion coefficient for electrons.
The code iterates the equations using Newton Raphson and Gunmel iteration method [22] to produce the results

After optimizing the performance parameters, we then vary the interface defect density in the range of 10^{10} to 10^{18} cm^{-2} to cover the low 10^{12} and high 10^{16} cm^{-2} defect densities as given by [16] at the 2D-$MoTe_2$/ $CH_3NH_3PbI_3$ and $CH_3NH_3PbI_3$/ Cu_2O interfaces with the corresponding $CH_3NH_3PbI_3$ thickness respectively and find out the effect on the cell performance parameters (PCE, Voc, Jsc and FF).

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3. Results and Discussion

The SCAPS simulations were performed based on parameters obtained from different experimental and theoretical research papers. Each component of the perovskite solar cell has a significant influence on the device's performance. After designing the cell FTO/2D-$MoTe_2$/$CH_3NH_3PbI_3$/Cu_2O/Au keeping all the parameters the same. we optimized the performance parameters, the result of the optimized cell is given in table 2. The cell gives an optimum power conversion efficiency of 24%.

Optimization of the electron transport layer is also very much important to achieve higher photovoltaic performance in perovskite solar cells. The ETL is responsible for extracting and transporting the photogenerated electrons. Optimization of ETL can control the charge recombination rates in perovskite solar cells. Fig. 3b represents the plots of performance parameters as a function of ETL thickness that is varied in the range of 10–100 nm. It was observed very insignificant decreases in open-circuit voltage as the layer thickness increases, then it becomes constant followed by a slight decrease which may be due to the increase in the series resistance and recombination in the device. The highest obtained VOC is at 10 nm with a value of ~1.09V. The short circuit current density(JSC) first goes through a small decrease as we increase the thickness, then the JSC decreases almost following a linear curve, getting a minimum value at 100 nm of ETL thickness. The fill factor (FF) and efficiency curves display a similar nature. Both of them increase as the thickness is varied in the range of 10 nm–40 nm. On further increasing the thickness, the FF and PCE become almost constant with a negligible variation. So, for the optimum device configuration, the ETL thickness should be in the range of 40 nm–60 nm which is nearly equal to carrier diffusion length.

It is observed that the device with Cu_2O shows better performance as compared to others. The performance parameters obtained after simulation with different HTLs are s

Table 2: Optimized performance parameters of the device.

Performance parameters	
Open circuit voltage (Voc)	1.1264 V
Short circuit current density (Jsc)	24.450764 mA/cm^2
Fill factor (FF)	86.34 %
Power Conversion Efficiency (PCE)	23.78 %

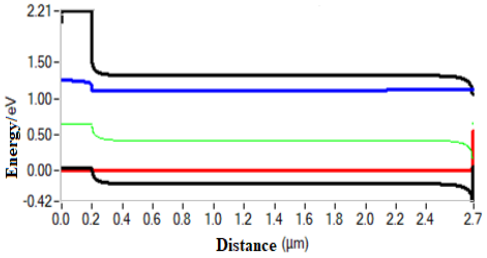

Figure 2: Band Diagram

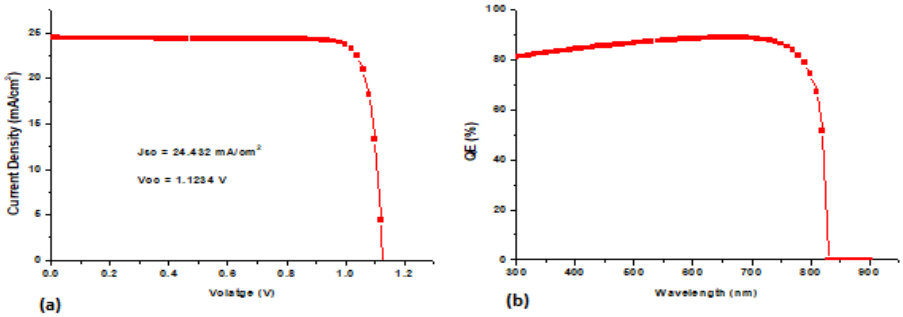

Figure 3: (a) The IV characteristics (b) Quantum Efficiency of the PSC

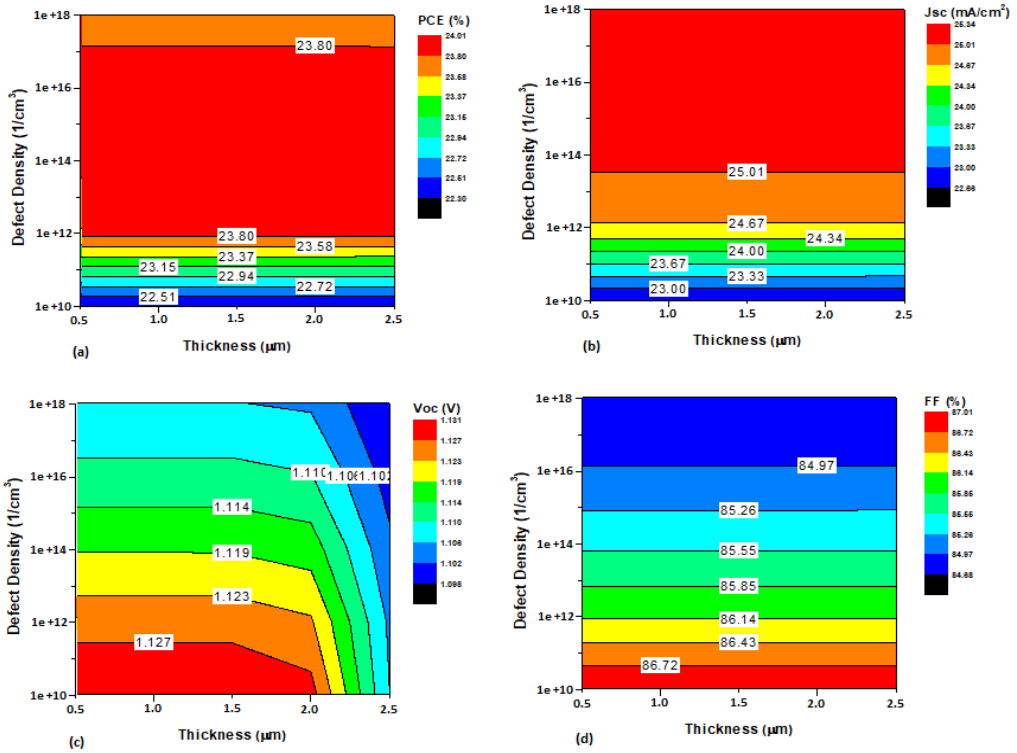

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Figure 4: Contour graphs of $CH_3NH_3PbI_3$ solar cell performance parameters dependency on of interface defect density at 2D-$MoTe_2$/ $CH_3NH_3PbI_3$ interface and $CH_3NH_3PbI_3$ thickness.

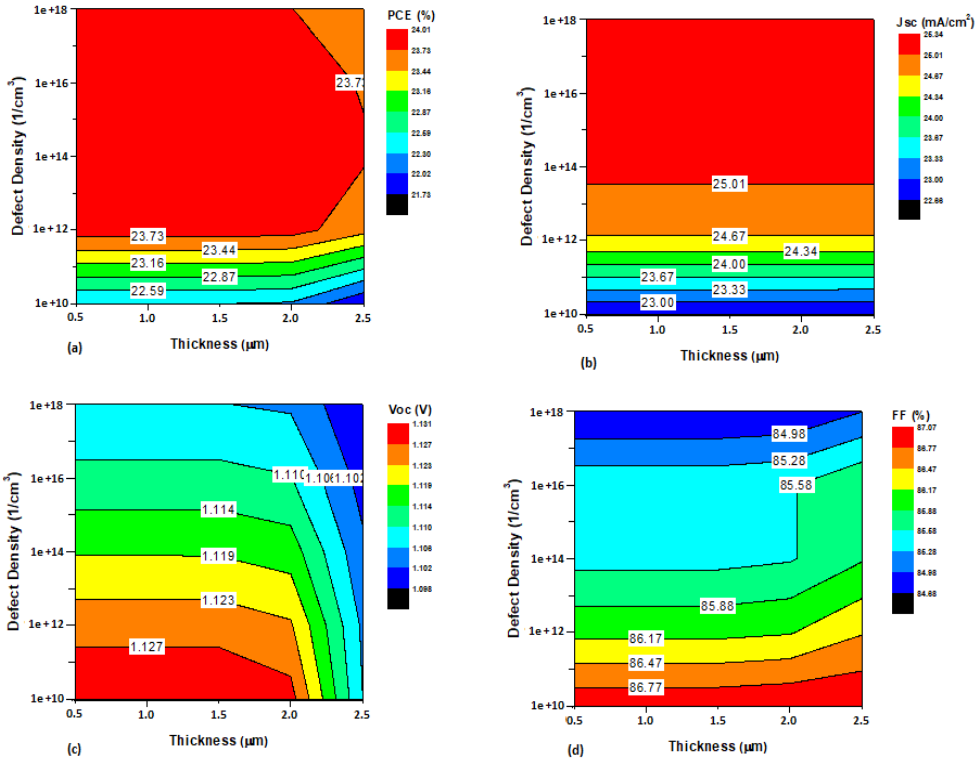

Figure 5: Contour graphs of $CH_3NH_3PbI_3$ solar cell performance parameters dependency on of interface defect density at Cu_2O/ $CH_3NH_3PbI_3$ interface and $CH_3NH_3PbI_3$ thickness.

Conclusion

This study optimized perovskite solar cell with a n-i-p configuration using SCAPS-1D simulator. 2D-$MoTe_2$/$CH_3NH_3PbI_3$/Cu_2O configuration was the primary modelled solar cell. Based on the simulation result, the PCE > 23% was obtained with V_{oc} of 1.2 V, FF 86%, and J_{sc} > 24 mA/cm^2. Increase in absorber layer thickness caused the perovskite solar cell efficiency to rapidly increase. Suitable absorber thickness > 1.0 µm and interfaces defect density of < 10^{14} cm^{-3} were found to be optimal for ETL and HTL/ $CH_3NH_3PbI_3$. In the second part, we obtained the CdS/absorber layer thickness. We changed the absorber layer thickness (0.5–2.0 µm) and tuned the defect density (10^{10}–10^{18} cm^{-3}).

A similar trend was observed although the device performance was more sensitive to the defect density. We discovered that the defect density has significant effect on perovskite solar cells, and increasing the thickness of absorber layer up to the certain point can overcome this issue. This work could provide important information for optimization of perovskite solar cells

Declaration of Competing Interest

The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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