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Impact of Absorbing Layer Band Gap and Light Illumination on the Device Performance of a Single Halide Cs_2TiX_6 Based PSC

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A comprehensive study on impact of active layer band gap and light illumination on the device performance has been analyzed for the FTO/TiO_2/Cs_2TiX_6/CuSCN/Ag based Perovskite Solar Cell (PSC) using the Solar Cell Capacitance Simulator – 1 Dimension (SCAPS-1D) simulator. The present design strategy of the device for optimizing the short circuit current (J_{SC}, mA/cm^2), power conversion efficiency (PCE, %) through the absorbing layer band gap variation, and light illumination spectrum has been studied at the optimal thickness, device temperature, and defect density. The value of the different parameters used in the device simulation has been taken from the previous work. From this study, it was revealed that Cs_2TiBr_6, and Cs_2TiF_6 absorbing layer based PSC device has recorded maximum PCE at the 1.80 eV band gap, whereas, for the Cs_2TiI_6, Cs_2TiCl_6 absorbing layer based PSC device has achieved maximum PCE at the 1.60 eV band gap. On the other side, optimum PCE can be achieved at 400 nm wavelength on the light illumination for the Cs_2TiBr_6, Cs_2TiI_6, and Cs_2TiF_6 absorbing layer based PSC. The Cs_2TiCl_6 absorbing layer based PSC device has recorded maximum PCE at 450 nm wavelength on the different light illumination.

Keywords: Perovskite solar cell, SCAPS-1D, Photovoltaic, Band gap, Illumination.

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1. INTRODUCTION

Solar cell is making for the conversion of solar energy into the electrical energy directly, which has undergone through tremendous development from past few years due to its photovoltaic (PV) properties and that creates a huge interest for researcher community to give their attention towards this area. Initially, 1st generation wafer based PV technology was developed but the production cost was relatively higher with lower conversion ability. The production cost became lower after the introduction of thin film based 2nd generation solar cell but still the power conversion efficiency (PCE) remained low. But both the problem including cost and PCE was nullified after the development of thin film based 3rd generation PV technology. Perovskite solar cells (PSCs) has great capability towards photovoltaic applications and is rapidly emerging as 3rd generation solar cell [1, 2]. Due to its highly suitable optoelectronic, physical, mechanical and electrical properties like direct band gap, large charge carrier mobility, higher optical absorption coefficient and higher diffusion length makes it ideal for photovoltaic use [3]. The journey started with Kojima et al. (2009) with halide Perovskite ABM_3 (A: organic CH_3NH_3+; B: Pb, X: Br, I) and recorded 3.8 % of power conversion efficiency (PCE, %) [1]. Later, further extensive research on material, deposition process, fabrication methods and device structure has enhanced the PCE up to 20.1 % experimentally and theoretically 31.4 % [4, 5]. Despite of such higher conversion efficiency in laboratory, it has several issues towards the commercialization like environment protection from toxic lead (Pb) component, stability under environment conditions due to organic component used in ABM_3 structure. To address such issues, researchers are thinking for use of lead-free inorganic material as absorbing material for the photovoltaic applications. Ju et al. (2018) first developed, Cesium Titanium (IV) mixed Halide Perovskite materials which has tunable band gap 1.0-1.8 eV [6]. Chen et al. (2018) achieved 3.28 % PCE, 1.02 V open circuit voltage (V_{OC}, V), 5.69 mA/cm^2 current density (J_{SC}, mA/cm^2) and 56.4 % Fill factor (*FF*, %) with Cs_2TiBr_6 absorbing material in FTO/TiO_2/Cs_2TiBr_6/P3HT/Au structure [7].

In this study, we have studied the photovoltaic parameters (J_{SC}, PCE) performance with the absorbing layer band gap, light illumination wavelength for the Cs_2TiBr_6, Cs_2TiI_6, Cs_2TiCl_6, and Cs_2TiF_6 based absorbing layer PSC.

2. DEVICE ARCHITECTURE AND SIMULATION

In our proposed FTO/TiO_2/Cs_2TiX_6/CuSCN/Ag based planar solar cell device model, band gap of ETL materials TiO_2 and HTL material CuSCN are taken to be 3.26 eV and 3.4 eV, respectively, the absorbing layer is tunable under 1.6-2.4 eV [8-11]. The working temperature for the simulation was maintained at 27 °C with – 0.8 V to 0.8 V bias voltage in the SCAPS-1D simulator. Here, Fig. 1 shows the schematic view of the proposed structure. All the simulation work was carried out with light illumination of 1.5 AM with the 1000 W/m^2 light power under Gaussian energy distribution where characteristic energy was set in 0.1 eV. The details of the various properties of the device and the base material taken for the work are shown in Table 1 and Table 2,

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respectively. The symbols i.e., E_g denotes the band gap energy, E_a is the electron affinity, ε_r is the relative permittivity, N_A is the acceptor density, N_D is the donor density, N_t is the defect density, N_C is the conduction band effective density of states, N_V is the valence band effective density of states, respectively. Default values of some parameters and settings are as: for electron mobility is 4.4 cm^2/V_s, the hole mobility is 2.5 cm^2/V_s, the electron and hole thermal velocity is 10^7 cm/s [12-14].

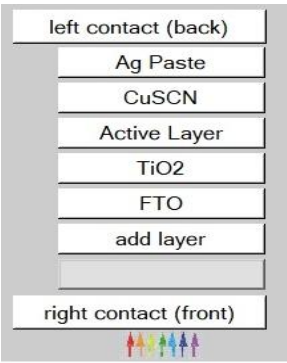

Fig. 1 – Schematic view of the proposed device structure

Table 1 – Base material properties [9, 11, 12]

Properties	CuSCN	TiO_2	FTO
Thickness (μm)	0.35	0.14	0.1
E_g (eV)	3.40	3.26	3.60
E_a (eV)	1.90	3.70	4.0
ε_r	9.0	55.0	9.0
N_D (1/cm^3)	0	4×10^{14}	2.4×10^{18}
N_A (1/cm^3)	1×10^{18}	0	1×10^{5}
μ_n (cm^2/Vs)	2×10^{-4}	100	100
μ_p (cm^2/Vs)	1×10^{-2}	25	25

Table 2 – Absorbing material properties [6, 7, 13-16]

Properties	Cs_2TiBr_6	Cs_2TiI_6	Cs_2TiF_6	Cs_2TiC_6
Thickness (μm)	1.5	1.0	1.0	2.5
E_g (eV)	1.78	1.65	1.90	2.23
E_a (eV)	4.47	4.20	3.70	4.0
ε_r	10	18	18	19
N_D (1/cm^3)	1×10^{19}	1×10^{19}	1×10^{19}	1×10^{19}
N_A (1/cm^3)	1×10^{19}	1×10^{19}	1×10^{19}	1×10^{19}
μ_n (cm^2/Vs)	4.4	4.4	4.4	4.4
μ_p (cm^2/Vs)	2.5	2.5	2.5	2.5

3. RESULTS AND DISCUSSION

3.1 Effect of Absorbing Layer Band Gap

In this section, various optimal values of the physical parameters, including absorbing layer thickness, device temperature and defect density of halide based absorbing materials (Cs_2TiBr_6, Cs_2TiI_6, Cs_2TiCl_6, and Cs_2TiF_6) have been taken for simulation study under the 300 K. The values of the absorbing layer band gap vary in the range of 1.6-2.4 eV. Here, Fig. 2 shows the changes in J_{SC} and PCE with the band gap variation of the absorbing layer. Theoretically, band gap optimization is important to synthesize an optimized band gap active layer experimentally. From Fig. 2a, it is clearly observed that J_{SC} decreases continuously with the band gap for Cs_2TiBr_6, Cs_2TiI_6, Cs_2TiCl_6 absorbing layer PSC and for Cs_2TiF_6 absorbing layer PSC; initially J_{SC} increases up to 1.8 eV band gap, then it decreases continuously. Similarly, PCE decreases drastically with the band gap of Cs_2TiI_6, Cs_2TiCl_6 absorbing layer based PSC and for Cs_2TiBr_6, Cs_2TiF_6 PSC the PCE decreases after the 1.8 eV which can be seen in Fig. 2b. The probable reason behind that decrement in the J_{SC} and PCE is much wider band gap of the absorbing layer is leads to less absorption of photons and as a result, low amount of photo-excited carrier is generated in the device. Thus, both the J_{SC} and PCE show decreasing trends with the band gap [17, 18].

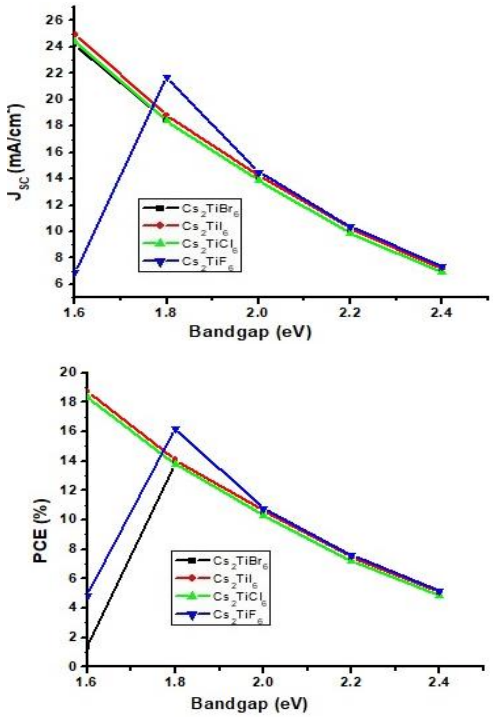

Fig. 2 – Variation in a) J_{SC} and b) PCE with the band gap of the absorbing material

3.2 Effect of Light Illumination Spectrum

In this section, the impact of various light illumination under wavelength of 400 1000 nm on the perovskite solar cell has been studied to analyze the photovoltaic performance of the device. Here, Fig. 3 shows the variation in J_{SC} and PCE with the different wavelength. From this figure it is clear that, Cs_2TiBr_6, Cs_2TiI_6, and Cs_2TiF_6 PSC have almost constant J_{SC} up to 800 nm and after that there is a slight jump in the J_{SC} is observed but for the Cs_2TiCl_6 PSC J_{SC} decreases after 800 nm wavelength. As the J_{SC} is constant up to 800 nm wavelength, the PCE starts to fall from the 400-800 nm wavelength for the Cs_2TiBr_6, Cs_2TiI_6, and Cs_2TiF_6 absorbing layer based PSC and the maximum PCE is recorded as 36 % approximately at 410 nm wavelength. On the other hand, PCE fall drastically from 450 nm wavelength for the Cs_2TiCl_6 absorbing layer based PSC and the highest PCE is recorded as 29 % at 460 nm wavelength. The PCE is depending upon the collection of electron-hole pair generation at the wider wavelength. So, as the illumination wavelength increases, electron-hole pair recombination also increases that leads to decrement in the PCE [19].

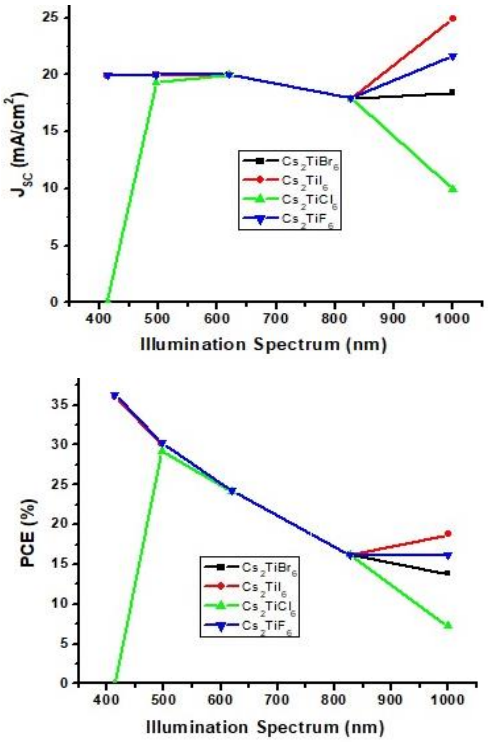

Fig. 3 – Variation in a) J_{SC} and b) PCE with the light illumination spectrum

4. CONCLUSIONS

This research article represents the two aspects of design issues of FTO/TiO_2/Cs_2TiX_6/CuSCN/Ag based PSC, band gap of the absorbing layer and light illumination spectrum. The studies show that Cs_2TiBr_6, Cs_2TiF_6 absorbing layers have maximum PCE at the 1.80 eV band gap, and Cs_2TiI_6, Cs_2TiCl_6 absorbing layers have maximum PCE at the 1.60 eV band gap. Similarly, at 400 nm wavelength highest PCE (36 %) can be achieved for Cs_2TiBr_6, Cs_2TiI_6, and Cs_2TiF_6 absorbing layers and at 450 nm wavelength 29 % PCE can be achieved for the Cs_2TiCl_6 absorbing layer based PSC. This simulation-based study can be useful for the selection of desired material at optimal design condition.

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Вплив ширини забороненої зони активного шару та освітленості на продуктивність пристрою PSC на основі одиночного галогеніду Cs_2TiX_6

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Комплексне дослідження впливу ширини забороненої зони активного шару та освітленості на продуктивність пристрою було проведено для перовскітного сонячного елемента (PSC) на основі FTO/TiO_2/Cs_2TiX_6/CuSCN/Ag з використанням одновимірного симулятора емності сонячних елементів

(SCAPS-1D). Сучасна стратегія проектування пристрою для оптимізації струму короткого замикання (J_{SC}, мА/см^2), ефективності перетворення енергії (PCE, %) за рахунок зміни ширини забороненої зони поглинаючого шару та спектру освітленості була досліджена при оптимальних значеннях товщини, температури пристрою і щільності дефектів. Величини різних параметрів, використаних при моделюванні пристрою, було взято з попередньої роботи. Дане дослідження виявило, що для пристрою на основі поглинаючих шарів Cs_2TiBr_6 та Cs_2TiF_6 максимальне значення PCE спостерігається при ширині забороненої зони 1,80 еВ, тоді як для пристрою PSC на основі поглинаючих шарів Cs_2TiI_6 та Cs_2TiCl_6 максимальне значення PCE досягнуто при ширині забороненої зони 1,60 еВ. З іншого боку, оптимальне значення PCE можна досягти при освітленні з довжиною хвилі 400 нм для PSC на основі поглинаючих шарів Cs_2TiBr_6, Cs_2TiI_6 та Cs_2TiF_6. Для пристрою PSC на основі поглинаючого шару Cs_2TiCl_6 зафіксовано максимальне значення PCE при довжині хвилі 450 нм і різному освітленні.

Ключові слова: Перовскітний сонячний елемент, SCAPS-1D, Фотоелектричний, Ширина забороненої зони, Освітленість.