Comparison of spectral responses of $\text{Cs}_2\text{TiI}_6-\text{xBr}_\text{x}$ based Perovskite device with CdS and TiO$_2$ Electron transport layer

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Abstract. This article represents the spectral responses of a planar FTO/CdS or TiO$_2$/Cs$_2$TiI$_6-\text{xBr}_\text{x/CuSCN/Ag}$ based structure where CdS and TiO$_2$ is used as Electron transport layer (ETL) and CuSCN as Hole transport layer (HTL) under 300 K temperature condition with the SCAPS-1D simulator. The simulation was performed at 750 nm thickness of Cs$_2$TiI$_6-\text{xBr}_\text{x}$ absorbing material where $x = 0$ to 6 to understand the quantum efficiency (QE) using two different ETL (CdS and TiO$_2$). This article shows that TiO$_2$ as ETL has better spectral responses from 300 nm to 900 nm wavelength compare to CdS.

1. Introduction
Perovskite solar cell (PSC) have undergone through a tremendous development for past few years due to its photovoltaic properties. It has created a huge interest for researchers towards its photovoltaic application. Recent reports suggest a power conversion efficiency above 22%. Moreover, researchers have proposed different Perovskite materials having different cell architecture to study the performance of solar cells. Despite of these progress in new generation solar cells, still stability remains a key issue for the Industrial Application & Commercialization. In early days when thin film based third generation Perovskite solar cell was made it was consists of an organic-inorganic lead compound with $\text{ABX}_3$ chemical formula $X$ is an anion which could be a halide element either Br, I, Cl or F and A and B are cations [1]. If we consider a most common organic-inorganic lead compound methyl ammonium lead Iodide Perovskite which has $(\text{CH}_3\text{NH}_3)^+$ cation and it is enclosed by octahedra of PbI$_6$ to form the crystal structure [2]. The position of anion is play important role towards formation of energy. Such organic-inorganic halide hybrid PSCs is most suitable to work as photo active layer as it has several advantages like greater light absorptivity, charge carrier mobility, higher exciton diffusion length, lower exciton binding energy and tunable band gap. As a result the power conversion efficiency (PCE, %) is also higher. Such hybrid halide was first introduced by Kojima et al. [1] with $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{CH}_3\text{NH}_3\text{PbBr}_3$ active material for solar cell and PCE was recorded up to 3.8%. Later he further improved the conversion efficiency by using the quantum dots technique with TiO$_2$ and spin coating as
fabrication method recorded up to 6.5% [1, 2, 3]. Then the researcher used organic spiro-MeOTAD as the HTM (Hole transfer material) in the solar cell which has further improved the PCE upto 9.7% [4]. Further extensive research on CH3NH3PbI3 solar cell recorded highest conversion efficiency >20% which is higher than any traditional DSSCs [4, 5]. The present article, an alternative structure of Cs2TiI6-xBrx based absorbing material (Cs2TiBr6, Cs2TiI5Br5, Cs2TiI4Br4, Cs2TiI3Br3, Cs2TiI2Br2, Cs2TiI1Br1 and Cs2TiI0) has been studied [6, 7] with two different ETL (CdS and TiO2) to find the quantum efficiency (QE, %) of the device. This result will help researcher to find the suitable ETL with this active layer for photovoltaic applications.

2. Simulation Process
The simulation work has been executed under 300 K ambient temperature, 1.5 AM light illumination with 1000 W/m² power which can be reset through the SCAPS-1D simulator software screen [4]. Here, Fig. (1) shows the schematic view of SCAPS tool screen-

![Figure 1. Schematic view of proposed solar cell model](image)

Here, both ETL has higher band gap which is 2.6 eV for CdS and 3.26 eV for TiO2. The above Fig. (1) shows a 5-layer structure and further it can be extended up to 7 layers as per the device structure. The active layer thickness was taken as 0.75 µm for Cs2TiBr6, Cs2TiI5Br5, Cs2TiI4Br4, Cs2TiI3Br3, Cs2TiI2Br2, Cs2TiI1Br1, Cs2TiI0 and 0.14 µm for both CdS and TiO2 ETL [6, 7, 8]. Here, Table 1 indicates the properties of basic material and Table 2 denoted the properties of absorbing material [9, 10].
TABLE 1. Basic Material Properties

| Properties       | CuSCN | CdS  | TiO₂ | FTO |
|------------------|-------|------|------|-----|
| Thickness (µm)   | 0.35  | 0.14 | 0.14 | 0.1 |
| Band gap (eV)    | 3.4   | 2.4  | 3.26 | 3.6 |
| Electron affinity (eV) | 1.9  | 4.18 | 3.70 | 4.0 |
| Permittivity     | 9.0   | 10   | 55.0 | 9.0 |
| \(N_D\) (1/cm\(^3\)) | 0    | 1×10\(^{15}\) | 4×10\(^{14}\) | 2.4×10\(^{18}\) |
| \(N_A\) (1/cm\(^3\)) | 1×10\(^{18}\) | 0    | 0   | 1×10\(^{5}\) |
| Electron mobility (cm\(^2\)/V S) | 2×10\(^4\) | 100  | 100 | 100 |
| Hole mobility   (cm\(^2\)/V S) | 1×10\(^{-2}\) | 25  | 25  | 25  |

TABLE 2. Absorbing Material Properties

| Properties       | \(Cs_2TiBr_6\) | \(Cs_2TiI_1Br_5\) | \(Cs_2TiI_2Br_4\) | \(Cs_2TiI_3Br_3\) | \(Cs_2TiI_4Br_2\) | \(Cs_2TiI_5Br_1\) | \(Cs_2TiI_6\) |
|------------------|----------------|------------------|------------------|------------------|------------------|------------------|----------------|
| Thickness (nm)   | 750            | 750              | 750              | 750              | 750              | 750              | 750            |
| Band gap, \(E_g\) (eV) | 1.78           | 1.58             | 1.38             | 1.26             | 1.15             | 1.07             | 1.02           |
| Electron affinity, \(E_a\) (eV) | 3.22           | 3.42             | 3.62             | 3.74             | 3.85             | 3.93             | 3.98           |
| Relative Permittivity, \(\varepsilon_r\) | 3.75-5.06     | 3.75-5.06       | 3.75-5.06       | 3.75-5.06       | 3.75-5.06       | 3.75-5.06       | 3.75-5.06     |
| Donor density, \(N_D\) (1/cm\(^3\)) | 1×10\(^{19}\) | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\) |
| Acceptor density, \(N_A\) (1/cm\(^3\)) | 1×10\(^{19}\) | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\)  | 1×10\(^{19}\) |
| Electron mobility, \(\mu_n\) (cm\(^2\)/V S) | 4.4            | 4.4             | 4.4             | 4.4             | 4.4             | 4.4             | 4.4           |
| Hole mobility, \(\mu_p\) (cm\(^2\)/V S) | 2.5            | 2.5             | 2.5             | 2.5             | 2.5             | 2.5             | 2.5           |

3. Result and Discussion

In that section, the effect of illumination on Perovskite solar cell device for FTO/CdS or TiO\(_2\)/Cs\(_2\)Ti\(_6\)-XBr\(_X\)/CuSCN/Ag structure has been studied at 300 nm to 900 nm wavelength light sources [11,12]. Quantum efficiency (QE) analysis at optimised thickness for the Perovskite material with TiO\(_2\) and CdS electron transport layer (ETL) will suggests the conversion of part of wavelength of the absorbing material into the electron-hole pair and
which will have collected in terms of current. Here, Fig. 2 shows the quantum efficiency comparison between two different ETL CdS and TiO$_2$ at the 0.75 µm thickness of Cs$_2$TiBr$_6$, Cs$_2$TiI$_5$Br$_5$, Cs$_2$TiI$_3$Br$_4$, Cs$_2$TiI$_4$Br$_2$, Cs$_2$TiI$_5$Br$_1$, Cs$_2$TiI$_6$ absorbing layer. The mathematical equation of the quantum efficiency is defined as [11, 12]-

$$\text{QE (\%)} = \frac{h \gamma I_{ph}}{e P} \quad \text{------------------------ (1)}$$

Where, $e$ is charge of electron ($1.6 \times 10^{-19}$ C), $I_{ph}$ is the electrons (holes) collected per second, $h$ is the Planck’s constant ($6.62 \times 10^{-34}$) and $P$ is the incident optical power (Watt).

Fig. 2(a) shows the QE comparison of Cs$_2$TiBr$_6$ absorbing layer with CdS and TiO$_2$ layer where highest 98% quantum efficiency is visible at the wavelength of 360-450 nm for CdS layer and 100% QE is visible at the 360-460 nm wavelength for TiO$_2$ layer. After that wavelength the QE is started to fall gradually, it means collection of charge carrier is also started to decrease after that wavelength. So, for the Cs$_2$TiBr$_6$ absorbing layer the collection of electron hole pair is higher at the 360-460 nm wavelength.

Similarly, Fig. 2(b) indicates up to 98% QE possible for Cs$_2$TiI$_5$Br$_5$ absorbing layer between 350-650 nm wavelength with CdS layer and 100% QE is achievable at the 360-650 nm wavelength for TiO$_2$ layer. After that wavelength the QE is started to fall. On the other hand, Fig. 2(c) shows Cs$_2$TiI$_3$Br$_4$ absorbing layer has 100% of QE at the wavelength of 330-750 nm with TiO$_2$ and 97% QE achievable between the 320-740 nm with CdS layer. Fig. 2(d) shows Cs$_2$TiI$_5$Br$_3$ absorbing layer with 0.75 µm thickness has 98% of QE with CdS ETL and 100% QE with TiO$_2$ ETL at the wave length of 350-760 nm. Similarly, the Fig. 2(e) shows 100% QE for Cs$_2$TiI$_4$Br$_2$ absorbing layer with TiO$_2$ ETL and 96% QE with CdS ETL at the 350-800 nm. Other two materials, Cs$_2$TiI$_5$Br$_1$, Cs$_2$TiI$_6$ has witnessed highest 100% QE with TiO$_2$ ETL and 95% QE with CdS ETL at the 350-830 nm wavelength which can be visible in the Fig. 2(f) and Fig. 2(g) respectively.
The above analysis shows that after 330 nm wavelength the QE started to increase, it means higher amount of solar irradiance is converted into the charge carrier is possible at the 330 nm wavelength and which will remain constant up to 650 nm wavelength for Cs$_2$TiI$_5$Br$_5$, 750 nm wavelength for Cs$_2$TiI$_6$Br$_6$, 760 nm wavelength for Cs$_2$TiI$_7$Br$_7$, 800 nm wavelength for Cs$_2$TiI$_8$Br$_8$, 830 nm wavelength for Cs$_2$TiI$_9$Br$_9$ and Cs$_2$TiI$_3$ absorbing layer. Due to the higher collection of electron-hole pair between that wavelength, the power conversion efficiency and maximum power generation is also enhanced. After that wavelength the conversion efficiency falls due to the less collection of charge carrier. The above comparison shows that TiO$_2$ will be most suitable as ETL compared to CdS for Cs$_2$TiI$_6$-XBr$_X$ Perovskite absorbing layer as at the same wavelength interval the TiO$_2$/Cs$_2$TiI$_6$-XBr$_X$ has 100 % QE.

4. Conclusion
This research article investigated the solar radiation intensity and the power conversion capability of the device with two different ETL for a Cs$_2$TiI$_6$-XBr$_X$ based Perovskite active layer. The spectral analysis shows that TiO$_2$ ETL has better conversion capability compare to CdS ETL as the opto-electronics properties of TiO$_2$ is superior compare to CdS ETL.
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5. References
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