Simulation studies on the electron transport layer based perovskite solar cell to achieve high photovoltaic efficiency

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Abstract. Perovskite solar cells have attracted the attention of the researchers in the last couple of years as a potential photovoltaic device. However, the use of expensive hole transport materials (HTM) in these devices often restricts their commercial adaptability. Thus exploring cost-effective, efficient HTL and ETL materials remain an important challenge to the researchers. In this work, simulation studies are carried out considering cupric oxide (CuO), a relatively inexpensive material as hole transport materials for planar heterojunction perovskite solar cells. The photo-voltaic performance of CuO based hole transport layer (HTL) has been estimated in combination with several electron transport materials (ETM) that include TiO₂, SnO₂, ZnO, CdS, ZnSe, PCBM and Cd₁₋ₓZnₓS. Studies predict that among these materials, the Cd₁₋ₓZnₓS electron transport layer (ETL) could be the most promising to result high photo-voltaic efficiency in combination to CuO based HTL. Also, the thickness and optical band gap of perovskite absorber are optimized in order to achieve maximum photo-voltaic efficiency. The cell efficiency of FTO/ Cd₁₋ₓZnₓS/ CH₃NH₃PbI₃/ CuO/carbon structure is predicted 25.24% under optimized operational conditions with Vₒc, Jₒc and Fill Factor of 1.1eV, 26.32mA/cm² and 87.14% respectively.

Keywords: Perovskite solar cell; Numerical simulation; ETM; Cd₁₋ₓZnₓS

1. Introduction

In the past few years, organic-inorganic metal halide based perovskite solar cells have attracted much attention due to its simple manufacturing process and high photo conversion efficiency. A typical perovskite solar cell is composed of transparent conducting glass substrate, ETL, perovskite layer and HTL, and metal back contact and the entire components play important role in achieving the performances. The role of perovskite layer is crucial since it absorbs the solar light for the photo-voltaic conversion. Among different organic-inorganic hybrid perovskite material, methylammonium lead triiodide (CH₃NH₃PbI₃, also known as MAPbI₃), remain a popular choice as absorber due to it’s low-cost with wide spectral absorption range throughout the ultraviolet–visible region up to about 825 nm, high mobility up to 66 cm²/V/s, tunable band gap and low carrier recombination rate [1]. At the same time, hole transport material and electron transport material are the important component to achieve the high performance perovskite solar cells (PSCs).
Currently, the compact or mesoporous scaffold TiO$_2$ is widely used as ETL, however its degradation under continuous ultraviolet sunlight leads to instability of PSC performance due to the activation of the oxygen vacancy charge trap, which is the major challenging issue [2]. And therefore alternative materials are required, the oxygen-free CdS is one of them. However there are two new problems arising when CdS is used as ETL. Firstly, CdS contains the toxic Cd element, which would pollute the environment. Second, it absorbs the short wavelength region of the solar spectrum due to its narrow band gap(2.45eV), which means that the perovskite layer could not absorb the green portion of photons, leading to deteriorate the device performance [3]. In order to solve these problems, ternary Cd$_{1-x}$Zn$_x$S compounds have been investigated to replace CdS. The electrical and optical properties of binary CdS compound can be adjust by introducing different molar concentrations of Zn into CdS [4]. As the molar concentrations of Zn increases, the band gap of Cd$_{1-x}$Zn$_x$S increases from 2.42eV for CdS(x=0) to 3.6 eV for ZnS(x=1) [5], which can increase the external quantum efficiency and improve device performance due to the green response of the solar cell. At the same time, it is less toxic when part of Cd is replaced with Zn in CdS. In this paper, we compared several materials commonly used for ETL, finally chose Cd$_{1-x}$Zn$_x$S as ETL, and specifically studied the influence of its proportion and thickness on the perovskite solar cells.As far as HTL are concerned, we chose CuO as HTL in this study. Copper oxide (CuO) is a typical p-type semiconductor with a low valence band energy level, which can be well matched with perovskite (CH$_3$NH$_3$PbI$_3$). The low cost, simple preparation of CuO again advantageous towards fabricating cost effective high-performance perovskite solar cells. X-ray diffraction (XRD) studies show that CuO has higher crystallinity than well explored hole transport materials PEDOT: PSS and thus CuO can promote the transport of charge carriers and improve device performance [6]. In order to achieve maximum photo-voltaic efficiency, the thickness and optical band gap of perovskite photo absorber are optimized based on the simulation algorithm. The cell efficiency of FTO / Cd$_{0.4}$Zn$_{0.6}$S / CH$_3$NH$_3$PbI$_3$/CuO/carbon structure is estimated 25.45% under optimized operational conditions.

The development of actual device as per the estimated efficiency may be challenging due to the unavoidable errors involved in fabricating the cells through several steps. The environmental impact on the stability of the cell has not been taken also into account for the simulation studies. However, the present study on the optimization of CuO HTL based perovskite solar cell could be insightful to the researchers towards developing cost effective and efficient perovskite solar cells.

2. Device structure and simulation method

Herein, wxAMPS software which simulates the photo-voltaic performance of solar cells by solving the boundary conditions of the entire device has been used to optimize the characteristics of key components i.e., ETL, HTL, absorber layer, front/back contacts. The coupled Poisson equation, continuity equation of electrons/holes are solved here based on the Shockley-Read-Hall reorganization model which is also known as trap assisted reorganization [1].

Table 1 and Table 2 summarize the material’s parameters (such as electron and hole mobility, electron affinity, relative permittivity, effective density of states in the conduction band and valence band) which are used for simulation These parameters are mostly taken from the experimental reports and few are obtained theoretically. The absorption spectra $\alpha(E)$ data are obtained from Spectroscopic Ellipsometry (SE) experimental publications results [5]. The $\alpha$ can be obtained from Eq. (1) according to the SE value of extinction coefficient $k$ and wavelength $\lambda$.

$$\alpha = \frac{4nk}{\lambda}$$

The solar spectrum of AM1.5G, working temperature of 300K are considered for the simulation. The reflectivity at the front and back contact is assumed 5% and 80% respectively and the recombination velocity (SRV) of electrons and holes are considered $10^7$ cm/s. Figure 1(a) shows the simulated structure of the device which is composed of glass substrate/FTO/ETL/ CH$_3$NH$_3$PbI$_3$/ HTL/carbon. The energy band diagram of electron transport materials and CH$_3$NH$_3$PbI$_3$ are presented in Figure 1 (b) and (c).
Table 1. Input Parameters for PSC device simulation [7-11].

| Parameters | FTO | TiO₂ | SnO₂ | ZnO | CdS | ZnSe | PCBM | CH₃NH₃PbI₃ | CuO |
|------------|-----|------|------|-----|-----|------|------|-------------|-----|
| Thickness (nm) | 500 | 50 | 50 | 50 | 50 | 50 | 600 | 200 |
| Eg(eV) | 3.5 | 3.2 | 3.5 | 3.3 | 2.4 | 2.18 | 2 | 1.55 |
| χ(eV) | 4 | 4 | 4 | 4 | 4.18 | 4.09 | 3.9 | 3.93 |
| εₚ | 2.2×10¹⁸ | 1×10¹⁰ | 4.3×10¹⁰ | 2.2×10¹¹ | 2.2×10¹³ | 2.5×10²¹ | 2.2×10¹⁸ | 2.5×1⁰²⁸ |
| 2Nₓ(cm⁻³) | 1.8×10¹⁹ | 2×1⁰²⁰ | 2.52×1⁰²⁰ | 1.8×1⁰²⁰ | 1.9×1⁰²⁰ | 1.9×1⁰²⁰ | 2.6×1⁰²⁰ | 3×1⁰²⁰ |
| Nₓ(cm⁻³) | 2×1⁰¹⁹ | 1×1⁰¹⁸ | 1×1⁰¹⁸ | 1×1⁰¹⁸ | 1×1⁰¹⁸ | 1×1⁰¹⁸ | 2.93×1⁰¹⁷ | 0 |
| Nₓ(cm⁻³) | 1×1⁰¹⁶ | 1×1⁰¹⁶ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁴ | 1×1⁰¹⁴ |

Table 2. Material parameters of Cd₁₋ₓZnₓS ETL [2][12-13]

| Parameters | X=1 | X=0.8 | X=0.6 | X=0.4 | X=0.2 | X=0 |
|------------|-----|-------|-------|-------|-------|------|
| Thickness(nm) | 50 | 50 | 50 | 50 | 50 | 50 |
| Eg(eV) | 3.5 | 3.33 | 3.07 | 2.78 | 2.58 | 2.45 |
| χ(eV) | 3.9 | 4.02 | 4.14 | 4.29 | 4.38 | 4.5 |
| εₚ | 8.3 | 9.3 | 9.3 | 9.3 | 9.3 | 9.4 |
| Nₓ(cm⁻³) | 1.3×10¹⁸ | 2.1×10¹⁸ | 2.1×10¹⁸ | 2.1×10¹⁸ | 2.1×10¹⁸ | 2.1×10¹⁸ |
| Nₓ(cm⁻³) | 1.8×10¹⁹ | 1.71×10¹⁹ | 1.71×10¹⁹ | 1.71×10¹⁹ | 1.71×10¹⁹ | 1.71×10¹⁹ |
| μₓ(cm²/V/s) | 50 | 60 | 65 | 80 | 85 | 100 |
| μₓ(cm²/V/s) | 10 | 15 | 20 | 30 | 50 |
| Nₓ(cm⁻³) | 1×1⁰¹⁶ | 1×1⁰¹⁷ | 1×1⁰¹⁷ | 1×1⁰¹⁷ | 1.7×1⁰¹⁷ | 1.7×1⁰¹⁷ |
| Nₓ(cm⁻³) | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ | 1×1⁰¹⁵ |

Fig 1. (a) schematic structure of the device. (b) and (c) energy band diagram of different ETLs and perovskite layer.
3. Results and discussion

3.1. Effect of ETL layer material

The photo-voltaic parameters ($V_{OC}$, $J_{SC}$, FF and η %) obtained experimentally for the perovskite cells prepared using CH$_3$NH$_3$PbI$_3$ absorber, CuO based HTL and TiO$_2$/SnO$_2$/ZnO/CdS/ZnSe/PCBM/$\text{Cd}_{1-x}\text{Zn}_x\text{S}$ based ETL are summarized in Table 3. As envisaged from the table, the short-circuit current ($J_{SC}$) densities of the cells composed of PCBM and CdS ETL are 22.78 mA / cm$^2$ and 23.33 mA / cm$^2$, respectively which are comparatively lower than the other studied ETLs. $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ based ETLs show the highest photovoltaic efficiencies of 24.70%. Figure 2 (a) represents the QE of different cells prepared using the already mentioned ETLs, CuO based HTL and CH$_3$NH$_3$PbI$_3$ absorber. The high QEs for the TiO$_2$, SnO$_2$, ZnSe and $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ based cells can be identified in the figure 2 (b). The band alignments of ETL and HTLs with the perovskite absorber influence the photovoltaic efficiencies as well as QEs of solar cells. Thus, the recommended alignment of conduction band (E$_c$) and valence band (E$_v$) for HTLs, ETLs, perovskite and FTO substrate to achieve high photo conversion efficiency should be similar to the alignment shown in Figure 1 (c) of TiO$_2$. The improper band alignments and the smaller band gap (E$_g$) values (shown in Figure 1 (c) of PCBM and CdS) lead to their lower photo-voltaic efficiencies.

| Parameters | TiO$_2$ | SnO$_2$ | ZnO | CdS | ZnSe | PCBM | $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ |
|------------|---------|---------|-----|-----|------|------|-------------------------------|
| $V_{OC}$ (V) | 1.09 | 1.09 | 1.08 | 1.08 | 1.09 | 1.09 | 1.09 |
| $J_{SC}$ (mA/cm$^2$) | 26.48 | 26.46 | 24.39 | 23.33 | 26.49 | 22.78 | 26.48 |
| FF (%) | 86.37 | 85.34 | 84.99 | 84.29 | 85.37 | 85.30 | 85.51 |
| η (%) | 24.66 | 24.64 | 22.54 | 21.33 | 24.67 | 22.99 | 24.70 |

Fig 2. (a) J-V curves and (b) Quantum efficiency curves for CH$_3$NH$_3$PbI$_3$ based solar cells with TiO$_2$, SnO$_2$, CdS, ZnSe, ZnO, PCBM and $\text{Cd}_{1-x}\text{Zn}_x\text{S}$

3.2. Effect of the composition on the ETL layer material

Figure 3 studies the ternary alloy $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ as the ETL, showing the changes in key parameters of the battery with different Zn molar concentrations. The x value is defined as the percentage of the Zn concentration in $\text{Cd}_{1-x}\text{Zn}_x\text{S}$, from 0 to 1, with a step size of 0.2, from the binary compound $\text{Cd}_S (x = 0)$ to the ternary compound $\text{Cd}_{1-x}\text{Zn}_x\text{S} (0 < x < 1)$ and finally back to the binary compound $\text{Zn}_S (x = 1)$). One of the reasons for choosing $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ is its band gap tunability. It can be observed from Fig. 3 that the change of x has little effect on $V_{OC}$ and $J_{SC}$. When x increases from 0 to 0.6, the fill factor and efficiency increase monotonically, which may be attributed to the band gap change of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ ETL. As the value of x increases, the electron affinity of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ decreases and the band gap increases, as shown in Table 2. The higher band gap of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ will reduce the spectral response of ETL in the green region.
Therefore, the perovskite layer will absorb more incident light and the efficiency will be improved. When $x$ further increases from 0.6 to 1, FF and efficiency decrease, which can be interpreted as the electron affinity of ZnS ($x = 1$) is higher than that of CH$_3$NH$_3$PbI$_3$ (Figure 1(b)). This hinders the flow of electrons from the light-absorbing layer to the ETL, resulting in reduced efficiency.

![Graph](image1)

**Fig 3.** Comparison of cell parameter variation with changing alloy composition ($x$) in Cd$_{1-x}$Zn$_x$S buffer layer with different perovskite layer thickness

### 3.3. Effect of Absorbing layer thickness

In order to achieve the optimum device performance, the simulations of thickness, band gap, doping concentration and defects of absorbing layer is very important. Accordingly, here simulation studies are carried out by varying the thickness of absorber layer within 100-1000nm It is observed that when the thickness of the absorption layer increases from 100 nm to 1000 nm, $V_{oc}$ decreases by a small amount (0.02eV). The increase in the thickness of the absorption layer, enhances the possibility of charge carrier recombination leading to the increment of dark saturation current ($J_0$) to a higher level. The decrease in $V_{oc}$ thus can be explained as per the relation shown in Eqn. 3,[14],

$$V_{oc} = \frac{nKT}{e} \ln \left( \frac{V_{oc}}{I_0} + 1 \right)$$

(2)

Therefore, $V_{oc}$ is influenced by the saturation current density which further depends on the recombination in the device. At the same time, as the thickness of the absorbing layer increases, the FF
decreases which is due to the increase in series resistance at both ends of the cell. $J_{sc}$ is found to increase significantly when the thickness of absorber layer increased from 100nm~400nm. The increase in the thickness of the absorber layer facilitates the absorption of more photons of longer wavelengths which in turn increases the $J_{sc}$ values. However, light absorption over the absorber layer saturates at particular thickness and thus significant change in current density is not predicted when the thickness is kept within 600-1000 nm. Similarly, the change of PCE with the thickness of the perovskite layer is shown in Figure 3. The PCE of the solar cell attains maximum of 24.70% when the thickness is about 600nm and $x=0.6$. For an overly thick perovskite layer, although the increase in absorption generates more carriers in the device, the increase in recombination and series resistance will reduce the collection efficiency of the device. The simulated results thus predict that by adjusting the thickness of the absorption layer to about 600 nm, a high-efficiency perovskite solar cell can be obtained.

3.4. Effect of Band gap of absorbing layer

![Figure 4](image)

**Fig 4.** Effect of variation of absorber layer doping concentration on photovoltaic parameters

The simulation studies also show that with the variation of band gap of absorbing layer, the open circuit voltage and short circuit current density of the cell change appreciably. Figure 4 represents the variation of open circuit voltage ($V_{oc}$) and short circuit current density ($J_{sc}$) with the band gap (from 1.2 to 1.9 eV) of absorbing layer. As shown in the figure, the Voc increases but Jsc decreases with the increase in the band gap of absorbing layer. The increase in the Voc can be explained due to the separation of photogenerated charge carriers by a larger potential barrier, resulting in the decrease in radiation recombination. The decrease in Jsc with the band gap is because of the decrease in the energy difference between the HTL/absorption layer ($\Delta E_{a}$). The band gap of CH$_3$NH$_3$PbI$_3$ can be adjusted by adjusting the Pb-I-Pb bond angle pair in the metal halide (PbI$_3$) When the band gap is reduced from 1.65eV to 1.40eV, the absorption layer can absorb the solar spectrum with a red shift. An increase in the band gap facilitates the absorption of more photons leading to the higher efficiency. Similarly, the reduction of band gap from 1.65eV to 1.40eV leads to the lowering of $\Delta E_{a}$ from 0.42eV to 0.17eV and in turn improves the hole collection efficiency. As the absorption band gap increases, the conduction band (Ec) also shifts and the energy gap between absorption layer/ETL interface becomes larger. A larger barrier difference will result higher interface contact resistance leading to the decrease in FF. The optimum PCE of the cell will be obtained when the band gap of CH$_3$NH$_3$PbI$_3$ absorber will be maintained at 1.6 eV. Further, Table 4 displays a comparison between our simulated results with the experimental work by the other researchers.
Table 4. Results comparison

| Parameters | structure | \(\text{Voc}(\text{V})\) | \(\text{Jsc}(\text{mA/cm}^2)\) | \(\text{FF}(\%)\) | \(\eta(\%)\) |
|------------|-----------|----------------------|----------------------|----------------------|----------------------|
| simulation | \(\text{CdTe/ Cd}_{1-x}\text{Zn}_x\text{S}[15]\) | 0.85 | 29.35 | 85 | 22.42 |
| | \(\text{Cd}_{1-x}\text{Zn}_x\text{S/CH}_3\text{NH}_3\text{PbI}_3\text{Cl}_x[/]spiro-OMeTAD[12]\) | 1.22 | 25.28 | 84.22 | 24.83 |
| | \(\text{Cd}_{1-x}\text{Zn}_x\text{S/CH}_3\text{NH}_3\text{PbI}_3/\text{MASnBr}_3[16]\) | 1.15 | 20.53 | 84.50 | 20.22 |
| This paper | \(\text{Cd}_{1-x}\text{Zn}_x\text{S/CH}_3\text{NH}_3\text{PbI}_3/\text{CuO}\) | 1.10 | 26.32 | 87.14 | 25.24 |

4. Conclusion
The development of a perovskite based photo-voltaic device requires several components which include conducting glass substrate, electron transport layer, photo-absorber, hole transport layer, interfacial layer and back contacts. These components need to be configured properly in sequence to achieve efficient solar cells. The selection of components and thereafter arranging them in order is again very challenging. The simulation studies are thus considered very important prior to start developing actual photovoltaic cells in laboratories. The present simulation based activities has concentrated to explore the photovoltaic characteristics of perovskite solar cells composed of CuO hole transport layer (HTL) along with other key components. Here, wxAMPS software has been used to numerically simulate the performance of target perovskite solar cell. Simulation studies have been started with the optimization of electron transport layer (ETL) appropriate with the CuO based HTL and \(\text{CH}_3\text{NH}_3\text{PbI}_3\) absorber. Several ETLs such as \(\text{TiO}_2,\ \text{SnO}_2,\ \text{ZnO, CdS, Cd}_{1-x}\text{Zn}_x\text{S, ZnSe, and PCBM}\) are taken into consideration, \(\text{Cd}_{1-x}\text{Zn}_x\text{S}\) ETL is found most promising to result high photo-voltaic efficiency when \(x=0.6\). The optimum thickness of the absorption layer is estimated to be 600 nm to obtain the maximum photo-voltaic efficiency. The band gap of the perovskite layer is recommended to be 1.6 eV. The simulation studies finally predict that the cell efficiency of FTO / \(\text{Cd}_{1-x}\text{Zn}_x\text{S/CH}_3\text{NH}_3\text{PbI}_3/\text{CuO/carbon}\) structure will be 25.24% under optimized operational conditions.

References
[1] Bag, A.; Radhakrishnan, R.; Nekovei, R.; Jeyakumar, R., Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation. Solar Energy. 2020; 196: 177-82.
[2] Ahmed, A.; Riaz, K.; Mehmoody, H.; Taqueer, T.; Ahmad, Z., Performance optimization of \(\text{CH}_3\text{NH}_3\text{PbI}_3(1-x\text{Br}_x)\) based perovskite solar cells by comparing different ETL materials through conduction band offset engineering. Optical Materials 2020, 105.
[3] Yu, X.; Zou, X.; Cheng, J.; Chang, C.; Zhou, Z.; Li, G.; Liu, B.; Wang, J.; Chen, D.; Yao, Y., Numerical simulation analysis of effect of energy band alignment and functional layer thickness on the performance for perovskite solar cells with \(\text{Cd}_{1-x}\text{Zn}_x\text{S}\) electron transport layer. Materials Research Express 2020, 7 (10).
[4] Horoz, S.; Ekinci, A.; Sahin, O., Synthesis, characterization and photovoltaic properties of \(\text{Cd}_{1-x}\text{Zn}_x\text{S}\) and Mn: \(\text{Cd}_{1-x}\text{Zn}_x\text{S}\) quantum dots. Journal of Materials Science: Materials in Electronics 2018, 29 (7), 5830-5836.
[5] Joishy, S.; Hebbar, D. N.; Kulkarni, S. D.; Rao, K. G.; Rajendra, B. V., Band structure controlled solid solution of spray deposited \(\text{Cd}_{1-x}\text{Zn}_x\text{S}\) films: Investigation on photoluminescence and photo response properties. Physica B: Condensed Matter 2020, 586.
[6] Rajeswari, R.; Mrinalini, M.; Prasanthkumar, S.; Giribabu, L., Emerging of Inorganic Hole Transporting Materials For Perovskite Solar Cells. Chem Rec 2017, 17 (7), 681-699.
[7] Rai, S.; Pandey, B. K.; Dwivedi, D. K., Modeling of highly efficient and low cost \(\text{CH}_3\text{NH}_3\text{PbI}_3(1-x\text{Cl}_x)\) based perovskite solar cell by numerical simulation. Optical Materials 2020, 100.
[8] Azri, F.; Meftah, A.; Sengouga, N.; Meftah, A., Electron and hole transport layers optimization by numerical simulation of a perovskite solar cell. Solar Energy 2019, 181, 372-378.
[9] Zhao, P.; Lin, Z.; Wang, J.; Yue, M.; Su, J.; Zhang, J.; Chang, J.; Hao, Y., Numerical Simulation of Planar Heterojunction Perovskite Solar Cells Based on \(\text{SnO}_2\) Electron Transport Layer.
Baig, F.; Khattak, Y. H.; Mari, B.; Beg, S.; Gillani, S. R.; Ahmed, A., Mitigation of interface recombination by careful selection of ETL for efficiency enhancement of MASnI3 solar cell. Optik 2018, 170, 463-474.

Tong, K.; Liu, Z.; Fan, J.; Shao, G., Numerical investigation of copper oxide-based heterojunction solar cells. Journal of Physics D: Applied Physics 2019, 52 (27).

Chowdhury, T. H.; Ferdaous, M. T.; Wadi, M. A. A.; Chelvanathan, P.; Amin, N.; Islam, A.; Kamaruddin, N.; Zin, M. I. M.; Ruslan, M. H.; Sopian, K. B.; Akhtaruzzaman, M., Prospects of Ternary Cd$_{1-x}$Zn$_x$S as an Electron Transport Layer and Associated Interface Defects in a Planar Lead Halide Perovskite Solar Cell via Numerical Simulation. Journal of Electronic Materials 2018, 47 (5), 3051-3058.

Xu, X.-B.; Wang, X.-Y.; Gu, W.-P.; Quan, S.; Zhang, Z., Study on influences of CdZnS buffer layer on CdTe solar cells. Superlattices and Microstructures 2017, 109, 463-469.

Huang, L.; Sun, X.; Li, C.; Xu, R.; Xu, J.; Du, Y.; Wu, Y.; Ni, J.; Cai, H.; Li, J.; Hu, Z.; Zhang, J., Electron transport layer-free planar perovskite solar cells: Further performance enhancement perspective from device simulation. Solar Energy Materials and Solar Cells 2016, 157, 1038-1047.

Md. Sharafat Hossain;N. A., M. M. Aliyu; M. A. M., Zn$_x$Cd$_{1-x}$S AS PROSPECTIVE WINDOW LAYER IN CdTe THIN FILM SOLAR CELLS FROM NUMERICAL ANALYSIS. IEEE Photovoltaic Specialists Conference 2011.

Xu, X.-B.; Wang, X.-Y.; Gu, W.-P.; Quan, S.; Zhang, Z., Study on influences of CdZnS buffer layer on CdTe solar cells. Superlattices and Microstructures 2017, 109, 463-469.