Numerical simulation analysis of effect of energy band alignment and functional layer thickness on the performance for perovskite solar cells with Cd_{1-x}Zn_xS electron transport layer

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Abstract
Energy band alignment between perovskite layer and charge transport layers is critical to the perovskite solar cell efficiency. The thickness of functional layers also has a great influence on the device performance. We have optimized the energy band alignment at the interface between electron transport layer (ETL) and perovskite layer by using appropriate Cd_{1-x}Zn_xS ETL (x represents the Zn molar concentration). Different hole transport layers (HTLs) have also been selected to address the mismatching energy band alignment at perovskite/HTL interface. Additionally, the thickness of Cd_{1-x}Zn_xS ETL and perovskite layer (MAPbI_3) has been optimized. We performed all the analysis via numerical simulation with wx Analysis of Microelectronic and Photonic Structures (wxAMPS) software. We also compared the results obtained in this study, with results reported in other literature to ascertain the validity of the results. The results show that the device performance could be improved by appropriately increasing the molar concentration of Zn in Cd_{1-x}Zn_xS. Spike-type energy band structure at the interface of MAPbI_3/HTL could favor the performance of perovskite solar cells when MASnBr_3 is adopted as HTL. Appropriate ETL and perovskite layer thickness would increase the short circuit current and reduce the recombination loss.

1. Introduction
In the past ten years, the perovskite solar cells have received tremendous attention [1–4]. Since the technology of dye-sensitized solar cell was initially employed to prepare PSCs, compact or mesoporous scaffold TiO_2 layer was typically used as ETL [5]. However, It’s reported in previous literature that the TiO_2 ETL exhibited degradation under continuous ultraviolet sunlight due to the activation of oxygen vacancy charge traps, which led to the unstable performance of PSCs [6, 7].

To address the issues of harmful effect of TiO_2 on perovskite layer, oxygen-free CdS was adopted to form ETL with different methods [8–16]. However, two issues about CdS couldn’t be ignored when it is used as ETL [17]. First, the short wavelength region of the solar spectrum could be well absorbed by CdS due to its small band gap (2.45 eV), which means that the green portion of photons could not be absorbed by perovskite layer, leading to the reduced external quantum efficiency. Second, CdS consists of the toxic Cd element, which would pollute the environment.
Table 1. Electric parameters for Cd$_{1-x}$Zn$_x$S electron transport layers used in this simulation (x represents the Zn molar concentration) [25, 27–34].

| Parameters                  | Symbols | x = 0  | x = 0.05 | x = 0.08 | x = 0.1 | x = 0.2 | x = 0.3 | x = 0.5 | x = 0.6 | x = 0.8 | x = 1 |
|-----------------------------|---------|--------|----------|----------|---------|---------|---------|---------|---------|---------|-------|
| Permittivity                | $\varepsilon$ |        |          |          |         |         |         |         |         |         |       |
| Band gap (eV)               | $E_g$   | [28]   | [6]      | [5]      | [4]     | [3]     | [2]     | [1]     | [1]     | [1]     | [1]   |
| Electric Affinity (eV)      | $\chi$  | [29]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Conduction Band Density (cm$^{-3}$) | $N_c$  | [29]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Value Band Density (cm$^{-3}$) | $N_v$  | [29]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Electron Mobility (cm$^2$v$^{-1}$s$^{-1}$) | $\mu_n$ | [29]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Hole Mobility (cm$^2$v$^{-1}$s$^{-1}$) | $\mu_p$ | [27]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Donor Concentration (cm$^{-3}$) | $N_D$  | [30]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Acceptor Concentration (cm$^{-3}$) | $N_A$  | [30]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Defect Density (cm$^{-3}$)  | $N_t$   | [30]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
| Thickness (nm)              |         | [30]   | [2]      | [2]      | [2]     | [2]     | [2]     | [2]     | [2]     | [2]     | [2]   |
The band gap of CdS should be larger and the percentage of Cd in CdS should be lower for high-efficiency and environment-friendly PSCs.

To allow more photons to be absorbed by the perovskite layer, fairly thin CdS film must be used. However, the ultra thin film would cause the pin-holes and lower shunt resistance at the interface, which would deteriorate the device performance [17].

Figure 1. Schematic of perovskite solar cell architecture. HTL: hole transport layer; ETL: electron transport layer; FTO: fluorine-doped tin oxide. MAPbI₃; CH₃NH₃PbI₃.

Figure 2. Energy level diagram of different materials. (a) for Cd₁₋ₓZnₓS electron transport layers (x represents the Zn molar concentration) and perovskite layer. (b) for perovskite layer and different hole transport layers.
**Table 2.** Electric parameters for all the hole transport materials and perovskite materials used in this simulation [45, 47–51].

| Parameters          | Symbols | MASnBr₃ | Cu₂O | CuSCN | NiO          | MAPbI₃ |
|---------------------|---------|---------|------|-------|--------------|--------|
| Permittivity        | ε       | 8.2 [45]| 7.11 [47]| 10 [48]| 10.7 [47] | 10.7 [51] |
| Band gap (eV)       | Eₕ     | 2.15 [45]| 2.17 [47]| 3.6 [48]| 3.8 [47]  | 3.55 [51]  |
| Electric Affinity (eV) | x     | 3.39 [45]| 3.2 [47] | 1.7 [48] | 1.46 [47] | 3.9 [51] |
| Conduction Band Density (cm⁻³) | Nc | 1E18 [45] | 2.02E17 [47] | 2.2E19 [48] | 2.8E19 [47] | 2.2E18 [51] |
| Value Band Density (cm⁻³) | Nv  | 1E18 [45] | 1.1E19 [47] | 1.8E18 [48] | 1E19 [47] | 1.8E19 [51] |
| Electron Mobility (cm²·V⁻¹·s⁻¹) | μₑ | 1.6 [45] | 200 [47] | 100 [48] | 12 [47]  | 10 [51] |
| Hole Mobility (cm²·V⁻¹·s⁻¹) | μₕ | 1.6 [45] | 80 [47] | 25 [48] | 2.8 [47] | 10 [51] |
| Donor Concentration (cm⁻³) | N_D | 0 [45] | 0 [47] | 0 [48] | 0 [47] | 1E13 [51] |
| Acceptor Concentration (cm⁻³) | N_A | 1E18 [45] | 1E18 [47] | 1E18 [50] | 1E18 [47] | 0 [51] |
| Defect Density (cm⁻³) | N_t | 1E15 [45] | 1E14 [47] | 1E14 [49] | 1E14 [47] | 2.5E13 [51] |
| Thickness (nm)      | /       | 50  | 50  | 50  | 450  |

To solve these problems, ternary Cdₓ-ZnₛS compounds have been investigated to modulate the electrical and optical properties of binary CdS compound by introducing Zn of different molar concentrations into CdS [18–22]. It’s reported that the band gap of Cdₓ-ZnₛS varies from 2.42 eV for CdS (x = 0) to 3.6 eV for ZnS (x = 1) [23]. Hence, the external quantum efficiency (for green response of the solar cells) could be improved when higher molar concentration of Zn is incorporated into CdS ETL. Thus, the short circuit current would be enhanced according to the relationship between short circuit current and external quantum efficiency spectra [24]. Moreover, the minimum conducting band (electrical affinity) changes monotonously with the band gap of Cdₓ-ZnₛS at low Zn molar concentration (shown in figure 2(a) and table 1), which is conducive to the energy band alignment at the perovskite layer/Cdₓ-ZnₛS ETL interface [25]. Thus the recombination loss would be reduced and the device performance would be improved [26]. In addition, CdS would be less toxic when part of Cd has been replaced with Zn in Cdₓ-ZnₛS [17].

Cdₓ-ZnₛS has been widely used as ETL in CdTe solar cells via experiments or numerical simulation [35–43]. However, few literatures reported the use of Cdₓ-ZnₛS as electron transport layer in perovskite solar cells [44, 45]. Cdₓ-ZnₛS ETL was adopted by Chowdhury et al to investigate the effect of Zn molar concentration in Cdₓ-ZnₛS on the sensitivity to interface defect levels via numerical simulation (with SCAPS software), where CH₃NH₃Pb₁₋ₓClₓ was used as perovskite layer and spiro-OMeTAD was used as HTL [44]. It’s reported by Baig through numerical simulation (with SCAPS software) that the energy band structure at Cdₓ-ZnₛS/perovskite interface could be modulated to provide better device performance, where the perovskite was determined to be MASnI₃ and HTL was determined to be MASnBr₃ [45].

In this paper, we have investigated the effect of energy band alignment between perovskite layer and charge transport layer on the performance of perovskite solar cells. Moreover, the thickness of ETL and perovskite layer has also been optimized. All the analysis has been performed via numerical simulation with wxAMPS software. The wxAMPS software has been developed at University of Illinois by Liu et al [46]. A combination of Newton and Gummel method is implemented in this software. The light absorption layer is determined to be MAPbI₃ perovskite. We have optimized the energy band alignment at ETL/perovskite layer interface by using appropriate Cdₓ-ZnₛS ETL (x represents the Zn molar concentration). P-type materials (MASnBr₃, Cu₂O, CuSCN, NiO) are used as HTL to optimize the energy band alignment at perovskite layer/HTL interface.

**2. Methods**

**2.1. Device structure**

Figure 1 shows the structure of solar cell model conducted in this simulation. The p-type materials (MASnBr₃, Cu₂O, CuSCN, NiO) are adopted as HTL. The n-type materials (Cdₓ-ZnₛS, where x represents Zn molar concentration) are adopted as ETL. The light absorption layer is determined to be MAPbI₃.
2.2. Electric parameters for materials

Figure 2 shows the energy level diagram for the materials used in this simulation. The defect layers at the ETL/MAPbI\textsubscript{3} interface and MAPbI\textsubscript{3}/HTL interface are ignored. The electric parameters for the materials are demonstrated in table 1 and table 2, which are reported in previous literature [25, 45, 27–34, 47, 48–51].

The value band offsets at perovskite/HTLs interfaces are shown in table 3. Capture cross sections for both holes and electrons are set to be 1 $\times$ 10\textsuperscript{−14} cm\textsuperscript{2} [24]. The defect energy levels for all the materials in this simulation are located at the center of their band gaps with Gaussian distribution (with deviation of 0.1) [24]. The density of band tail states is 1 $\times$ 10\textsuperscript{14} cm\textsuperscript{−3}\textsuperscript{eV}\textsuperscript{−1} and the tail characteristic energy is 0.01 eV [24]. The

Figure 3. Parameters of solar cells with Cd\textsubscript{1−x}Zn\textsubscript{x}S ETL (x represents Zn molar concentration). (a). Open circuit voltage; (b). Short circuit current; (c). Fill factor; (d) Power conversion efficiency for Zn molar concentration (x) ranging from 0 to 1; (e) Power conversion efficiency for Zn molar concentration (x) ranging from 0.6 to 1.

Figure 4. External quantum efficiency spectra of solar cells with Cd\textsubscript{1−x}Zn\textsubscript{x}S ETL (x represents Zn molar concentration). (a). for wavelength ranging from 200 nm to 1000 nm; (b). for wavelength ranging from 200 nm to 500 nm.
The absorption coefficients for all the layers are determined to be $10^5$ [52–60]. The band-to-band recombination rate is set to be $1 \times 10^{-11}$ cm$^3$ s$^{-1}$ [48, 61].

2.3. Environment settings for wxAMPS software

The AM1.5 solar radiation spectrum is used as light source in our work and the temperature is fixed at 300 K [24]. The light reflection coefficient for the bottom and top contacts are set to be 0.8 and 0.2, respectively [43, 62]. The surface recombination velocities for both holes and electrons at the top and bottom electrodes are set to be $1.0 \times 10^7$ cm$^{-1}$ s$^{-1}$ [24].

2.4. Investigation methodology

We improve the performance of perovskite solar cells with the following approaches:

- The light absorption layer is determined to be MAPbI$_3$. The HTL is determined to be MASnBr$_3$ initially. The thickness of ETL, light absorption layer and HTL is initially set to be 50 nm, 450 nm and 50 nm, respectively.

- We analyze the effect of Zn concentration in Cd$_{1-x}$Zn$_x$S ETL on the performance of perovskite solar cells.

- The ETL is determined to be Cd$_{1-x}$Zn$_x$S with optimum Zn concentration discussed above (in terms of efficiency). Then we analyze the effect of different p-type HTLs (MASnBr$_3$, Cu$_2$O, CuSCN, NiO) on the performance of perovskite solar cells.
The ETL is determined to be Cd_{1-x}Zn_xS with optimum Zn concentration discussed above (in terms of efficiency). The HTL is determined to be the optimum p-type material (in terms of efficiency). Then we analyze the effect of thickness of ETL and perovskite layer on the performance of perovskite solar cells.

3. Results and discussion

3.1. Effect of energy band alignment at Cd_{1-x}Zn_xS/MAPbI_3 Interface on the perovskite solar cell performance

The Cd_{1-x}Zn_xS (x represents Zn molar concentration) was used as ETL of perovskite solar cells. The x value ranges from 0 to 1. As x value increases from 0 to 1, Cd_{1-x}Zn_xS shifts from binary compounds (x = 0) to ternary compounds (0 < x < 1) and finally returns to binary compound (x = 1). The HTL is determined to be MA_{0.3}SnBr_{3}, and the perovskite is determined to be MAPbI_3 initially. The reason for selecting Cd_{1-x}Zn_xS ascribed to its bandgap tunability [63]. As the x value increases, the electronic affinity of Cd_{1-x}Zn_xS decreases and the band gap increases (table 1). However, the summation of electronic affinity value and band gap value change little at low Zn concentration, indicating that the maximum value band shows negligible fluctuation (shown in figure 2(a), table 1). Therefore, the selection of Cd_{1-x}Zn_xS ETL with different Zn molar concentration (x) wouldn’t affect the transporting of holes at the ETL/perovskite interface, simplifying the discussion [64].
It’s clearly observed from figure 3 that the device performance could be optimized by appropriately increasing the Zn molar concentration \(x\) in Cd\(_{1-x}\)Zn\(_x\)S. The open circuit voltage increases when \(x\) (Zn molar concentration) increases from 0 to 0.6. While \(x\) further increases from 0.6 to 1, the open circuit voltage decreases. Both the short circuit current and fill factor monotonously increase when \(x\) (Zn molar concentration) increases from 0 to 0.8. While \(x\) further increases from 0.8 to 1, both the short circuit current and fill factor decrease. The power conversion efficiency rocks to the highest at \(x = 0.8\).

Figure 4 shows the external quantum efficiency spectra of solar cells with Cd\(_{1-x}\)Zn\(_x\)S ETL of different Zn molar concentration \(x\). In figure 4(b), the external quantum efficiency increases as the \(x\) value increases from 0 to 1, which could be attributed to the bandgap variation of Cd\(_{1-x}\)Zn\(_x\)S ETL. As \(x\) (Zn molar concentration in Cd\(_{1-x}\)Zn\(_x\)S) increases, the bandgap of Cd\(_{1-x}\)Zn\(_x\)S increases (figure 2(a)). Similar to the previous research reported by Oladeji et al [65], the higher bandgap of Cd\(_{1-x}\)Zn\(_x\)S would reduce the the spectral response of ETL in green region. Thus, more incident light would be absorbed by perovskite layer. Therefore, the external quantum efficiency would be higher. Our results are also similar to previous reported research employing Cd\(_{1-x}\)Zn\(_x\)S as ETL [66]. As reported in previous research, the short circuit current density could be defined as the following formula [24, 67]:

\[
J_{sc} = q \cdot \int_{\lambda_{min}}^{\lambda_{max}} [\Phi(\lambda) \cdot EQE(\lambda)] d\lambda
\]

where \(J_{sc}\) is short circuit current density, \(q\) is quantity of electric charge, \(\lambda\) is wavelength, \(\Phi(\lambda)\) is spectral photon flux of AM 1.5 G solar irradiation and \(EQE(\lambda)\) is external quantum efficiency. Therefore the short circuit current density \(J_{sc}\) increases when external quantum efficiency \((EQE(\lambda))\) is enhanced. Thus, the short circuit current increases as \(x\) value increases from 0 to 0.8. The slight decrease for \(x > 0.8\) could be explained by the higher
Figure 9. External quantum efficiency spectra of solar cells with different HTL (different value band offset).

Figure 10. Energy level of solar cells with different HTL (different value band offset). (a), for position ranging from 0 to 0.55 μm; (b), for position ranging from 0.48 μm to 0.52 μm; (c) illustration for Ea at cliff-like band structure; (d) illustration for Ea at spike-like band structure. Noting: Ea represents active energy of recombination and VBO represents value band offset.
The electronic affinity of ZnS ($x = 1$) is lower than MAPbI$_3$ (figure 2(a)), which impeded the flowing of electrons from light absorption layer to ETL [64].

Figure 5(b) shows the different band structures at the ETL/absorption layer interface. Cliff ($E_{c(ETL)} < E_{c(Absorber)}$) and Spike ($E_{c(ETL)} > E_{c(Absorber)}$) are the two kinds of band structures at the ETL/absorption layer interface [68]. When the band structures exhibit cliff-like structures, the activation energy ($E_a$) of recombination is lower than the bandgap of light absorption layer (figure 5(c)), thus the main recombination process is interface recombination. However, as the $E_a$ increases, the interface recombination decreases [69–71], which leads to the increase of open-circuit voltage for $x$ increasing from 0 to 0.6 (as shown in figure 3(a)). The decrease of open-circuit voltage for $x > 0.6$ may be attributed to the lattice mismatch induced recombination [43]. According to Vegard’s law, the lattice constant of Cd$_{1-x}$Zn$_x$S (ternary compound) could be estimated with the following formula (2) [66]:

$$a = a_{CdS} - x \cdot \left(a_{ZnS} - a_{CdS}\right)$$

Where $a$ represents the lattice constant, $x$ represents the Zn molar concentration in Cd$_{1-x}$Zn$_x$S. As reported in previous research, the lattice constant of MAPbI$_3$ [72], Cds [73] is 6.274 Å, 5.8304 Å, respectively. It means that there is a lattice mismatch between MAPbI$_3$ and Cds. The lattice constant of ZnS is 5.428 Å [74], which is lower than that of Cds. Therefore the lattice constant of Cd$_{1-x}$Zn$_x$S decreases with $x$ (Zn molar concentration) increasing according to formula (2), which is also consistent with the previously reported results [75]. Thus it would create further lattice mismatch between Cd$_{1-x}$Zn$_x$S ETL and MAPbI$_3$ perovskite, which would deteriorate the device performance when $x > 0.6$ (shown in figure 3(a)).
Another difference between the two band structures lies in the built-in electric field at Cd$_{1-x}$Zn$_x$S/MAPbI$_3$ interface (figure 6). Therefore, the band structure would affect the injection of electrons from light absorption layer to ETL [68].

When the cliff is large (the conduction bands between ETL and light absorption layer exhibit a great difference at the interface), the built-in electric field is small [68]. As x value increases from 0 to 0.8, the increment of Zn molar concentration in Cd$_{1-x}$Zn$_x$S lowers the $\Delta$Ec ($E_{c(Absorber)} - E_{c(ETL)}$) (figure 5(b)). Therefore, the built-in electric field at the interface increases gradually (as shown in figure 6(b)), resulting in the efficient extraction of electrons from light absorption layer. Thus the recombination loss would be reduced (as shown in figure 7) and the fill factor would be improved [76] (as shown in figure 3(c)). The discussion mentioned above is consistent with the previous reports that the recombination at the interface could be modulated by designing suitable band structure at ETL/absorption layer interface [26] and the fill factor would be influenced by the recombination [76].

As the Sunlight is incident from Cd$_{1-x}$Zn$_x$S ETL side, more charge carriers would be generated at Cd$_{1-x}$Zn$_x$S ETL/MAPbI$_3$ perovskite interface. Thus, the recombination would be much higher in a region close to Cd$_{1-x}$Zn$_x$S ETL. Therefore, a strong built-in electric field (used to separate electron-hole pairs) at Cd$_{1-x}$Zn$_x$S ETL/MAPbI$_3$ perovskite interface is preferred [77], which is consistent with our above discussion.

When the x value further increases from 0.8 to 1, the ternary Cd$_{0.2}$Zn$_{0.8}$S compound shifts to the binary ZnS compound. The conduction band position of ZnS (−3.8 eV) is higher than that of MAPbI$_3$ (−3.9 eV), leading to the formation of spike band structure. Although the electric field becomes higher, compared with cliff band structure, the spike band structure is not beneficial to the flowing of electrons into the ETL from light absorption layer [45, 64], which would lower the current density (figure 3(b)) and deteriorate the fill factor (figure 3(c)).
Our results are similar to the reported work about the effect of different Zn concentration in Cd$_{1-x}$Zn$_x$S solar cell performance [38].

3.2. Effect of energy band alignment at MAPbI$_3$/HTL interface on the perovskite solar cell performance

Figure 8 depicts the electric parameter variation with the different value band offset (different HTL), where the ETL is determined to be Cd$_{0.2}$Zn$_{0.8}$S. It’s clearly observed that the HTL in our work has a minor impact on the current density. The open-circuit voltage, fill factor and power conversion efficiency all monotonously decrease with value band offset increasing. In addition, the trend in efficiency variation is similar to previous reported results [78]. The MASnI$_3$ (Value Band Offset = −0.09, shown in table 3) is considered as the optimum HTL, yielding the best performance (in terms of efficiency).

As we know, the Sunlight is transmitted from ETL to HTL for solar cells of normal structure and the light absorption layer is sandwiched between ETL and HTL. In addition, the perovskite layer exhibits high absorption ability. As a consequence, the most photons have been captured by ETL and light absorption layer, leading to the negligible absorption for HTL. Therefore, the number of photo-generated charge carriers does not change when different HTL is used. Thus, the external quantum efficiency (figure 9) remains invariable, giving constant current density.

When Cu$_2$O, CuSCN, NiO are used as HTLs, the band structures exhibit cliff-like structures, which decrease the activation energy (Ea) of recombination (figure 10(c)). While MASnBr$_3$ is used as HTL, the band structure
exhibits a small spike-like structure. Therefore, the $E_a$ becomes equal to the bandgap energy (figure 10(d)), leading to the increase of the device open-circuit voltage [64].

As we discussed above, compared with cliff band structure, spike band structure is beneficial to the formation of high built-in electric field [68], which is also verified by figure 11. It’s clearly observed from figure 11(b) that the electric field is highest when MASnBr$_3$ is used as HTL. Thus, the separation of photo-generated electron-hole pairs at perovskite/MASnBr$_3$ interface would be facilitated. Therefore, the device performance could be improved [77]. Different from Cd$_{1-x}$Zn$_x$S ETL/MAPbI$_3$ perovskite interface, the MAPbI$_3$ perovskite/MASnBr$_3$ HTL interface could form p-n junction because the perovskite absorption layer used in our work is n-type while the HTL is p-type. The p-n junction favors the injection of holes into HTL from light absorption layer [77]. Therefore the spike band structure has little adverse impact on the flow of holes to the HTL and the device performance.

As discussed above, when the cliff is lager (figure 10(b)), the electric field is lower (figure 11(b)). Thus, the separation of photo-generated electron-hole pairs at perovskite/HTL interface would be deteriorated, which increases the recombination loss (figure 12). Therefore, the fill factor would be reduced [76] (figure 8(c)). So does the efficiency (figure 8(d)).

3.3. Effect of thickness of Cd$_{0.2}$Zn$_{0.8}$S ETL and MAPb$_3$ light absorption layer on the perovskite solar cell performance

We determine the thickness in the range of 30 nm to 50 nm with a step of 5 nm. It’s clearly observed that 40 nm is the optimum value (In terms of efficiency) (figure 13). It’s worth noting that MASnBr$_3$ is adopted as HTL based on above discussion.
No significant effect of Cd$_{0.2}$Zn$_{0.8}$S thickness on voltage is observed in figure 13(a), which is similar to the previous reported results [79]. When the thickness increases, the current density and power conversion efficiency improve at first then decline dramatically. As the Cd$_{0.2}$Zn$_{0.8}$S ETL thickness increases from

Figure 17. Parameters of solar cells with light absorption layer of different thickness (ranging from 300 nm to 500 nm). (a). Open circuit voltage; (b). Short circuit current; (c). Fill factor; (d) Power conversion efficiency.

Figure 18. Carrier Density of solar cells with light absorption layer of different thickness (ranging from 300 nm to 500 nm), where n represents electrons and p represents holes.
30 to 40 nm, it could generate more photo-generated carriers, which leads to the enhanced short circuit current density. As the Cd$_{0.2}$Zn$_{0.8}$S ETL thickness further increases, it would exceed the depletion width of Cd$_{0.2}$Zn$_{0.8}$S formed at the interface, which leads to the inefficient separation and collection of photo-generated carriers [24]. Therefore, the current density decreases, which is also verified by the external quantum efficiency spectra (as shown in figure 14).

As the Cd$_{0.2}$Zn$_{0.8}$S thickness increases, the shunt resistance decreases (as shown in figure 15), responsible for the damping of fill factor [43].

The effect of light absorption layer thickness on the device performance has also been investigated. It’s worth noting that the thickness of Cd$_{0.2}$Zn$_{0.8}$S is set to be 40 nm and HTL is determined to be MASnBr$_3$. First, we determine the thickness in the range of 200 nm to 700 nm, with a step of 100 nm. It’s clearly observed from figure 16 that the optimum thickness is 400 nm (in terms of efficiency). Further simulations were performed to optimize the thickness in the range of 300 nm to 500 nm, as shown in figure 17.

The current density depends largely on the light absorption which is affected by the thickness of MAPbI$_3$ layer. A thicker light absorption layer could capture more photons [80], which would in turn generate more electron-hole pairs (as shown in figure 18). This is consistent with previous reported results [81].

In addition, as reported in previous research [82], the thicker absorption layer would cause bandgap decrease, which improves the absorption of long wavelength photons. Therefore, a higher external quantum efficiency is obtained (as shown in figure 19). Thus, the current density is enhanced according to formula (1).
The decrease of open circuit voltage may be ascribed to the higher recombination caused by the thicker absorption layer [80, 83]. In addition, the thicker absorption layer causes the bandgap decrease [82], which would also lead to the reduction of open circuit voltage.

The fill factor monotonously declines with thickness increasing, which is ascribed to the decrease of shunt resistance (as shown in figure 20) [43].

In addition, too thick light absorption layer would increase the photo-generated carrier diffusion length. Thus, the photo-generated carrier collection would be impeded and the recombination loss would be increased (as shown in figure 21). Therefore the fill factor would be reduced [76].

4. Conclusion

The issue of energy band alignment mismatch at ETL/MAPbI3 interface and MAPbI3/HTL interface could be addressed by using appropriate Cd1-xZnxS ETL (x represents the Zn molar concentration) and appropriate HTL. In addition, the thickness of ETL and perovskite layer could be adjusted to enhance the short circuit current and reduce recombination loss. The optimum ETL is Cd0.2Zn0.8S (the Zn molar concentration in Cd1-xZnxS is x = 0.8). Higher Zn molar concentration (0 < x < 0.8) in Cd1-xZnxS increases the band gap of ETL, which would reduce the minimum conduction band difference between Cd1-xZnxS ETL and MAPbI3 layer. Therefore, the recombination loss at the Cd1-xZnxS ETL/MAPbI3 interface could be decreased, which favors the device performance. However, as x value further rises from 0.8 to 1, the performance decreases slightly. This could be explained by the higher electric affinity of Cd1-xZnxS than MAPbI3. When the electric affinity of Cd1-xZnxS is higher than MAPbI3, the flowing of electrons from MAPbI3 to Cd1-xZnxS ETL would be impeded. The optimum HTL is MASnBr3. Spike-type energy band structure at the interface of MAPbI3/MASnBr3 could also improve the performance of perovskite solar cells. Because the sharply enhanced electric field at the MAPbI3/MASnBr3 interface resulted from spike band structure facilitates the separation of electron-hole pairs. The optimum thickness for Cd0.2Zn0.8S ETL and MAPbI3 perovskite layer is 40 nm and 400 nm, respectively. Perovskite film thinner than 400 nm could not capture all the incident photons, which leads to the low short circuit current. Perovskite film thicker than 400 nm increases the diffusion length, which impedes the efficient collection of photo-generated carriers and causes the higher recombination loss. Based on the comprehensive investigation as discussed above, an optimal device structure of Cd0.2Zn0.8S/MAPbI3/MASnBr3 (in terms of functional layers) yields the best performance in our work, where the optimum thickness for Cd0.2Zn0.8S and MAPbI3 is 40 nm and 400 nm, respectively.

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