Quantum Dotes of Perovskites Solar Cells based on ZnSe as ETM

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Abstract: Numerical analysis and performance improvements of nanostructured Cu2O / CH3NH3PbI3 / ZnSe in heterojunction solar cells have been documented in this paper. The choice for conventional solar cells reaching maximum efficiency of 22.1 percent is predominant for Perovskite photovoltaics. In recent years, organic-inorganic hybrid perovskite solar cells in the photovoltaic research community have gained great interest because of their ease of processing. Low manufacturing costs, excellent characteristics of light-harvesting, A relatively high performance Making it more appealing than other current materials from solar cells. In this study, a numerical simulation using the Solar Cell Capacitance Simulator (SCAPS) of a thin film heterojunction perovskite solar cell to study some parameters that can affect the performance of CH3NH3PbI3 PSC with Cu2O as HTL and ZnSe as ETL performed. The absorber material thickness, ETL and HTL, the absorber material bandgap, and ETL were investigated. Results have shown that the thickness of ZnSe greatly influences the device's Process / Analysis: The Capacitance Simulator(SCAPS) is used to perform the study of solar cell design. It is a computer-based software tool and is well adapted for homo and heterojoint, multi-junction, and photovoltaic structure analysis. This software instrument is based on the continuity and Poisson equation of the Holes and Electrons. It is used to optimize the different parameters, such as thickness and temperatures, for this model.CE. As the thickness of ZnSe decreases, the efficiency of the cell increases.

1. Introduction

Hybrid perovskites solar cells was received considerable foucassing as an hybrid layer in thin film solar cells after Kojima et al. introduced methylammonium lead halide based solar cells in 2009[1]. The characteristics of these materials, such as the strong coefficient of absorption[2], indicate excellent transport properties. [3], tunable bandgap [4]. The materials are ideal for low-cost photovoltaic ( PV) applications due to the absence of deep trap states within the bandgap[5-6], low temperature processing, etc. perovskite solar cells have involved substantial interest in the photovoltaic research field as result their ease of handling, low manufacture charges and its has high performance, making them more preferable than other present-day solar cell materials[7]. Improving the efficiency and substantial possessions of the architecture of the solar cell is of great significance. The intention in this field is to study the act of optimized zinc selenide (ZnSe) such as electron transporting material (ETM), cuprous oxide (Cu2O) used as hole transporting material (HTM).
2. **Modeling and Computer Simulation**

Simulation is a critical technique to gain a deep insight into the physical activity, the feasibility of the physical interpretation suggested, and the impact of physical changes on the efficiency of the solar cell devices. The solar cell factors used to determine the efficiency of a solar cell system. The one-dimensional simulation program SCAPS-1D was established by Burgelman et al. The flow diagram under displays measures for running SCAPS and its act panel for simulation.

![Flow diagram of SCAPS](image)

The perovskites are based on FTO / ETL / perovskite / HTL / Ag where the transparent conducting oxide is referred to by the FTO electron transport layer, ETL and HTL. The hole transportation layer and the Perovskite semiconductor are the central of the solar cell. The energy bandgap for this work is given in Figure 2.

![Energy bandgap diagram](image)

**Figure 1.** map and action panel SCAPS [8].

**Figure 2.** Model of layer structure simulated and diagram of energy levels of various perovskite solar cell ETMs
### 3. Numerical Method

SCAPS-1D extracts solar cell parameters such as quantum efficiency and I-V characteristics, which are depend on the succeeding Poisson equation [9]:

\[
\frac{d}{dx} \phi(x) = \frac{e}{\varepsilon_0 \varepsilon_r} \left[ P(x) - N_D(x) - N_A(x) + \rho_p(x) - \rho_n(x) \right] \tag{1}
\]

Here \( \Phi \) is electrostatic potential, \( \varepsilon_0 \) is the vacuum dielectric permittivity and \( \varepsilon_r \) is relative, \( N_D \) and \( N_A \) are donor and acceptor charged impurities, \( e \) is the electron charge, \( \rho_n \) and \( \rho_p \) are electrons and holes densities. The electrons and holes continuous mathematical expression areas [10]:

\[
\frac{d}{dx} J_n(x) - e \frac{\partial n(x)}{\partial t} - e \frac{\partial n(x)}{\partial t} - e \frac{\partial p(x)}{\partial t} = G(x) - R(x) \tag{2}
\]

\[
\frac{d}{dx} J_p(x) + e \frac{\partial p(x)}{\partial t} + e \frac{\partial p(x)}{\partial t} = G(x) - R(x) \tag{3}
\]

\( G(x) \) and \( R(x) \) are generation and recombination rate \( J_p \) and \( J_n \) are hole and electron current density [10].

**Table 1. Summary of parameters used for perovskite SCAPS modeling [11,12]**

| parameters                      | Cu2O      | CH3NH3PbI3 | ZnSe       |
|---------------------------------|-----------|------------|------------|
| Band gap (ev)                   | 2.17      | 1.5        | 1.4        |
| Electron effinity (ev)          | 3.20      | 3.9        | 4.1        |
| Dielectric permittivity         | 7.11      | 10         | 10         |
| CB effective density of states (1/cm²) | 2.02E+17 | 2.75E+18 | 1.800E+18 |
| VB effective density of states (1/cm²) | 1.10E+19 | 3.9E+18  | 1.800E+19 |
| Electron mobility (cm²/v.s)     | 2.000E+2 | 1.00E+1   | 1.000E+2  |
| Hole mobility (cm²/v.s)         | 8.00E+18 | 1.0E+1    | 2.500E+1  |
Table 2: Devise Parameters use in Scaps.

| Right contact electrical properties (Au)                  |     |
|----------------------------------------------------------|-----|
| Thermionic emission /surface recombination               |     |
| Velocity of electron (cm/s)                              | $10^5$ |
| Thermionic emission /surface recombination               |     |
| Velocity of hole (cm/s)                                  | $10^7$ |
| Metal (Au) work function (ev)                            | 5.1 |
| Left contact electrical properties                        |     |
| Thermionic emission /surface recombination               |     |
| Velocity of electron (cm/s)                              | $10^7$ |
| Thermionic emission /surface recombination               |     |
| Velocity of hole (cm/s)                                  | $10^5$ |
| the work function of ITO (ev)                            | 4.4 |

4. Result and discussion

4.1- Effect of layer thickness and Temperatures change on the Cu2O/CH3NH3PbI3/Znse solar cells devices

4.1.1- Impact of a change in Cu2O layer thickness on solar cells

The absorber layer should be set to the optimal thickness to absorb the maximum number of photons and to create electron-hole pairs. The absorber layer thickness ranged from 0.3μm to 1.8μm. The longer wavelength of the illumination causes a reasonable amount of electron-hole pair generation as the thickness of the absorber's layer rises. The depletion layer gets very close to the back contact, by increasing the thickness of the absorber layer, and the back contact collects more electrons for recombination. Via these fewer electrons, the generation process will participate and eventually lead to the Voc, Jsc increase, Decreased fill factor, and enhanced performance. The variance of PV parameters with the thickness of the absorber layer is seen in Figure 3. Due to the increased exciton performance, the graph shows an efficiency gain as we switch from the thinner absorber to the thicker absorbers. But in the fill factor, there is a fast drop.
| Thickness (µm) Cu₂O | Voc (V) | Jsc (mA/cm²) | F.F (%) | η (%) |
|--------------------|--------|--------------|---------|-------|
| 0.3                | 0.829  | 23.875       | 22.23   | 4.42  |
| 0.8                | 0.9229 | 33.966       | 22.64   | 7.10  |
| 1.300              | 0.997  | 36.175       | 21.29   | 7.68  |
| 1.800              | 1.049  | 37.388       | 20.53   | 8.06  |
| 2.300              | 1.085  | 38.209       | 20.14   | 8.36  |
| 2.800              | 1.111  | 38.821       | 19.95   | 8.61  |
| 3.300              | 1.131  | 39.297       | 19.86   | 8.83  |
| 3.800              | 1.146  | 39.690       | 19.84   | 9.03  |
| 4.300              | 1.158  | 40.013       | 19.86   | 9.21  |
| 4.800              | 1.168  | 40.288       | 19.92   | 9.38  |
| 5.300              | 1.177  | 40.535       | 19.98   | 9.54  |
| 5.800              | 1.187  | 40.743       | 20.07   | 9.69  |
| 6.300              | 1.191  | 40.927       | 20.16   | 9.83  |
| 6.800              | 1.196  | 41.091       | 20.26   | 9.97  |
| 7.300              | 1.201  | 41.239       | 20.37   | 10.10 |
| 7.800              | 1.206  | 41.387       | 20.47   | 10.22 |
| 8.300              | 1.210  | 41.509       | 20.58   | 10.34 |
| 8.800              | 1.214  | 41.580       | 20.71   | 10.46 |
| 9.300              | 1.217  | 41.68        | 20.82   | 10.57 |
| 9.800              | 1.220  | 41.752       | 20.95   | 10.68 |
| 1.300              | 0.983  | 35.850       | 21.52   | 7.59  |
| 1.800              | 1.049  | 37.388       | 20.53   | 8.06  |
4.1.2. Effect of the CH3NH3PbI3 layer thickness change on solar cells

The absorber layer thickness ranged from 0.2 µm to 0.6 µm. The variance of PV parameters with absorber layer thickness is shown in Figure 4. The graph shows that, as we're switching from a thinner absorber to a thicker one, the performance, Voc, and Jsc are decreased. But there is an improvement. Table number four displays the data on the drawing. One shows that the optimal thickness for perovskite solar cells is 0.2 micrometer as listed in table 4 where 0.2-micrometer thickness corresponds to the efficiency of (10.77)%.

| Thickness (µm) | Voc (V) | Jsc (mA/cm²) | F.F (%) | η (%) |
|----------------|--------|--------------|--------|------|
| CH3NH3PbI3     |        |              |        |      |
| 0.2            | 1.220  | 41.876       | 21.06  | 10.77|
| 0.250          | 1.230  | 35.001       | 17.86  | 7.69 |
| 0.3            | 1.206  | 26.186       | 18.62  | 5.88 |
| 0.350          | 1.165  | 19.540       | 21.39  | 4.87 |
| 0.4            | 1.136  | 14.967       | 25.78  | 4.39 |
| 0.450          | 1.124  | 11.843       | 31.25  | 4.16 |
| 0.5            | 1.120  | 9.728        | 37.27  | 4.06 |
| 0.550          | 1.117  | 8.344        | 43.07  | 4.02 |
| 0.6            | 1.117  | 7.49         | 47.73  | 4   |
4.1.3-Effect of the ZnSe layer thickness change on solar cells

The effect of zinc selenide (ETL) thickness on cell output parameters fluctuating from 0.01 to 0.140μm is shown in Fig 5. Table 5 shows that the thickness of the electron transporting material is increased, JSC, FF, and system efficiency are decreased while VOC increases. This indicates that the semiconductor material is thicker, it provides a longer diffusion path for the electron to reach the electrode Which limits the efficiency of charge collection, and transmission of an incident photon (the solar cell parameters) decreases with increasing thickness. High output was achieved when ETL thickness was obtained, 0.01µm with JSC of 41.876 mA/cm², VOC of 1.2209V, FF of 21.06%, and high efficiency of 10.77%.
Table 5: Variation of Thickness for ZnSe with device parameters

| Thickness (µm) | Voc (V) | Jsc (mA/cm²) | F.F (%) | η (%) |
|---------------|---------|--------------|---------|-------|
| ZnSe          |         |              |         |       |
| 0.01          | 1.2209  | 41.876       | 21.06   | 10.77 |
| 0.02          | 1.220   | 41.819       | 21.06   | 10.75 |
| 0.03          | 1.2207  | 41.813       | 21.07   | 10.75 |
| 0.04          | 1.2207  | 41.788       | 21.02   | 10.72 |
| 0.05          | 1.2209  | 41.752       | 20.95   | 10.68 |
| 0.06          | 1.2210  | 41.713       | 20.87   | 10.63 |
| 0.07          | 1.2211  | 41.675       | 20.80   | 10.59 |
| 0.08          | 1.2213  | 41.638       | 20.74   | 10.55 |
| 0.09          | 1.2214  | 41.604       | 20.68   | 10.51 |
| 0.100         | 1.2215  | 41.572       | 20.62   | 10.47 |
| 0.110         | 1.2216  | 41.542       | 20.57   | 10.44 |
| 0.120         | 1.2217  | 41.514       | 20.53   | 10.41 |
| 0.130         | 1.2218  | 41.488       | 20.48   | 10.38 |
| 0.140         | 1.2219  | 41.464       | 20.44   | 10.36 |
| 0.150         | 1.2219  | 41.4416      | 20.41   | 10.33 |

Figure 5: Variation of PV parameters by adjusting the thickness of PV parameters ZnSe
4.1.4 Effect of annealing temperatures for ZnSe

The results of simulation I-V characteristic such as PCE, FF, Jsc, and Voc of the perovskite solar cells with varying environment temperature as shown in Table 6 where the highest efficiency is 10.77% with Jsc = 41.876 mA/cm², FF = 21.06% and Voc = 1.2209 is achieved when the temperature at 333.15 K. Consequently, the best outcome at very high levels. The temperature is very good for working in a vacuum. When the temperature is decreased, due to the decrease in the generation of electron-hole pairs in the perovskite materials with increasing temperature, the PCE, Voc and Jsc degrees are from 333.15 K to 233.15 K, as shown in Illustration 6. The open-circuit voltage steadily decreases with a decrease in Figure 6. Due to the regulation of the temperature, the performance can be modified by temperature.

Table 6: The parameter of the Cu2O/CH3NH3PbI3/ZnSe hetrojunction solar cell

| Temperature (K) | Voc (V)  | Jsc (mA/cm²) | F.F (%) | η (%) |
|-----------------|----------|--------------|---------|-------|
| 333.15          | 1.2209   | 41.876       | 21.06   | 10.77 |
| 313.15          | 1.220    | 41.819       | 21.06   | 10.75 |
| 293.15          | 1.2207   | 41.813       | 21.07   | 10.75 |
| 273.15          | 1.2207   | 41.788       | 21.02   | 10.72 |
| 253.15          | 1.2209   | 41.752       | 20.95   | 10.68 |
| 233.15          | 1.2210   | 41.713       | 20.87   | 10.63 |

Figure 6: The variation of solar cell parameters with the temperature

5. Conclusions
In this study, the thickness was changed for CH3NH3PbI3, ZnSe, and Cu2O, were observed for each substance and after that. Also, the study with a variety of temperature, defect and work function to get optimum condition corresponding to best efficiency of the structure Cu2O/CH3NH3PbI3/ZnSe device which reached to 10.77% to be amazing device structure and best Efficiency while the structure of Cu2O/CH3NH3PbI3/ZnSe device reaches to 10.77% at 0.01µm. And all other parameter solar cells improved as result to use ZnSe as electron transport materials.
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