High Efficiency (41.85) of Br Perovskites base solar cells with ZnO and TiO2 comparable study as ETM

Dhuha E.Tareq *1,2, Samir M.AbdulAlmohsin2 and Hussein H. Waried2

*1 College of Health and Medical Technology, Al-Ayen University, Iraq.
*2 Department of Physics, Thi Qar University, Nasiriyah, Iraq.

Correspondence: Email: dhuhaimad333@gmail.com

Abstract: Due to its ease of processing, low production costs, superb light-harvesting characteristics, and high efficiency, organic-inorganic perovskite solar cells have attracted great attention in the photovoltaic research community in recent years, making it more preferable than other existing solar cell materials. Lead-based perovskites (CH3NH3PbX3, X= Cl, I, Br) solar cells have recently achieved high efficiency of ~19.3 percent, well exceeding most thin-film and organic solar cells' efficiencies despite its potential for photovoltaic applications, organometal halide perovskites have attracted considerable attention recently and are also considered as promising materials in light-emitting devices. In particular, photovoltaic devices with efficiencies above 20 percent have been prepared using organometal halide perovskites as absorbent materials in the last few years A planar. The standard design for a planar hetero-junction perovskite-based solar cell is: Back electrode/ Hole Transport Material (HTM)/ Perovskite absorber / Electron Transport Material (ETM) / Transparent electrode. The hole mobility and acceptor concentration of the HTM, interface trap density, and work-function of back contact metal have shown a significant influence on the device performance. Also with these good merits. In this research, two types of ETM (TiO2 and ZnO) were used with the Perovskite CH3NH3PbBr3 and was found that the use of TiO2 with perovskite achieved high efficiency of 41.85% while the use of ZnO with perovskites we obtained an efficiency 17.67%.

Method/Analysis: Solar cell architecture assessment is conducted using Solar Cell Power Simulator(SCAPS). This is a computer-based software tool and is well equipped to research photovoltaic structures with barriers to homo and heterojunctions, multi-junctions, and Schottky. This model optimizes various parameters such as thickness, absorber layer density, Electron Transport Material (ETM) Density of accepter and donor (ND and NA), and Hole Transport Material (HTM) doping concentrations. Achievement and simulates electrons and holes based on the Poisson's and continuity equation. The effected thickness of CH3 NH3 PbBr3 different from 0.05µm to 1.2µm and the finest results are observed at 0.05µm.
1-Introduction

Perovskite solar cells based on CH3NH3PbX3 have recently drawn massive attention as a result of their simple manufacturing process and their dramatically increasing photoelectric conversion efficiency (PCE) from 3.81% in 2009 to 22.1% in 2016 [1-6]. To obtain the high-performance devices, it is important to consider the balance of thickness and carrier diffusion length in perovskite thin films. While increasing the thickness of the perovskite absorption layer can improve its light-harvesting efficiency, the PCE of the corresponding perovskite solar cell is not always improved due to the restriction of the length of the electron and the hole diffusion in perovskite absorption layers. Additionally, other perovskite parameters, such as high absorption coefficient, strong carrier transmission capacity, low-temperature manufacturing, and low sensitivity in crystal defects, prepared the likelihood of PCE solar cells being produced by absorbers around 20 percent [7, 8, 9, 10]. The related simulation work has given the basic information from the literature to build this model [11–15]. In this device, we examined and analyzed the effect of absorber layer properties (thickness) and the impact of HTM and ETM doping on system output SCAPS is software for window application, Developed with laboratory windows / CVI of a national instrument at the University of Ghent. The software is arranged in a Set of panels where the consumer can set parameters or calculate outcomes [16]. SCAPS analyzes model physics and explains the recombination profiles, the distribution of electric fields, the carrier transport mechanism, and the individual current densities. Generally, ETL and HTL are used in the PSCs for broad bandgap hole blocking and electron blocking materials respectively. The PSCs use different types of organic and inorganic materials, such as TiO2, ZnO, SnO2, and Al2O3, as ETL [17,18]. TiO2 among them is the most promising material for the ETL because of its wide bandgap, high stability, and attractive bending with perovskite material [19]

1.2. Perovskites

The key concern in the design of a solar photovoltaic cell is to optimize the cost-efficiency ratio, i.e., to reduce the overall cost, increase the performance and longevity of the PV module[20]. Different factors affect a solar cell 's efficiency. The first and primary consideration is the percentage of electromagnetic energy that enters the absorber layer to covert the solar cell into electricity. Secondly, different material types have different absorption coefficients , band gaps and hence different maximum theoretical efficiency[21]. Higher solar cell output is predicted and is typically observed in perfect crystalline structure. For the former, the thickness may not be appropriate for the distribution of charge carriers, while in the latter case the intensive increases and the output reduces. The fifth element is the amount of light that enters the absorbing material, i.e., the material's reflection, transmittance, and absorption. The temperature is the sixth-factor affecting efficiency since different materials have different temperature responses
1.3 Structure and working of perovskites

On a cubo-octahedral site, A cation is occupied in perovskite structures with general formula ABX₃ (X = oxygen, carbon, nitrogen, or halogen), and at an octahedral site B cation is occupied (Fig 1). When used with O₂ anion, A and B are usually divalent and tetravalent. At sites A and B, however, perovskite with halogen anions allows for monovalent and divalent cations. In CH₃NH₃PbI₃, the A-site cation is CH₃NH₃⁺ and the B-site cation is Pb²⁺, as shown in Fig. 2b. The formability of perovskite is estimated based on its geometric tolerance factor (t) [22], t = (rA + rX)/[H₂(rB + rX)], where rA, rB and rX are the effective ionic radii for A, B and X ions, respectively. For transition metal cations containing oxide perovskite, an ideal cubic perovskite is expected when t = 1 while octahedral distortion is expected when t < 1 [23].

The perovskite layer firstly absorbs photons to produce excitons (electron-hole pairs). Due to the difference in the exciton binding energy of the perovskite materials, such excitons may produce free carriers to generate a current (free electrons and holes) or may recombine into excitons. The carrier's distance and the service life is long due to low carrier recombination probabilities of CH₃NH₃PbI₃ (MAPbI₃) and other perovskite products, and improved carrier mobility. For example, the carrier diffusion distance is at least 100 nm for MAPbI₃ and longer than 1 µm for MAPbI₃-xClₓ [25, 26]. The longer spreading distance and lifespan of the carrier are the foundation of the superior performance of perovskite solar cells. Ten, these free electrons and holes are obtained using an Electron Transport Material (ETM) and a Hole Transport Material (HTM). The electrons are moved from perovskite to TiO₂, used for ETM layers, and finally obtained by FTO. Around the same time, the holes are passed to the HTM sheet, and the metal electrode is stored. Finally, the FTO and metal electrode are connected, and the outer circuit generates the photocurrent. The electron-hole pairs separated TiO₂ / perovskite and Cu₂O / perovskite at the two heterojunction interfaces, followed by injecting electrons into TiO₂ /perovskite and Spiro-OMeTAD/perovskite, followed by electrons injecting into TiO₂ (process (i) in Figure 3) and holes injecting into HTM process (ii) to achieve charges transport [27]. At the same time, several behaviors may also be detrimental.
to cell efficiencies, such as exciton annihilation process (iii), photoluminescence or non-radiative recombination, and reverse transmission of electrons and holes (process (iv) and (v) and recombination at the TiO2 / HTM interface process (vi). The transport processes of electrons and holes in an HTM/perovskite/TiO2 cell are shown in Fig 2.

![Schematic diagram of energy levels and transport processes of electrons and holes in an HTM/perovskite/TiO2 cell](image)

**Figure 2**: Schematic diagram of energy levels and transport processes of electrons and holes in an HTM/perovskite/TiO2 cell

### 1.4 Description of working

SCAPS concepts The Burgelman et. developed the SCAPS 1D simulator. Al. Simulating the electrical characteristics of thin-film heterojunction solar cells by solving equations of basic semiconductor devices under stable conditions[28]. In this work, it was used to explore the real device (MASnI3) solar cell with modified material parameters for better performance. The program allows for the inclusion of deep bulk level and interfaces defect recombination (non-radiative recombination). Many of the recombination losses in the system being considered are radiative recombination (i.e. direct band-to-band recombination) and interface recombination, compensated by the Shockley-Read-Hall recombination (propagated by defects or traps). The flow chart below shows step-by-step stages in simulating with SCAPS

![Flow chart showing simulation procedure](image)

**Figure 3** simulation procedure
1.5. Numerical Simulations

Simulation is a crucial technique for realizing a deep insight into the physical activity, the viability of the suggested physical interpretation, and the effect of physical changes on the solar cell devices’ performance. Various simulation models exist for the simulation of solar cells (SCAPS, AMPS, SCAP, etc). SCAPS (Solar Cell Power Simulator) is a one-dimensional simulation program with seven semiconductor input layers developed by a group of solar cell researchers from the Electronics and Information System Department, University of Ghent, Belgium[29]. Building a solar cell without stimulation works is unpractical, as is waste of time and money. It not only minimizes the risk, time, and money but also analyzes the properties of the layers and their function to maximize the efficiency of the solar cell. To simulate a computer all the basic input parameters should be well specified to function as a real counterpart. The different structure has been used by perovskite-based solar cells with inorganic semiconductor solar cells, such as CIGS, and exciting form Wannier is contained in perovskite. Thus SCAPS like a 1D simulator can be used to model solar cells based on perovskite [30].
Figure 4. SCAPS panel showing the Cu2O/CH3NH3PbI3/TiO2, Cu2O/CH3NH3PbBr3/ZnO heterojunction solar cells

definition

Table 1: Summary of the basic device equations[31]

| Equation          | Expression                                                                 |
|-------------------|-----------------------------------------------------------------------------|
| Poisson equation  | \( \frac{\partial}{\partial x} (-\varepsilon(x) \frac{d\phi}{dx}) = q \left[ p(x) - n(x) + N_d^+ - N_A^- + P_i(x) - n_i(x) \right] \) |
| Continuity Eq. for| \( \frac{\partial n(x,t)}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n(x,t) - R_n(x,t) \) |
| Continuity Eq. for| \( \frac{\partial p(x,t)}{\partial t} = \frac{1}{q} \frac{\partial J_p}{\partial x} + G_p(x,t) - R_p(x,t) \) |
| Current density   | \( J_p = q (p \mu_p E - D_p \frac{dp}{dx}) \)                               |
| Current density   | \( J_p = q (p \mu_p E - D_p \frac{dp}{dx}) \)                               |

1.6. SCAPS simulation of Cu2O/Perovskite/ZnO or TiO2

Note that all simulation parameters for each layer in the architecture are carefully selected from those reported experimental data and other literature [32]. Table 2 summarizes all the primary parameters used in the simulation.

Table 2 Material properties of ETM, absorber, and HTM.[33-38]

| Parameters                        | Cu2O | CH3NH3PbBr3 | TiO2 | ZnO |
|-----------------------------------|------|-------------|------|-----|
| Band gap (eV)                     | 2.17 | 2.33 [18]   | 3.26 | 3.3 [16] |
| Electron affinity (eV)            | 3.20 | 3.70 [19]   | 4.2  | 4.0 [16] |
| Dielectric permittivity           | 7.11 | 7.50 [21]   | 10   | 9.0 [15] |
| CB effective density of states    | 2.02E+17 | 1.00+17 [21]| 2.0E+17 | 3.7 × 10^{18} [15] |
| VB effective density of states    | 1.10E+19 | 1.00+17 [21]| 6.0E+17 | 1.8 × 10^{18} [16] |
| Electron mobility (cm²/v.s)       | 2.000E+2 | 24 [22]    | 100  | 100 |
| Hole mobility (cm²/v.s)           | 8.00E+18 | 24 [22]    | 25   | 25 |
Table 3: Devise Parameters use in the numerical analysis.

| Left contact electrical properties (Pt) |  |
|----------------------------------------|--|
| Thermionic emission /surface recombination | $10^7$ |
| Velocity of electron (cm/s) |  |
| Thermionic emission /surface recombination | $10^7$ |
| Velocity of hole (cm/s) |  |
| Metal (Pt) work function (ev) | 5.65 |

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

Result and discussion

1-Effect of layer thickness, Temperatures, Defects and Work function change on the Cu2O/CH3NH3PbBr3/TiO2 solar cells devices

1.1- Effect of the thickness of CH3NH3PbBr3

The absorber layer should be set for optimum thickness to absorb the maximum number of photons and to generate electron-hole pairs. Absorber layer thickness has been varied from 0.05μm to 0.7μm. When the thickness of the absorber layer increases, a good amount of electron-hole pair generation will result from the longer wavelength of the illumination. Through raising the thickness of the absorber layer, the depletion layer is very similar to the back contact, and more electrons are collected for recombination by the back contact. This will involve fewer electrons in the generation process and ultimately lead to a reduced filling factor and reduced efficiency. Fig5 describes the variation of PV parameters with absorber layer thickness. By looking at the Voc / thickness graph, we can say that by increasing the thickness, Voc increases. From Jsc/ thickness graph; short circuit current decreases, by increasing the thickness. Table number three shows the drawing data
Table 4 Variation of Thickness for CH$_3$NH$_3$PbBr$_3$ with device parameters

| Thickness(µm) | $V_{oc}$ (V) | $J_{sc}$ (mA/cm$^2$) | F.F (%) | η (%) |
|---------------|--------------|----------------------|---------|-------|
| CH$_3$NH$_3$PbBr$_3$ |              |                      |         |       |
| 0.05          | 1.6820       | 46.575               | 51.89   | 40.65 |
| 0.1           | 1.7897       | 46.1818              | 38.50   | 31.82 |
| 0.150         | 1.8186       | 45.6120              | 28.91   | 23.98 |
| 0.2           | 1.8401       | 44.578               | 21.19   | 17.38 |
| 0.250         | 1.8597       | 41.567               | 15.96   | 12.34 |
| 0.3           | 1.8794       | 35.1010              | 13.47   | 8.89  |
| 0.350         | 1.8994       | 27.186               | 13      | 6.71  |
| 0.4           | 1.9200       | 20.339               | 13.82   | 5.40  |
| 0.450         | 1.9406       | 15.3229              | 15.43   | 4.59  |
| 0.5           | 1.9607       | 11.823               | 18.57   | 4.31  |
| 0.550         | 1.9790       | 9.3819               | 23.27   | 4.32  |
| 0.6           | 1.9912       | 7.640                | 28.50   | 4.34  |
| 0.650         | 2.0013       | 6.3590               | 34.13   | 4.34  |
| 0.7           | 2.0084       | 5.3857               | 40.18   | 4.35  |

Figure 5. Variation of PV parameters by varying the thickness of CH$_3$NH$_3$PbBr$_3$. 


1.2- Effect of annealing Temperatures for CH$_3$NH$_3$PbBr$_3$

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 2 where the highest efficiency is 40.65% with Jsc = 46.575 mA/cm$^2$, FF = 51.89% and Voc = 1.6820 is achieved when the temperature at 333.15 K, therefore the best result at very low temperature to be very appropriate to work in space. When the temperature is increasing from 333.15 K to 213.15 K, the PCE, and Jsc degrees due to reducing in the generation of the electron-hole pairs in the perovskite materials with increasing temperature as shown in Fig 6. From the Fig 6 the open-circuit voltage increases gradually with increasing temperature, it can adjust the efficiency with temperature due to control of the recombination, generation, and a collection of the charge carriers so the best temperature of perovskites solar cells with CH$_3$NH$_3$PbBr$_3$ as PVSC is 333.15 K.

Table 5. The parameter of the Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/TiO$_2$ heterojunction solar cells

| Temperature(K) | Voc (volt) | Jsc (mA/cm$^2$) | FF | Efficiency% |
|----------------|------------|-----------------|----|--------------|
| 333.15         | 1.6820     | 46.575          | 51.89 | 40.65        |
| 313.15         | 1.7897     | 46.1818         | 38.50 | 31.82        |
| 293.15         | 1.8186     | 45.6120         | 28.91 | 23.98        |
| 273.15         | 1.8401     | 44.578          | 21.19 | 17.38        |
| 253.15         | 1.8597     | 41.567          | 15.96 | 12.34        |
| 253.15         | 1.8794     | 35.1010         | 13.47 | 8.89         |
| 213.15         | 1.8994     | 27.816          | 13   | 6.71         |

Figure 6: The variation of solar cell parameters with the temperature.
1.3- Effects of the Defect State of the Interface Defect Layer (Cu₂O/CH₃NH₃PbBr₃/TiO₂).

defect layer has been considered for the simulations of the proposed CH₃NH₃PbBr₃ solar cell structures. The HTM/CH₃NH₃PbBr₃ /ETM layer has been represented by IDL. Numerical simulation has been performed on the defect density at both interfaces from $2 \times 10^{15}$ cm$^{-3}$ to $10 \times 10^{15}$ cm$^{-3}$. Fig 7 show the effect of interface defect density versus efficiency curves for perovskite solar cells. From the graphs, it can be deduced that the Voc, Jsc, and $\eta$ decreasing with increasing defect but the FF increases. When the defect density exceeds $2 \times 10^{15}$ cm$^{-3}$, a decrease in efficiency is observed. With increasing defect density, the recombination rate also increases which in turn decreases the efficiency. So, it can be realized from the simulated results that interface defect density of $2 \times 10^{15}$ cm$^{-3}$ is optimum for device simulation ($\eta=41.85$).

| Defect Nt(1/cm$^3$) | Voc (volt) | Jsc (mA/cm$^2$) | FF | Efficiency% |
|---------------------|------------|-----------------|----|--------------|
| $2\times10^{15}$    | 1.4918     | 46.954          | 59.74 | 41.58        |
| $4\times10^{15}$    | 1.4904     | 46.946          | 59.76 | 41.81        |
| $6\times10^{15}$    | 1.4891     | 46.938          | 59.77 | 41.78        |
| $8\times10^{15}$    | 1.4878     | 46.930          | 59.79 | 41.75        |
| $10\times10^{15}$   | 1.4866     | 46.922          | 59.80 | 41.71        |
1.4 -Effect of Different Back Contacts

Simulations were performed using silver (Ag), iron (Fe), copper (Cu) graphite alloy, gold (Au), nickel (Ni), and platinum (Pt) as a prospective back touch electrod for solar perovskite cells. Fig8 illustrates the impact of different back contact with efficiency. The simulated output of solar cells improves but saturates after a certain value with the increasing function of the work. The majority carrier barrier height (relative to Ef) decreases due to band bending at the metal-semiconductor interface, thus making contact more ohmic [39]. As the metal 's work function increases, the Voc becomes bigger. Hence, perovskite solar cell efficiency is also increasing. Holes traveling towards the electrode is energetically unfavorable because the electric field close to HTM / back contact becomes negative [40]. For this reason, it can be expected that the lower function of the work is responsible for the lower efficiency. The simulation results show that Pt is one of the potential rear contact materials that can develop PSC performance.

Table 7 shows the effect of various metal back contact on different candidates of the HTM layer.

| Work Function (ev) | Voc (volt) | Jsc (mA/cm²) | FF | Efficiency % |
|-------------------|------------|--------------|----|--------------|
| 4.5               | 1.0319     | 44.1952      | 14.93 | 6.81 |
| 4.6               | 1.1319     | 44.5522      | 20.41 | 10.29 |
| 4.7               | 1.2319     | 44.7378      | 25.46 | 14.03 |
| 4.8               | 1.3319     | 44.8783      | 29.98 | 17.92 |
| 4.9               | 1.4319     | 44.9937      | 34.01 | 21.91 |
| 5                 | 1.5318     | 45.0913      | 37.59 | 25.97 |
| 5.1               | 1.6253     | 45.1733      | 40.36 | 29.83 |
| 5.25              | 1.6393     | 45.1868      | 41.06 | 30.42 |
| 5.15              | 1.6534     | 45.2044      | 41.53 | 31.04 |
| 5.25              | 1.6646     | 45.2555      | 41.79 | 31.62 |
| 5.65              | 1.6820     | 46.575       | 51.89 | 40.65 |
2-Effect of the Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/ZnO layer thickness, Temperatures, Defects and Work function change on solar cells

2.1-Effect of the thickness of ZnO on the solar cell.

The absorber layer should be set for optimum thickness to absorb the maximum number of photons and to produce electron-hole pairs. Absorber layer thickness has been varied from 0.05μm to 1.2μm. When the thickness of the absorber layer increases the longer wavelength of the illumination produces a good amount of electron-hole pair generation. Fig9 indicates variation in the thickness of an absorber sheet of PV parameters. By looking at the Voc / thickness graph we can say that by increasing its thickness Voc is reduced. From Jsc/ thickness graph; the short circuit current decrease, by increasing the thickness. From the efficiency/thickness graph we can say that there is decreasing with increasing thickness and filling factor increases with increasing thickness we can observe that from the graph. optimum thickness at (0.05) the efficiency is (17).

Table 8 Variation of Thickness for ZnO with device parameters

| Thickness(μm) | Voc (volt) | Jsc (mA/cm$^2$) | FF | Efficiency % |
|---------------|------------|-----------------|----|--------------|
| ZnO           |            |                 |    |              |
| 0.05          | 1.0953     | 46.7049         | 33.23 | 17           |
| 0.1           | 1.0940     | 46.4504         | 33.01 | 16.77        |
| 0.2           | 1.0932     | 46.6525         | 33.05 | 16.71        |
| 0.3           | 1.0930     | 46.1776         | 33.06 | 16.69        |
| 0.4           | 1.0928     | 46.1275         | 33.07 | 16.67        |
| 0.5           | 1.0927     | 46.0875         | 33.08 | 16.66        |
| 0.6           | 1.0927     | 46.0529         | 33.08 | 16.65        |
| 0.7           | 1.0926     | 46.0219         | 33.09 | 16.64        |
| 0.8           | 1.0925     | 45.9937         | 33.10 | 16.63        |
| 0.9           | 1.0924     | 45.9678         | 33.10 | 16.62        |
| 1             | 1.0924     | 45.9438         | 33.11 | 16.61        |
| 1.1           | 1.0923     | 45.9215         | 33.11 | 16.61        |
| 1.2           | 1.0922     | 45.9007         | 33.11 | 16.60        |
Figure 9. Variation of PV parameters by varying the thickness of ZnO

2.2-Effect of annealing Temperatures for ZnO

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 2 where the highest efficiency is 17 with Jsc = 46.7049 mA/cm$^2$, FF = 33.23% and Voc = 1.0953 is achieved when the temperature at 333.15 K, therefore the best result at very low temperature to be very appropriate to work in space. When the temperature is increasing from 333.15 K to 213.15 K, the PCE, Voc and Jsc degrees due to reducing in the generation of the electron-hole pairs in the perovskite materials with increasing temperature as shown in Fig10. From Fig 10 the open-circuit voltage decreases gradually with increasing temperature, it can adjust the efficiency with temperature due to control of the recombination, generation, and a collection of the charge carriers so the best temperature of perovskites solar cells with ZnO as PVSC is 333.15 K.

Table 9. The parameter of the Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/TiO$_2$ heterojunction solar cells

| Temperature (K) | Voc (volt) | Jsc (mA/cm$^2$) | FF  | Efficiency % |
|-----------------|------------|-----------------|-----|--------------|
| 333.15          | 1.0953     | 46.7049         | 33.23 | 17           |
| 313.15          | 1.0940     | 46.4504         | 33.01 | 16.77        |
| 293.15          | 1.0932     | 46.6525         | 33.05 | 16.71        |
| 273.15          | 1.0930     | 46.1776         | 33.06 | 16.69        |
| 253.15          | 1.0928     | 46.1275         | 33.07 | 16.67        |
| 233.15          | 1.0927     | 46.0875         | 33.08 | 16.66        |
| 213.15          | 1.0927     | 46.0529         | 33.08 | 16.65        |

Figure 10: The variation of solar cell parameters with the temperature.

2.3- Effects of the Defect State of the Interface Defect Layer (Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/ZnO).

Numerical simulation has been performed on the defect density at both interfaces from $2 \times 10^{15}$ cm$^{-2}$ to $10 \times 10^{15}$ cm$^{-2}$. Fig 11 show the effect of interface defect density versus efficiency curves for perovskite solar cells. From the graphs, it can be deduced that the Voc, Jsc, and η
decreasing with increasing defect but the FF increases. When the defect density exceeds $2 \times 10^{15} \text{ cm}^{-3}$, a decrease in efficiency is observed. So, it can be realized from the simulated results that interface defect density of $2 \times 10^{15} \text{ cm}^{-3}$ is optimum for device simulation ($\eta=17.67$)

Table 10: Variation of defect for Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/ZnO with device parameters

| Defect Nt(1/cm$^3$) | Voc (volt) | Jsc (mA/cm$^2$) | FF | Efficiency% |
|---------------------|-----------|----------------|----|------------|
| $2 \times 10^{15}$  | 1.1105    | 47.4692        | 33.53 | 17.67      |
| $4 \times 10^{15}$  | 1.1001    | 47.4516        | 33.82 | 17.65      |
| $6 \times 10^{15}$  | 1.0947    | 47.434         | 33.96 | 17.63      |
| $8 \times 10^{15}$  | 1.0918    | 47.416         | 33.02 | 17.61      |
| $10 \times 10^{15}$ | 1.0902    | 47.399         | 34.05 | 17.59      |

Figure 11: Defect density of the Cu$_2$O/CH$_3$NH$_3$PbBr$_3$/ZnO Device solar cells

2.4 - Effect of Different Back Contacts as electrodes

Simulations were performed using silver (Ag), iron (Fe), copper (Cu) graphite alloy, gold (Au), nickel (Ni), and platinum (Pt) as a prospective back touch for solar perovskite cells. Fig 12 shows the effect of the back contacts having different performances. When the metal becomes more practical, the Voc, Jsc, and FF increase. Hence solar cell efficiency in perovskite is also increasing. Because the electrical field near HTM / back contact becomes negative[40], it is energetically unfavorable for the holes to travel towards the electrode.
The results of the simulation show that Pt is one of the possible rear contact materials that can develop PSC performance.

Table 11 shows the effect of various metal back contact on different candidates of the HTM layer.

| Work Function (ev) | Voc (volt) | Jsc (mA/cm²) | FF | Efficiency % |
|-------------------|------------|--------------|----|--------------|
| 4.2               | 0.7431     | 573.945      | 8.09| 0.03         |
| 4.3               | 0.7431     | 573.945      | 8.09| 0.03         |
| 4.4               | 0.4731     | 573.945      | 8.09| 0.03         |
| 4.5               | 1.0269     | 2.5711       | 9.45| 0.25         |
| 4.6               | 1.0520     | 3.6606       | 10.59| 0.41        |
| 4.7               | 1.0747     | 7.5370       | 7.31| 0.59         |
| 4.8               | 1.1131     | 19.5829      | 3.66| 0.80         |
| 4.9               | 1.1819     | 35.903       | 4.65| 1.97         |
| 5                 | 1.2189     | 43.076       | 8.10| 4.25         |
| 5.1               | 1.1546     | 44.585       | 13.77| 7.09       |
| 5.12              | 1.1463     | 44.678       | 14.77| 7.56       |
| 5.15              | 1.1388     | 66.764       | 15.82| 8.06       |
| 5.25              | 1.1335     | 44.872       | 16.76| 8.53       |
| 5.65              | 1.0953     | 46.704       | 33.23| 17        |

Figure 12: Metalwork function versus Voc, Jsc, FF and η%
Conclusions

In this study, the thickness was changed for CH3NH3PbBr3,TiO2 and ZnO, where 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/CH3NH3PbBr3/TiO2 device which reached to 41.85% at 2*10^15 Nt(1/cm3) to be amazing device structure and best Efficiency while the structure of Cu2O/CH3NH3PbBr3/ZnO device reach to 17.67% at 2*10^15,And all other parameter solar cells improved as result to use TiO2 as electron transport materials.

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