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Efficient design of perovskite solar cell using mixed halide and copper oxide

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Solar cells based on perovskites have emerged as a transpiring technology in the field of photovoltaic. These cells exhibit high power conversion efficiency. The perovskite material is observed to have good absorption in the entire visible spectrum which can be well illustrated by the quantum efficiency curve. In this paper, theoretical analysis has been done through device simulation for designing solar cell based on mixed halide perovskite. Various parameters have efficacy on the solar cell efficiency such as defect density, layer thickness, doping concentration, band offsets, etc. The use of copper oxide as the hole transport material has been analyzed. The analysis divulges that due to its mobility of charge carriers, it can be used as an alternative to spiro-OMeTAD. With the help of simulations, reasonable materials have been employed for the optimal design of solar cell based on perovskite material. With the integration of copper oxide into the solar cell structure, the results obtained are competent enough. The simulations have shown that with the use of copper oxide as hole transport material with mixed halide perovskite as absorber, the power conversion efficiency has improved by 6%. The open circuit voltage has shown an increase of 0.09 V, short circuit current density has increased by 2.32 mA/cm^2, and improvement in fill factor is 8.75%.

Keywords: perovskite solar cell, band offset, device simulation, hole transport material

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1. Introduction

Perovskite materials used in fabricating solar cells as absorber have significantly improved the efficiency of solar cells for power conversion. They have proved to have a great impact on photovoltaic (PV) devices. They have power conversion efficiencies (PCE) considerably higher than their other counter parts such as the organic solar cell. They also have an efficiency higher than the dye sensitized devices. They are reported to have a PCE of around 20%.[1,2] There has been an impressive increase in the efficiency of solar cells using perovskite materials. This improvement was just reported in the last three years. The power conversion efficiency has been increased from a value of 9.6% in 2012 to a value of 20.1% in 2015 for lead based halides. For halides employing tin the efficiency is still at around 8%. So to increase the performance of the perovskite based solar cells, numerous fabrication processes are being developed. Various concepts are being developed for the devices.[2–4] Various organic and inorganic hole transport media are also being developed. For developing high-performing devices, there are a lot of issues which need to be addressed in order to commercialize the perovskite solar cell device. Some issues are being addressed, but the stability in particular is not that well documented in the literature. Various options for different layers in the cell structure have been suggested like Al_2O_3 for the electron transport layer.[5,6]

CuSCN when used as the hole transport medium (HTM) is reported to have an efficiency of 12.4%. The molecule based HTM is also being studied. Polymeric HTM's have attained an efficiency of 12%. Perovskite shows BX_6 octahedral structure. The structure of perovskite solar cells evolved firstly by introducing it as a sensitizer in DSCC where the molecular dye was replaced by perovskite. The increase in the carrier mobility and also the concentration density of the transport layers also increases the performance of the device. CuSCN and ZnO are used as the hole transport and electron transport layers and the donor density of ZnO is less than the acceptor density of CuSCN.[7–9] Carbon nanotube (CNT) films are then used as the efficient contact for the perovskite solar cell without hole-transport medium. The concept of clamping solar cells such as direct and chemically promoted has been evolved. The cell without HTM has attained an efficiency of 7.84%. It has been suggested that the efficiency of CNTs can be increased by doping the CNT. With doping the conductivity increases. Processing CNT electrodes on top of perovskite possesses vast possibilities to be chosen so as to optimize the device materials and structure. The band structure of the perovskite and the adjacent charge transport materials should have matching compatibility so as to enable efficient transportation of charge across the layers. The substitution of the halide with another is possible because of the lattice compatibility between different pure halides based compounds. The energy offset between the VBM of perovskite and the HOMO of HTM needs to be small so as to prevent a decrease in V_{OC}.[10–13]

Silicon single junction solar device when used in conjunction with perovskite absorbers in a tandem fashion increases the efficiency of the device. Efficiency of about 18% has been

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achieved enabling V_{OC} of 1.78 V. Silicon is used as a bottom cell with perovskite as the top cell. Its efficiency is basically reduced due to the silicon bottom cell, in which photo generated current is limited by the reflectance losses. FTO electrodes reduce the hysteresis effect, which is pronounced while using ITO electrodes. Doping spiro-OMeTAD enables it to have broader absorption peaks at 500 nm and 380 nm. Use of SiC as the rear contact diminishes the interface recombination which is more pronounced in the earlier reported silicon bottom sub cell. Increasing mobility of the HTM layer also increases the efficiency. Decreasing mobility increases the resistance in the hole transport layer and there will be a drop in the FF and J_{SC}.[14–17] This is because of the increase in the series resistance. The short circuit current density depends on the number of holes being collected at the interface of the perovskite and the HTM layer. Increasing mobility of the HTM layer also increases the efficiency. Decreasing mobility increases the resistance in the hole transport layer and there will be a drop in the FF and J_{SC}. This is due to the increase in the series resistance. The drift diffusion model is adapted for obtaining the current–voltage characteristics of the hysteresis free perovskite solar cells. The carrier recombination has a value of above 1 μs and also it is suggested that there is less recombination velocities at the interface between the layer of perovskite material and the other transport layers of around 1000 cm/s. The built-in voltage is slightly smaller than the open-circuit voltage of around 1.05 V. The interface between the tin oxide and the perovskite layer resembles the Schottky diode and is found to act as a heterojunction for the dissociation and the excitation of the charge carriers. The hybrid structure comprising of a silicon p–i–n structure of nanowire array which is filled with $CH_3NH_3PbI_3$ shows the highest efficiency of absorption in broader wavelength region of 300–800 nm. The power conversion efficiency achieved with this structure is around 13.3%. The J_{SC} is found out to be 28.8 mA/cm^2 with a thin absorber.[17–22]

The performance of the tin-based solar cell has been improved by reducing the acceptor doping concentration in the absorbing or the active layer. Due to this, the efficiency increases and reaches up to a value greater than 18%. The optimum position for VBO of the HTM is calculated to be 0.0–0.2 eV lower than the absorber, and the conduction band of the buffer is 0.0–0.3 eV higher than the absorber. With the removal of the HTM layer, a back junction is formed between the perovskite absorber and the metal back contact. Hence the built in voltage is high if the work function is equal to or deeper than $E_{\text{v-absorber}}$. It is important to match the work function of the back contact to design HTM-free perovskite based solar cells.[23–28] The tin based halide perovskite is used because lead used is a toxic material and possesses serious health hazards. So there is a drive to replace the toxic materials by the non toxic tin based perovskite. Reducing the defect density can further enhance the efficiency of the solar cell. The band offset between the buffer and absorber layers is a decisive factor for the carrier recombination at the interface which determines the open circuit voltage. The optimum position of VBO of the HTM is calculated to be 0.0–0.2 eV lower than the absorber and the conduction band of the buffer is 0.0–0.3 eV higher than the absorber.[29–34] Some of the notable reasons for using copper oxide as HTM are as follows. (i) Cu-based materials are gathering attention owing to their higher charge mobility and low cost engaged in their fabrication because the materials used in the fabrications of copper oxide are also less in cost. (ii) These materials are proved to have high current density and for this reason their conductivity is elevated when they are matched up with other hole transport materials such as spiro-OMeTAD having smaller molecular size and higher weight of molecules. (iii) These metal oxides substantiate robust behavior and market friendly characteristics as their cost is less. (iv) Metal oxides enjoy long term durability because of their environment friendly nature. (v) Their chemical stability tests prove that the copper oxide material does not allow water to disseminate in comparison to organic hole transport media such as spiro-OMeTAD. They are more resistant to scratching and serration as they are mechanically stronger. (vi) The copper oxide layer absorbs more light incident on its surface when compared with spiro-OMeTAD because of its narrower band gap.

Mixed halide perovskites have enhanced diffusion length of carriers and due to chloride substitution there is elevation in the photovoltaic performance because of the enhanced carrier transport across the junction of the hetero-structure. The halide substitution leads to band gap narrowing due to which electroluminescence is tuned to green region of the solar spectrum from blue region.

2. Basic structure and physics based model

The perovskite solar cell devices are originally evolved from DSSC research with the fact that there is no requirement of oxide scaffold. Their device architecture seems very much similar to the thin film PVs with a difference that here the active layer is composed of a perovskite material. The precursors of perovskite based solar cells used polar solvents for the deposition which enabled the development of this kind of devices. The structure in the figure represents a generic non inverted structure of the perovskite based solar cell. The structure is based on standard substrates of glass/ITO along with back contact of metal which in most cases is silver. The main requirement to get a device working effectively is the presence of two interface layers which are charge selective in nature, one for electrons and the other for holes. There are a number of interface layers which work very well in the field of organic PV devices. Some of them are PEDOT: PSS, PTAA polymers work very effectively as the hole transport medium,

while oxides such as tin oxide work well as the electron transport layer. Various practical issues like the quality and thickness of the film limit the device fabrication process. Also the width of the perovskite active needs to be of several hundred of nanometers, which is more than that of the organic photovoltaic devices by several times.

After the absorption of light, the photo generated charge carriers get transferred to the hole and electron interface layers from the perovskite layer from where they are transported to their respective charge selective contacts. The typical structure of perovskite solar cell usually has an absorber layer made up of a perovskite material which has a thickness of around 300–500 nm. Also it comprises of a hole transporting medium which is p-type and an electron transporting medium which is n-type. Together with these layers there are the front and the back contacts which are arranged in various different configurations.[14] There have been numerous suggestions regarding the dielectric constant of the perovskite, where it is suggested that its high value makes the dissociation of excitons generated, into free charge carriers very swiftly. The electrons and holes then get drifted and diffused through their absorber layers and the transporting layer. After that they get collected at their respective contacts. Hence an analytical model has been developed after getting solution by solving the various steady state continuity equations for electrons and the holes within the absorber layer[15]

$$D\frac{\partial^2 n(x)}{\partial x^2}+\mu E(x)\frac{\partial n(x)}{\partial x}+G(x)-R(x)=0, \quad (1)$$

$$D\frac{\partial^2 p(x)}{\partial x^2}-\mu E(x)\frac{\partial p(x)}{\partial x}+G(x)-R(x)=0, \quad (2)$$

where $n(x)$ is the electron concentration and $p(x)$ is the hole concentration. D denotes the diffusion constant and μ denotes the mobility of the two charge carriers. Here $G(x)$ denotes the rate of photo generation which is dependent on the position. The perovskite material has a long diffusion length, due to which the effect of charge recombination can be ignored within that layer. So we can assume $R(x)=0$. Lastly the electric field inside the absorber layer is position resolved and is denoted as $E(x)$.

3. Proposed device simulation

The simulator used for simulating device is SCAPS ver. 3.3.05. Here the solar cell employing perovskite has a planar structure. The configuration includes substrate of glass/ transparent conducting oxide (TCO)/ buffer layer (TiO_2)/ defect layer 1/ perovskite ($CH_3NH_3PbI_{3-X}Cl_X$)/ defect layer 2/ hole transport medium (Cu_2O)/ back contact as shown in Fig. 1. The parameters of all layers in simulation are listed in Table 1. N_A and N_D are the acceptor and the donor densities. The parameter ε_r denotes the relative permittivity, while the parameter χ denotes the electron affinity. E_g is the band gap of different layers, while μ_n and μ_p are the mobilities of electron and hole, respectively. N_t here is the defect density present in each layer. The parameters based on physics for the TCO layer are those of SnO_2:F. The thicknesses of the layers in the architecture are adopted from some experimental report where solar cells having high efficiency were reported. The choice of planar structure simplifies the device structure preparation and helps reducing the cost of the materials.

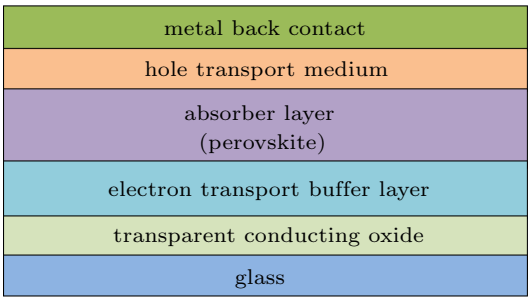


Fig. 1. (color online) Basic structure of perovskite solar cell.

In order to account for the recombination at the interfaces, two interface defect layers have been inserted between the interface of the absorber and buffer layers and the other one between the absorber and HTM layer. The parameters of the defect layers are summarized in Table 1 and kept almost indistinguishable to that of the perovskite layer except the defect density. The defect density N_t is a predominant and overriding parameter which sways the efficiency of the perovskite solar

Table 1. Design parameter selection.

Parameter	TCO (SnO_2:F)	Buffer layer (TiO_2)	IDL 1 (defect layer 1)	Perovskite ($CH_3NH_3PbI_{3-X}Cl_X$)	IDL 2 (defect layer 2)	HTM (copper oxide)
Thickness/nm	500	50	10	500	10	350
E_g/ev	3.5	3.2	1.55	1.55	1.55	2.1
χ/ev	4	3.9	3.9	3.9	3.9	3.2
ε_r	9	9	6.5	6.5	6.5	7.11
$\mu_n/cm^2\cdot V^{-1}\cdot s^{-1}$	20	20	2	2	2	3.4
$\mu_p/cm^2\cdot V^{-1}\cdot s^{-1}$	10	10	2	2	2	3.4
N_D/cm^{-3}	2×10^{19}	1×10^{16}	1×10^{15}	1×10^{15}	1×10^{15}	-
N_A/cm^{-3}	–	–	–	–	–	1×10^{18}
N_t/cm^{-3}	10^{15}	10^{15}	10^{15}	$10^{10}-10^{17}$	10^{15}	10^{15}

cells. The defect density influences the performance and is based on Shockley–Read–Hall (SRH) recombination model. The model is given as

$$R = \frac{np - n_{\mathrm{i}}^2}{\tau_{\mathrm{p}}\left(n + N_{\mathrm{C}}\,\mathrm{e}^{(E_{\mathrm{g}}-E_{\mathrm{t}})/kT}\right) + \tau_{\mathrm{n}}\left(p + N_{\mathrm{V}}\,\mathrm{e}^{E_{\mathrm{t}}/kT}\right)}, \quad (3)$$

where n and p represent the concentrations of mobile electrons and holes, respectively, which are obtained by the solution of Poisson and continuity equations. Neglect n_{i}^2 term, because $qV > 3kT$ for adequate forward bias. Also we have

$$\tau_{\mathrm{n,p}} = \frac{1}{\sigma_{\mathrm{n,p}} v_{\mathrm{th}} N_{\mathrm{t}}}, \quad (4)$$

where N_{t} and E_{t} are the concentration and the energy level of defects. $\tau_{\mathrm{n,p}}$ denotes the lifetime of charge carriers whereas $\sigma_{\mathrm{n,p}}$ depicts the capture cross-section and v_{th} is the thermal velocity. The diffusion length hence can be calculated as

$$l = \sqrt{D\tau}, \quad (5)$$

where D denotes the diffusion constant and is given as

$$D = \mu kT/q. \quad (6)$$

By combining the above equations, the diffusion length can be calculated and is in agreement with the simulated values. The other parameters like the conduction and valence band effective densities of states are kept the same and identical for all the layers and are set to be equal to 2.2×10^{18} cm^{-3} and 1.8×10^{18} cm^{-3}. The thermal velocity is kept at 10^7 cm/s for both electrons and holes for all the layers. The absorption coefficient is obtained using $\alpha = A_\alpha(h\nu - E_{\mathrm{g}})^{1/2}$. For this the pre factor A_α is chosen to be 10^5 to get the value of absorption coefficient. In this simulation the conduction band offset (CBO) is set to zero and valence band offset (VBO) is calculated as -0.15. These values are in the range of optimum position of the CB and VB for the buffer layer and HTM layer. With this, the absorber will be fully depleted and the solar cell here has a p–i–n structure. Here in the simulation no series or shunt resistances are being considered for the contacts and the TCO layer. The back contact work function is calculated from flat bands. The difference between $E_{\mathrm{V_absorber}}$ and the work function of metal back contact affects the performance of the solar cell.

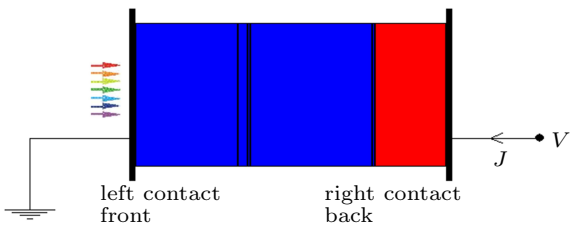


Fig. 2. (color online) Simulated device structure.

The defects have been taken to be neural for every layer having placed at centre of the band gap. It has the characteristic energy of 0.1 eV with a Gaussian distribution. The capture cross-section of holes and electrons has a value of 2×10^{-14} cm^{-2} for all the layers.

4. Results and discussion

On launching the recorder set-up and the batch set-up, we obtain the results shown below. Figure 3 presents the band diagram of the solar cell based on perovskite. The structure here is in p–i–n configuration. The structure exhibits higher values of PCE = 24.13%, $FF = 87.75\%$, $V_{\mathrm{OC}} = 1.12$ V, and $J_{\mathrm{SC}} = 24.52$ mA/cm^2, when the defect density is kept at 10^{10} cm^{-3}. On further increasing the defect density there is not much effect on the short circuit current density and V_{OC}. When the defect density is 10^{13} cm^{-3}, the results are PCE = 23.16%, $FF = 85.31\%$, $V_{\mathrm{OC}} = 1.10$ V, and $J_{\mathrm{SC}} = 24.51$ mA/cm^2. The overall performance of the perovskite solar cell is elevated with improvement in open circuit voltage and short circuit current density because of the minimal interconnection losses at this stage. Here the Poisson equation and continuity equations are solved iteratively for both electrons and holes.

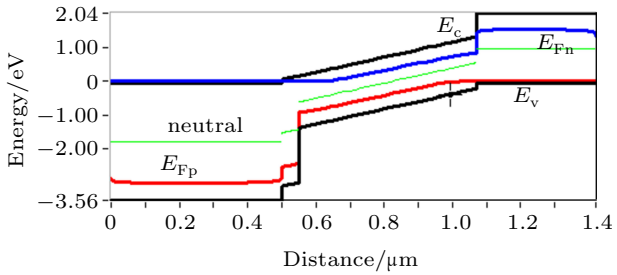


Fig. 3. (color online) Proposed device energy band diagram.

But on further increasing the defect density to 10^{15}, there is a sharp decrease in all the observed parameters and when it is further increased to 10^{17}, the PCE reduces to as low as 0.43%, $FF = 24.39\%$, $V_{\mathrm{OC}} = 0.65$ V, and $J_{\mathrm{SC}} = 2.67$ mA/cm^2. The decreased performance of the solar cell is mainly attributed to the increased defect density because of which the recombination of the charge carriers becomes dominant in the absorption layer and the quality of the film is decreased. Figure 4 below depicts the energy band diagram with CBO.

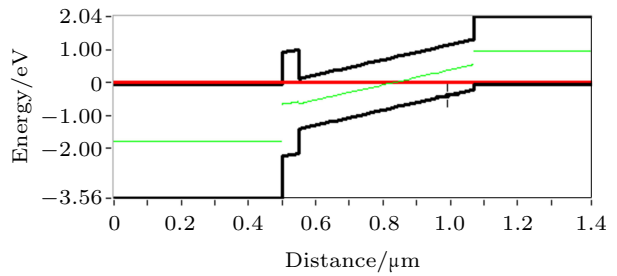


Fig. 4. (color online) Energy band diagram with CBO.

The effect on the short circuit current density can be seen from the J–V characteristics as shown in Fig. 5.

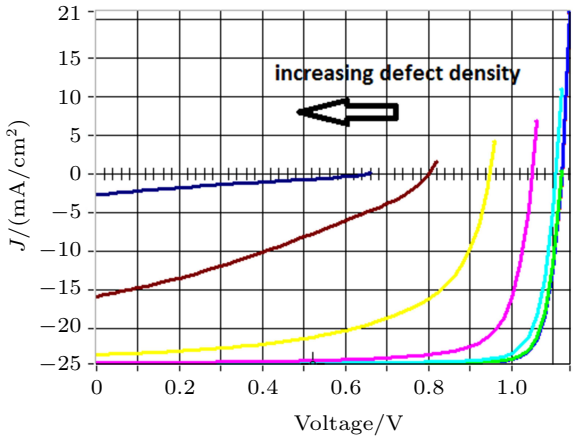


Fig. 5. (color online) Current density versus voltage response.

The variation of the cell parameters with the variation in the electron affinity of the HTM layer is illustrated in Fig. 6, where it can be seen that with the change in electron affinity, the valence band offset also changes. Due to the presence of offset at the interface of HTM and absorber layer, there is the formation of a barrier because of the bridging effect. With the bridging, there will be recombination and the charge carriers will not be able to reach their respective electrodes and hence hamper the performance of the cell. This decrease in the cell parameters is depicted in Fig. 7. This can be explained by the SRH recombination model. Whenever the defect density of absorber is increased, the length decreases, which in turn increases the recombination and inhibits the progression and diffusion of photo generated charge carriers towards their respective electrodes.

Figure 8 illustrates the generation–recombination profiles for a defect density of 10^{13} cm^{-3}, where the recombination rate is less than the e–h pair generation. The same reason can be stated for using the material having high mobility.

The conduction band offset has been set to 0, which is an ideal condition and hence does not restricts the flow of photo generated carriers across the respective electrodes. But if there is significant CBO, then there is formation of spike, which results in a behavior similar to the double-diode and restricts the flow of electrons. On the other hand, there is a slight valence band offset of -0.15 eV. On making it more negative, there is a drop in the V_{OC} and FF whereas the value of J_{SC} is not much affected. The change or decrease in the fill factor is not much prominent. The decrease in V_{OC} is mainly attributed to the decrease in the activation energy. The decreased activation energy basically increases the recombination at the interface and hence V_{OC} decreases. The effect of band offsets is not much discussed here. The band offsets have pronounced effect in case of perovskite solar cells without HTM layer. This is so because the difference between the valence band of absorber and the work function of metal contact leads to the formation of a spike when the offset is positive.

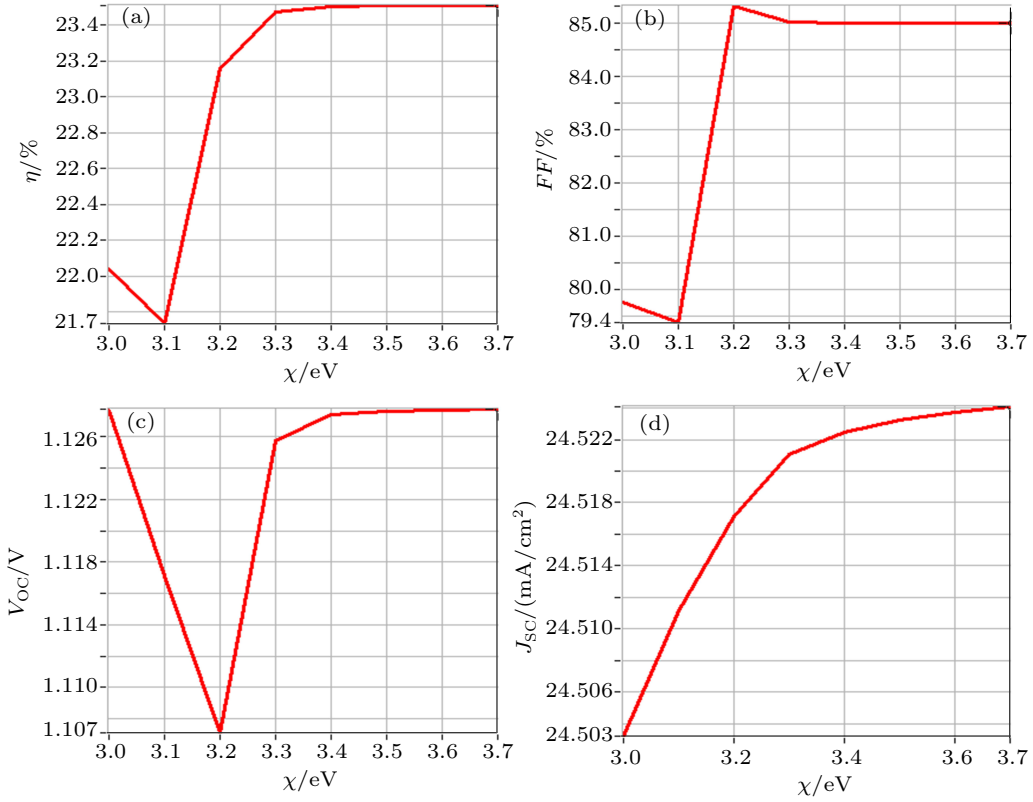


Fig. 6. (color online) Variation of cell parameters with electron affinity of copper oxide.

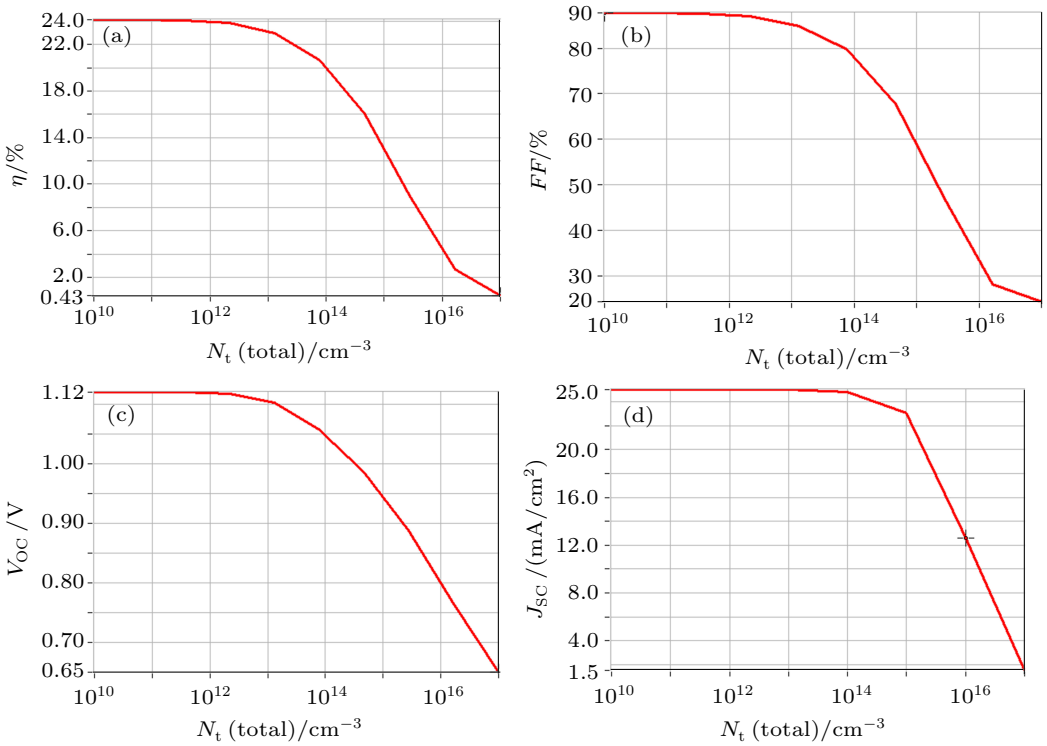


Fig. 7. (color online) Effect of defect density on cell parameters.

The efficiency reported in Refs. [18] and [19] is around 18% when the HTM layer used is spiro-OMeTAD having mobility of 2×10^{-4} cm^2/Vs for both electrons and holes. But by Cu_2O as HTM, the efficiency is certainly improved because high mobility ensures less series resistance, low diffusion length, and efficient carrier transport.

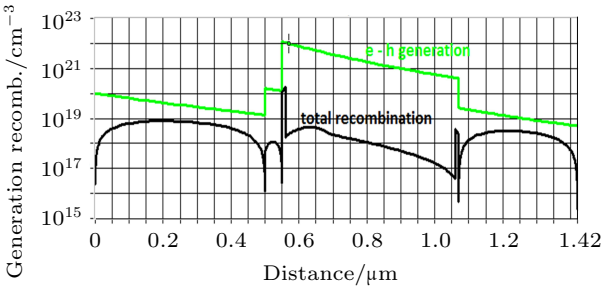


Fig. 8. (color online) Generation and recombination curves.

The donor density also has a crucial role. With the increase in donor density from 10^{13} cm^{-3} to 10^{15} cm^{-3}, there is an increase in efficiency from 21.4% to 24% but the further increase decreases the V_{OC} of the device due to recombination, which becomes dominant with increasing doping concentration. Figure 9 shows the quantum efficiency curve as a function of wavelength for different values of defect density. The efficiency curve is spanned over almost entire visible range of the solar spectrum. The quantum efficiency decreases for the increase in defect density. The quantum efficiency is constant in the region from 360 nm to 600 nm and then it decreases and has an onset even up to 800 nm.

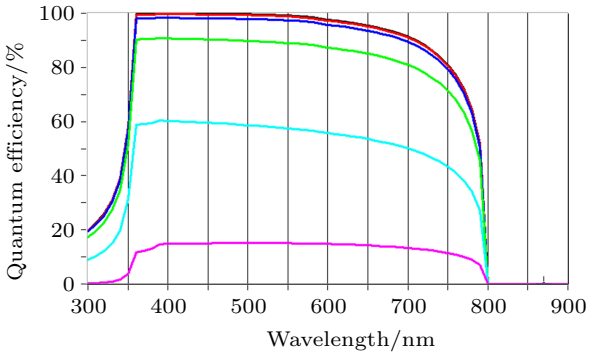


Fig. 9. (color online) Quantum efficiency response.

5. Conclusion

With the use of perovskite materials, the efficiency of solar cells has been increased manifold. The main consideration here lies to increase the efficiency of the device. Various techniques have been proposed to enhance the efficiency of the device like use of mixed halide perovskite i.e. $CH_3NH_3PbI_{3-X}Cl_X$ and copper oxide as HTM. Also the effect of the defect density and band offsets is crucial and here the effect of the defect density is studied. The best way to increase the efficiency and fill factor is to use high mobility oxides as the hole transport layer. Some of the notable highly efficient oxides are copper oxide and, nickel oxide. If the work function of the contacts is also increased then also the efficiency would tend to increase. The doping concentration of the HTM layer can also be varied to get desired results. By incorporating some of these methods, the efficiency and the fill

factor of the solar cell will be improved upto certain extent. The simulated results have PCE of 24.13%, V_{OC} of 1.12 V, J_{SC} of 24.52 mA/cm^2, and FF of 87.75%. The use of mixed halides also increases the efficiency because they have good band alignment with the HTM and buffer layer. With the help of device simulation the role and influence of various factors can be studied effectively. There is still a left on improving the efficiency of tin based halides as lead based halides are toxic in nature.

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References

[1] Prasanthkumar S and Giribabu L 2016 *Current Science* **111** 1173
[2] Sharma S, Jain K K and Sharma A 2015 *Materials Sciences and Applications* **6** 1145
[3] Snaith H J 2013 *Physical Chemistry Letters* **4** 3626
[4] Green M A, Baillie A H and Snaith H J 2014 *Nat. Photon.* **8** 506
[5] Park N G 2015 *Materials Today* **18** 65
[6] Zhang A, Chen Y and Yan J 2016 *Quantum Electronics* **52** 90
[7] Yin W J, Shi T and Yan Y 2014 *Appl. Phys. Lett.* **104** 063903
[8] Yin W J, Shi T and Yan Y 2014 *Adv. Mater.* **26** 4653
[9] Chandu V V M, Mallineni G, Prabakar V and Kim H J 2017 *Photochemistry and Photobiology A: Chemistry* **332** 265
[10] Ou Q D, Li C, Wang Q K, Li Y Q and Tang J X 2017 *Advanced Materials Interfaces* **4** 1
[11] Albrecht S, Saliba M, Pablo J, Baena C, Lang F, Kegelmann L, Mews M, Steier L, Abate A, Rappich J, Korte L, Schlatmann R, Khaja M, Anders N, Grätzel H and Rech B 2016 *Energy and Environmental Science* **9** 81
[12] Pandey R and Chaujar R 2016 *Superlattices and Microstructures* **100** 656
[13] Alnuaimi A, Almansouri I and Nayfeh A 2016 *Computational Electronics* **15** 1110
[14] Bansal S and Aryal P *Proceedings of* 43rd *Photovoltaic Specialists Conference*, June 2016, p. 747
[15] Taretto K, Soldera M and Frischknecht A 2017 *Journal of Photovoltaics* **7** 206
[16] Yadav P, Pandey K, Bhatt P, Raval D, Tripathi B, Kanth C, Manoj P, Pandey K and Kumar M 2015 *Solar Energy* **122** 773
[17] Yan X, Zhan C, Wang J, Zhang X and Ren X 2017 *Nanoscale Research Letters* **12** 128
[18] Toshniwal A, Jariwala A, Kheraj V, Opanasyuk A S and Panchal C J 2017 *Nano and Electronic Physics* **9** 030381
[19] Du H J, Wang W C and Zhu J Z 2016 *Chin. Phys. B* **25** 803
[20] Mohammad A, Mirzaei B, Vahid M and Mohsen M 2000 *American Journal of Optics and Photonics* **3** 94
[21] Mandadapu U, Vedanayakam S V and Thyagarajan K 2017 *Indian Journal of Science and Technology* **10** 65
[22] Minemoto T and Murata M 2015 *Solar Energy Materials and Solar Cells* **133** 8
[23] Minemoto T and Murata M 2014 *Current Applied Physics* **14** 1428
[24] Hossain M I, Andrabi F H and Tabet N 2015 *Solar Energy* **120** 370
[25] Alnuaimi A, Almansouri I and Nayfeh A 2016 *American Institute of Physics Advances* **6** 110
[26] Masuko K, Shigematsu M, Hashiguchi T, Fujishima D, Kai M, Yoshimura N, Yamaguchi T, Ichihashi Y, Yamanishi T, Takahama T, Taguchi M, Maruyama E, Okamoto S, Mishima T, Matsubara N, Yamanishi T, Takahama T, Taguchi M, Maruyama E and Okamoto S 2014 *Journal of Photovoltaics* **4** 1433
[27] Wehrenfennig C, Eperon G E, Johnston M B, Snaith H J and Herz L M 2014 *Adv. Mater.* **26** 1584
[28] Tan K, Lin P, Wang G, Liu Y, Xu Z and Lin Y 2016 *Solid-State Electron.* **126**
[29] Zhou H, Chen Q, Li G, Luo S, Song T B, Duan H S, Hong Z, You J, Liu Y and Yang Y 2014 *Science Journal* **345** 542
[30] Edri E, Kirmayer S, Kulbark M, Hodes G and Cahen D 2014 *Physical Chemistry Letters* **5** 429
[31] Jeffrey A, Raymon C, Fung C M and Kamal P V 2014 *J. Am. Chem. Soc.* **136** 758
[32] Chin Q, Zhou H, Song T B, Luo S, Hong Z, Duan H S, Dou L, Liu Y and Yang Y 2014 *Nano Lett.* **14** 4158
[33] Wang D, Naveen M W, Elumalai K and Uddin A 2016 *Solar Energy Materials and Solar Cells* **147** 255
[34] Huang L, Hu Z, Xu J, Sun X, Du Y, Ni J, Cai H, Li J and Zhang J 2016 *Solar Energy Materials and Solar Cells* **149** 1