Original Article

IJCIH
Converging Healthcare & Technology

INTERNATIONAL JOURNAL OF CONVERGENCE IN HEALTHCARE

Published by
IJCIH & Pratyaksh Medicare LLP

www.ijcih.com

Effect of Intensity on Perovskite Solar Cells Parameters by SCAPS-1D Simulation

Deepika[1], Upkar Kumar Verma[2], Arjun Singh[3]

[1]Research Scholar, Department of Applied Sciences, The Northcap University, Gurugram, India, [2]Assistant Professor, Department of Physics, B S N V PG College, Lucknow, India, [3]Assistant Professor Department of Applied Sciences, The Northcap University, Gurugram, India

Abstract

In recent years, climate mitigation and limited fossil fuel resources have increased the necessity for electricity, especially from renewable sources. Therefore, the sun is an abundant renewable energy source. The solar cell is one of the better choices for future clean energy. Due to low prices and high efficiency, the perovskite solar cell has emerged lately as a solar cell technology compared to other solar cells. The performance of solar cells varies according to weather conditions such as humidity, temperature, and sunlight intensity. This work studied the illumination impact on the perovskite solar cell.The perovskite solar cells having n-i-p device structure i.e, FTO/ SnO_2/$FA_{0.85}Cs_{0.15}Pb(I_{0.85}$ $Br_{0.15})3$/BiI_3/CuI/Au was used. The illumination depended on solar cell parameters such as Voc, Jsc, and FF was reported. It has been observed that light intensity affects the device's performance significantly. Hence, this study can have a way for an optimal design of effective performance and economical solar cells.

Keywords: *Perovskite solar cell,SCAPS-1D, Fill factor, efficiency, short circuit current.*

Introduction

A key technology for producing electricity from renewable sources is solar cells. Solar cells are an excellent source of clean energy that does not contribute to climate change or air pollution because they generate electricity without emitting any emissions or pollution. Being abundant and never running out, solar energy is renewable, and we can use solar energy as long as the sun is out. The cost of solar panels and cells has declined rapidly over the years, making them increasingly affordable and cost-effective. In many cases, solar energy is now cheaper than traditional energy sources such as coal and natural gas. Overall, solar technology is crucial for the shift to a low-carbon, sustainable economy[1, 2]. Due to their potential for high efficiency and low cost, perovskite solar cells are a type of solar cell that has recently attracted much attention. These cells' use of perovskite materials, which are inexpensive and straightforward to produce, makes them a suitable replacement for conventional silicon-based solar cells. Perovskite solar cells are increasingly in demand due to the rising demand for renewable energy sources and the need to reduce greenhouse gas emissions. The efficiency and cost of solar energy production could significantly increase and decrease, respectively using

Corresponding Author:
Dr. Arjun Singh
Assistant Professor, Department of Applied Sciences, The NorthCap University, Gurugram (India)
e-mail: arjunsingh@ncuindia.edu

perovskite solar cells. One of the most plentiful and pure renewable energy sources is solar energy.

In addition, perovskite solar cells can be used in a wide range of applications, from large-scale solar farms to portable devices, such as smartphones and wearable electronics. Their flexibility and lightweight design make them ideal for applications where traditional solar cells may not be suitable. Overall, the urgent need to switch to a more sustainable and clean energy system and the potential for perovskite solar cells to offer a low-cost, high-efficiency substitute for conventional solar cells are driving the demand for perovskite solar cells. The improvement in solar cell technologies can be seen from 1st generation to 4th generation, and the perovskite solar cells (PSCs) turned out to be a leading source of energy(3).

The perovskite structure is represented by the formula ABX3, where X, A, and B are anions and cations, respectively, with sizes A>B. Using α-FAPbI3, PSCs achieved record efficiency of 26.08% (certified 25.73%) and have the potential to be used in solar-scale development due to their exceptional light absorption, carrier lifetime, and mobilities(4).

The performance of PSCs is limited by issues like material toxicity and device hysteresis, despite having the potential to replace Si-based solar cells for long periods of time. PSCs are capable of stacking up to seven layers of various materials, but because of the problem of carrier recombination at the interfaces, trap sites that are extremely sensitive to moist air appear, which lowers the device's performance.(5)

To be commercialized, PSCs must overcome significant obstacles such as material toxicity, defect formation, device hysteresis, non-uniformity at the interface, and perovskite material stability.(6, 7). The enormous capacitance under light conditions compared to dark conditions, which is only observed in PSCs, is another difficulty. (8)

Although $FA_{0.85}$ $Cs_{0.15}$ $Pb(I_{0.85}$ $Br_{0.15})$ $_3$-based PSCs are less toxic and can withstand harsh environmental conditions like high temperatures and moisture without corroding, they still fall short in many areas. This work, SCAPS-1D simulation is used to examine the impact of intensity on PSC. The authors of this study observed and reported the results of the light-dependent current-voltage (J-V) characteristics and capacitance-voltage (C-V) relationships using simulations of $FA_{0.85}Cs_{0.15}Pb(I_{0.85}$ $Br_{0.15})3$ perovskite materials as a basis for perovskite solar cells.

Methodology

In this work, the device simulation is performed based on planar heterojunction n-i-p structure, composed of FTO/SnO2/$FA_{0.85}Cs_{0.15}Pb(I_{0.85}Br_{0.15})_3$/$BiI_3$/CuI/Au using SCAPS-1D which proved to be a key to developing new inexpensive devices. The simulation was performed at different intensities by varying the frequency. The schematic representation of the used device structure is shown below in figure 1.

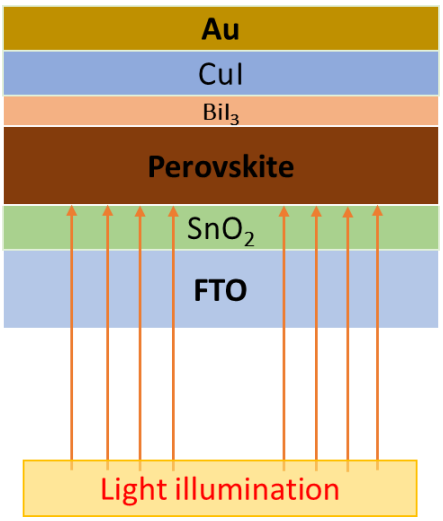


Figure 1: Schematic representation of planar heterojunction (n-i-p) device structure with BiI_3 as an interface layer.

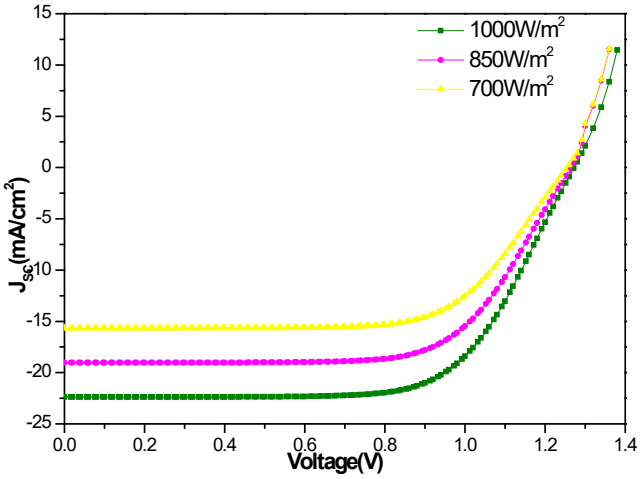
The work function of the Au electrode and FTO were 5.1eV and 4.0eV, respectively. By keeping the velocities of e- and h+ as 1 * 10^7 cm/s at a constant temperature of 300K. The voltage range kept for C-V simulation is from 0 to 1.2V.

Table 1: Simulation parameters of $FA_{0.85}Cs_{0.15}Pb(I_{0.85}Br_{0.15})_3$ based PSC using SCAPS-1D(9).

Parameters	FTO	ETL (SnO_2)	$FA_{0.85}Cs_{0.15}Pb(I_{0.85}Br_{0.15})_3$	BiI_3 (IL)	HTL (CuI) (10)	Ref.
Thickness (nm)	500	70 [1]	500	30	100	(11)
Band gap (eV)	3.50	3.50	1.59	1.72	2.98	(12)
E Affinity (eV)	4.00	4.00	4.09	4.10	2.10	(13, 14)
Permittivity	9.00	9.00	6.600	5.78	6.50	(15)
Effective density of states at CB (cm^{-3})	$2.2 * 10^{18}$	$2.2 * 10^{17}$	$2.0 * 10^{19}$	$2.5 * 10^{19}$	$2.8 * 10^{19}$	
Effective density of states at VB (cm^{-3})	$2.2 * 10^{18}$	$2.2 * 10^{17}$	$2.0 * 10^{18}$	$2.5 * 10^{19}$	$1.0 * 10^{19}$	
Mobility of e^- ($cm^2 V^{-1} s^{-1}$)	20	20	8.16	600	$1.69 * 10^{-4}$	(13, 16)
Mobility of h^{+-} ($cm^2 V^{-1} s^{-1}$)	10	10	2	200	$1.69 * 10^{-4}$	
Density of n-type doping (cm^{-3})	$1.0 * 10^{15}$	$1.0 * 10^{17}$	$1.3 * 10^{16}$	$1.0 * 10^{16}$	0	
Density of p-type doping (cm^{-3})	0	0	$1.3 * 10^{16}$	$1.0 * 10^{16}$	$1 * 10^{18}$	
Density of defects (cm^{-3})	Donor- $1.0 * 10^{18}$	Donor- $1.0 * 10^{15}$	Neutral- $4 * 10^{13}$	Neutral-$1 * 10^{15}$	Neutral- $1 * 10^{15}$	

Results and Discussion

Each layer in a perovskite solar cell has a unique set of optoelectronic characteristics. Table 1 explains the parameters needed for each layer. SCAPS-1D is fed with the defects at the interface and in the materials of each layer to produce the results. Figure 2 depicts the characteristics of the current-voltage (J-V) relationship as (a) dark J-V characteristics and (b) intensity-dependent (J-V).



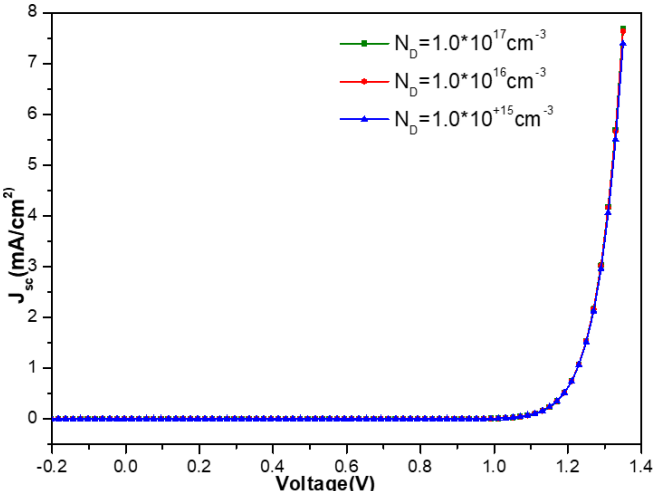


Figure 2: Current-Voltage characteristics of (a) light dependent as well as (b) dark.

With Voc= 1.27 V, Jsc= 22.38 mA/cm^2, and Fill Factor (FF)=66.78%, the device had the highest power conversion efficiency (PCE) of 19.02% at 1000W/m^2. All other parameters, except FF, decreased as the intensity increased, resulting in the device's lower power conversion efficiency (PCEs). When the light intensity is reduced from 1000 W/m^2 to 700 W/m^2, a rise in non-radiative recombination in the device and a decrease in Jsc and Voc values may be referred to as the reduction in generated

carrier concentration with light intensity[17]. The PCEs of the device increase with increases in light illuminations. Even at higher defect in ETLs leads to higher performnce at higher light intensity, this may be due to higher carrier concentartion. It is common to see this behavior in all light intensities. The intensity-dependent results of all the devices are shown in table 2.

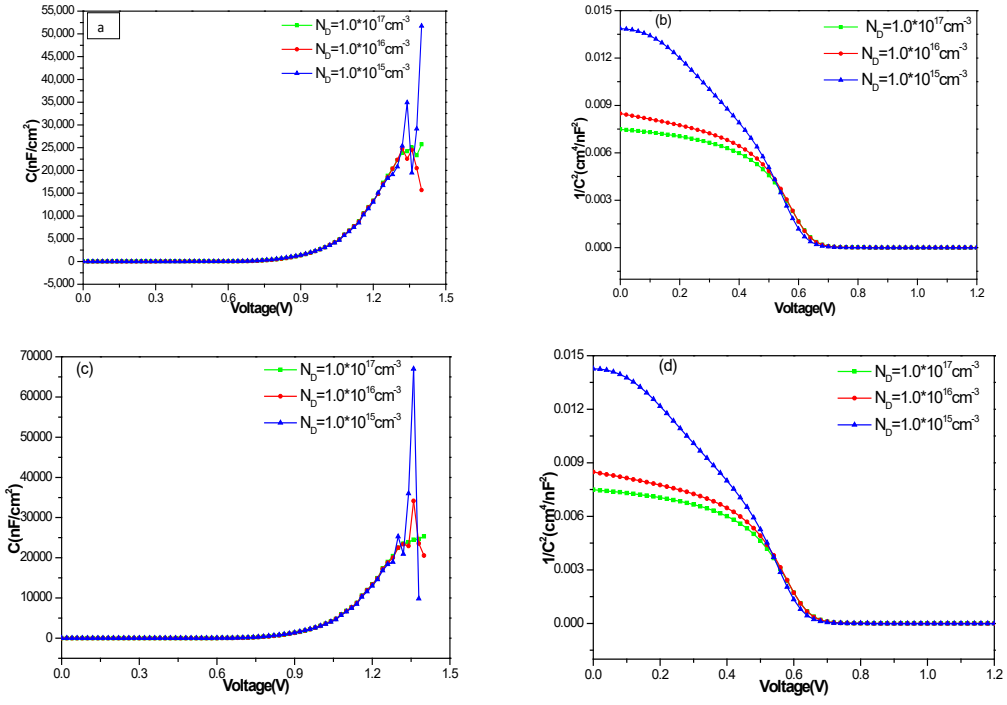
Table 2: Obtained device parameters at different intensities and defect densities.

Intensity (W/m^2)	N_D (cm^{-3})	Efficiency (%)	FF (%)	J_{sc} (mA/cm^2)	V_{oc} (V)
1000	$1.0*10^{17}$	19.02	66.78	22.38	1.27
	$1.0*10^{16}$	18.91	66.45	22.38	1.27
	$1.0*10^{15}$	18.59	65.32	22.39	1.27
850	$1.0*10^{17}$	18.93	66.88	19.02	1.26
	$1.0*10^{16}$	18.82	66.55	19.03	1.26
	$1.0*10^{15}$	18.52	65.51	19.03	1.26
700	$1.0*10^{17}$	18.82	67.01	15.66	1.25
	$1.0*10^{16}$	18.72	66.69	15.66	1.25
	$1.0*10^{14}$	18.44	65.72	15.67	1.25

The most popular technique to be applied to C-V data is Mott-Schottky (MS) analysis used to calculate both built-in-voltage as well as doping density with the help of relation,

$$\frac{1}{C^2} = \frac{2}{A^2 \in q N_A} \frac{1}{} (V_{bi} - V)$$

Where C denotes capacitance, A denotes device area, ε denotes permittivity, q denotes unit charge, NA denotes doping density, and Vbi denotes built-in voltage. The C-V simulation, along with MS plot, is shown in figure 3 (a), (b) and (c) where different parts of the cell decide different parts of C-V curve. Here, MS plots are taken at different intensities keeping frequency fixed at 1000Hz and the outcome reported in figure 3 (a), (b) and (c).



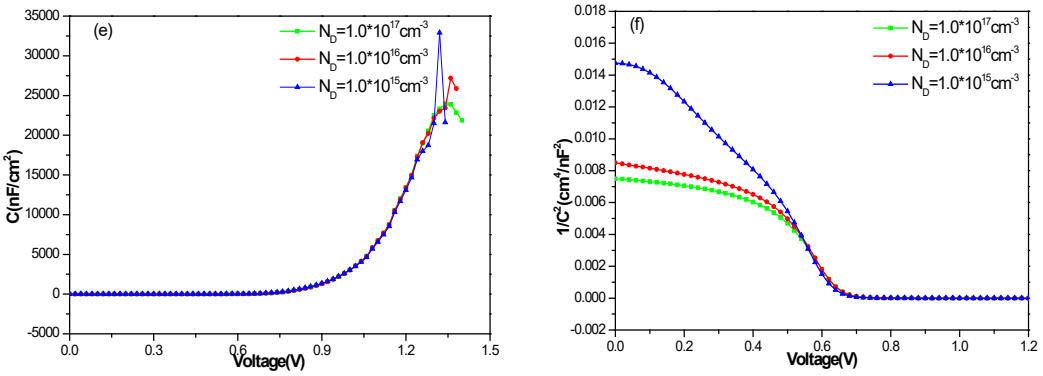


Figure 3: (a&b) C-V and MS plot at 1000W/m^2. (c&d) C-V and MS plot at 850W/m^2. (e&f) C-V and MS plot at 700W/m^2.

The MS plot's x-axis intercept typically represents the built-in potential(Vbi) of a perovskite solar cell, and the slope of $1/C^2$ (V) is interpreted as a concentration of occupied trapping centers[18-20]. Nevertheless, given the disparity in electrode work functions, the obtained values are less than anticipated[21-23]. The system's capacitance under reverse polarization (for the metal/SnO_2 interface) is the product of the capacitances of the junction and the contact[22] . As a function of the donor density (N_D) and light intensity, The proposed perovskite solar cells' C-V characteristics and Mott-Schottky plot analysis are shown in Figure 3. While other variables remained constant, the donor density (ND) concentration ranged from 10^{15} cm^{-3} to 10^{17} cm^{-3}.

Figures 3a, c, and e show that the capacitance rises gradually with applied voltage, sharply at higher voltages, and reaches its maximum when ND is 10^{17} cm^{-3}. A well-known and reliable tool to evaluate a device's built-in potential (Vbi), or the difference between its doping level and electrode operation[24] is the Mott-Schottky (MS). The MS theory is primarily based on the characteristics of the p-n junction[25] but it is also applied to solar cell technology[18, 19, 26]. The MS plot's x-axis intercept typically represents the built-in potential(Vbi) of a PSCs, and the slope of $1/C^2$ (V) is interpreted as a concentration of occupied trapping centers [18-20]. As a result, capacitance grows along with an increase in forward bias voltage and behaves in accordance with the Mott-Schottky relationship. Despite earlier reports that it was significantly lower than the saturation current at low voltages, the current was only permitted to reach the contact's saturation current at high voltages[27]. The lower value of the built-in potential (Vbi), which was determined from the Mott-Schottky plot under illumination, is most likely caused by the capacitance resulting from the photogenerated charge carriers that can accumulate in the low-mobility materials, even at reverse bias[28]. As the doping concentration increases, there is an increase in charge accumulation at the interface and a corresponding increase in capacitance. As a result, there is a drop in voltage at the metal/SnO_2 interface. Figure 3(b,d,f) shows the calculation of the built-in potential (Vbi) Mott- Schottky relation at $1/C^2 = 0$ on the potential axis[29]. According to research, the built-in potential (Vbi) rises from 0.69 V to 0.72 V as N_D increases.

Conclusion

In summary, in this article $FA_{0.85}Cs_{0.15}Pb(I_{0.85}Br_{0.15})_3$ based perovskite solar cell structure is analyzed with SCAPS-1D simulation software. The effect of light intensity on device performance was studied, and reported that with the decrease in light intensity, the PCE decreased–the maximum obtained efficiency is19.02%.

Defect formation is a major challenge to control during fabrication. The effect of defect concentration was also studied in SnO_2 and the performance was studied using the C-V and MS plot. Even though the built-in potential is lower than the expected one, the capacitance changes with the defect concentrations. Thus reducing the donor concentration (N_D) to 1.0E+15 cm^{-3} at the perovskite/ETL interface can lead to a highly efficient PSC reaching 19.02% PCE with 66.78% as a FF at 1000W/m^2. With the decrease in donor density (N_D) concerning the intensity from 1000W/m^2 to 700W/m^2, accumulation of the charges decreases at the interface, resulting in decreased capacitance and variation in built-in voltage (V_{bi}).

Conflict of Interest: The authors declare no competing interests.

Ethical Clearance: Not applicable

Source of Funding: There is no funding for this article available.

References

1. Shahzad U. The Need For Renewable Energy Sources. 2015.
2. Fraas L, Partain L. Solar Cells: A Brief History and Introduction. Solar Cells and their Applications2010. p. 1-15.
3. Chapter 41 - Engineered Nanomaterials for Energy Applications. In: Mustansar Hussain C, editor. Handbook of Nanomaterials for Industrial Applications: Elsevier; 2018. p. 751-67.
4. Park J, Kim J, Yun H-S, Paik MJ, Noh E, Mun HJ, et al. Controlled growth of perovskite layers with volatile alkylammonium chlorides. Nature. 2023.
5. K. Rao M, Sangeetha DN, Selvakumar M, Sudhakar YN, Mahesha MG. Review on persistent challenges of perovskite solar cells' stability. Solar Energy. 2021;218:469-91.
6. Juarez-Perez EJ, Sanchez RS, Badia L, Garcia-Belmonte G, Kang YS, Mora-Sero I, et al. Photoinduced Giant Dielectric Constant in Lead Halide Perovskite Solar Cells. The journal of physical chemistry letters. 2014;5(13):2390-4.
7. Almora O, Garcia-Belmonte G. Light capacitances in silicon and perovskite solar cells. Solar Energy. 2019;189:103-10.
8. Samiul Islam M, Sobayel K, Al-Kahtani A, Islam MA, Muhammad G, Amin N, et al. Defect Study and Modelling of SnX3-Based Perovskite Solar Cells with SCAPS-1D. Nanomaterials [Internet]. 2021; 11(5).
9. Karthick S, Bouclé J, Velumani S. Effect of bismuth iodide (BiI3) interfacial layer with different HTL's in FAPI based perovskite solar cell – SCAPS – 1D study. Solar Energy. 2021;218:157-68.
10. Muhammed OA, Danladi E, Boduku PH, Tasiu J, Ahmad MS, Usman N. Modeling and Simulation of Lead-Free Perovskite Solar Cell Using SCAPS-1D. East European Journal of Physics. 2021;0(2):146-54.
11. Chen S, Liu T, Zheng Z, Ishaq M, Liang G, Fan P, et al. Recent progress and perspectives on Sb2Se3-based photocathodes for solar hydrogen production via photoelectrochemical water splitting. Journal of Energy Chemistry. 2022;67:508-23.
12. Coutinho NF, Cucatti S, Merlo RB, Silva Filho JMC, Villegas NFB, Alvarez F, et al. The Thermomechanical Properties of Thermally Evaporated Bismuth Triiodide Thin Films. Scientific Reports. 2019;9(1):11785.
13. Prathapani S, Bhargava P, Mallick S. Electronic band structure and carrier concentration of formamidinium–cesium mixed cation lead mixed halide hybrid perovskites. Applied Physics Letters. 2018;112(9):092104.
14. Lee LC, Huq TN, MacManus-Driscoll JL, Hoye RLZ. Research Update: Bismuth-based perovskite-inspired photovoltaic materials. APL Materials. 2018;6(8):084502.
15. Brandt RE, Stevanović V, Ginley DS, Buonassisi T. Identifying defect-tolerant semiconductors with high minority-carrier lifetimes: beyond hybrid lead halide perovskites. MRS Communications. 2015;5(2):265-75.
16. Han H, Hong M, Gokhale SS, Sinnott SB, Jordan K, Baciak JE, et al. Defect Engineering of BiI3 Single Crystals: Enhanced Electrical and Radiation Performance for Room Temperature Gamma-Ray Detection. The Journal of Physical Chemistry C. 2014;118(6):3244-50.
17. Partain L. Solar Cell Device Physics. Solar Cells and their Applications2010. p. 67-109.
18. Bisquert J, Garcia-Belmonte G, Munar A, Sessolo M, Soriano A, Bolink HJ. Band unpinning and photovoltaic model for P3HT:PCBM organic bulk heterojunctions under illumination. Chemical Physics Letters. 2008;465(1):57-62.
19. Nolasco JC, Sánchez-Díaz A, Cabré R, Ferré-Borrull J, Marsal LF, Palomares E, et al. Relation between the barrier interface and the built-in potential in pentacene/C60 solar cell. Applied Physics Letters. 2010;97(1):013305.
20. Ray D, Burtone L, Leo K, Riede M. Detection of trap charge in small molecular organic bulk heterojunction solar cells. Physical Review B. 2010;82(12):125204.
21. Boix PP, Garcia-Belmonte G, Muñecas U, Neophytou

M, Waldauf C, Pacios R. Determination of gap defect states in organic bulk heterojunction solar cells from capacitance measurements. Applied Physics Letters. 2009;95(23):233302.

22. Mingebach M, Deibel C, Dyakonov V. Built-in potential and validity of the Mott-Schottky analysis in organic bulk heterojunction solar cells. Physical Review B. 2011;84(15):153201.
23. Hosenuzzaman M, Rahim NA, Selvaraj J, Hasanuzzaman M, Malek ABMA, Nahar A. Global prospects, progress, policies, and environmental impact of solar photovoltaic power generation. Renewable and Sustainable Energy Reviews. 2015;41:284-97.
24. Malliaras GG, Salem JR, Brock PJ, Scott C. Electrical characteristics and efficiency of single-layer organic light-emitting diodes. Physical Review B. 1998;58(20):R13411-R4.
25. p-n Junctions. Physics of Semiconductor Devices2006. p. 77-133.
26. Garcia-Belmonte G, Munar A, Barea EM, Bisquert J, Ugarte I, Pacios R. Charge carrier mobility and lifetime of organic bulk heterojunctions analyzed by impedance spectroscopy. Organic Electronics. 2008;9(5):847-51.
27. Decock K, Khelifi S, Burgelman M. Modelling multivalent defects in thin film solar cells. Thin Solid Films. 2011;519(21):7481-4.
28. Zonno I, Martinez-Otero A, Hebig J-C, Kirchartz T. Understanding Mott-Schottky Measurements under Illumination in Organic Bulk Heterojunction Solar Cells. Physical Review Applied. 2017;7(3):034018.
29. Burgelman ANaM. Numerical modelling of ac-characteristics of CdTe and CIS solar cells. In: Proceedings of the 25th IEEE Photovoltaic Specialists Conference, IEEE, New York. 1996:4.