American Journal of Materials Research
2018; 5(2): 30-34
http://www.aascit.org/journal/ajmr
ISSN: 2375-3919

American Association for Science and Technology

Simulation of core@shell Type II Solar Cell by SILVACO ATLAS Software

Masood Mehrabian[1, *], Elham Mirzapoor[2], Mohammadreza Akbarpour[2]

[1]Department of Physics, Faculty of Basic Science, University of Maragheh, Maragheh, Iran
[2]Department of Materials Engineering, Faculty of Engineering, University of Maragheh, Maragheh, Iran

Email address
masood.mehrabian@yahoo.com (M. Mehrabian), masood.mehrabian@maragheh.ac.ir (M. Mehrabian)
[*]Corresponding author

Citation
Masood Mehrabian, Elham Mirzapoor, Mohammadreza Akbarpour. Simulation of core@shell Type II Solar Cell by SILVACO ATLAS Software. *American Journal of Materials Research.* Vol. 5, No. 2, 2018, pp. 30-34.

Received: January 7, 2018; **Accepted**: January 22, 2018; **Published**: February 27, 2018

Abstract: A numerical simulation is performed to characterize the power conversion efficiency of a PbS Quantum Dot sensitized solar cell and a solar cell containing of type-II semiconductor core shell layer. Simulation results showed much higher efficiency for a core-shell solar cell as compared to PbS QD sensitized solar cells, reaching an overall efficiency of 3.5% under simulated solar illumination (AM1.5, 100 $mW\cdot cm^{-2}$). In addition, simulation results in this work demonstrated that the shell effectively could passivate the surface traps on PbS, resulting in highly improved in the short-circuit current density. Therefore, presented approach in present simulation provides a new method for simulation of high performance core-shell solar cells.

Keywords: PbS QD, Core Shell Type II, Photovoltaic, Simulation

1. Introduction

Quantum dots (QDs) have attracted much attention due to their unique optical properties, size-dependent band gap tenability, cost-effective solution process ability, and stability which make them attractive candidates for optoelectronic applications. QDs have large surface to volume ratio which leads to create many defect states at the surface that turns to cause of charge trapping [1]. Due to charge recombination at the interface of the quantum dots, QDSSCs still show limited power conversion efficiencies. This considerably affects the photovoltaic performance of the devices.

Lead sulfide (PbS) is a p-type semiconductor with large Bohr radius of 20 nm and wide band gap tuning range of 0.4 eV (Bulk) to 1.3 eV (D~3.7 nm) [2-4]. Its tunable band gap energy across the near infrared region (NIR) of the solar spectrum makes it good candidate for solar cell applications. Partial passivation arising from organic ligands, the incomplete bonds remaining on the QDs surface, may act as carrier trapping sites which downgrade the solar cell performance [5]. Inorganic materials such as CdSe and ZnS are known to provide more complete passivation for the QD surface [6].

In present work, a QDSSC with ITO/ZnO/PbS QD/Au structure, denoted as reference cell, is simulated by using SILVACO-ATLAS software. Then for the first time a new model to simulate a solar cell containing of core-shell structure (PbS@CdSe) is proposed. Finally the thickness of core-shell layer is optimized so that a maximum power conversion efficiency is reached.

The effects of the photo generation rate, electron and hole concentrations, and thickness of core-shell layer on the photovoltaic properties is studied.

It is shown that the CdSe shell reduces interface recombination and provides additional photo-generated carriers, resulting in significantly higher photovoltaic properties for ITO/ZnO/PbS@CdSe/Au solar cells in comparison to reference cell.

2. Method

Figure 1 (a) depicts the cross section scanning electron microscopy (SEM) of PbS QDSSC (reference cell). The schematic representation of reference cell and SEM image of PbS

QDs are depicted in Figure 1 (b) and (c), respectively. Compared to the commonly reported PbS QDSSCs, a CdSe shell on the PbS core was introduced to make a core-shell structure.

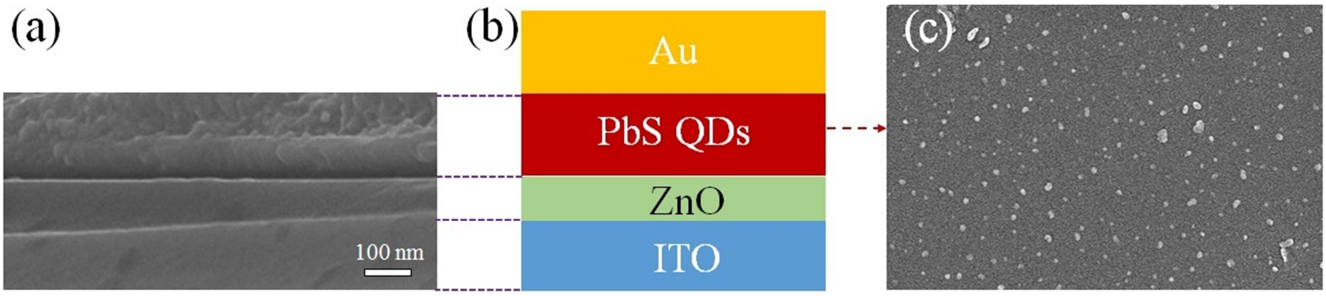


Figure 1. *(a) SEM cross-sectional image, (b) schematic of reference solar cell, and (c) SEM image of PbS QDs.*

2.1. Simulation

The simulation of reference cell was performed at room temperature (27°C) and under standard terrestrial solar spectral irradiance distribution (AM 1.5). The Current density-voltage (J-V) characteristics of reference device obtained using ATLAS is shown in Figure 2(a).

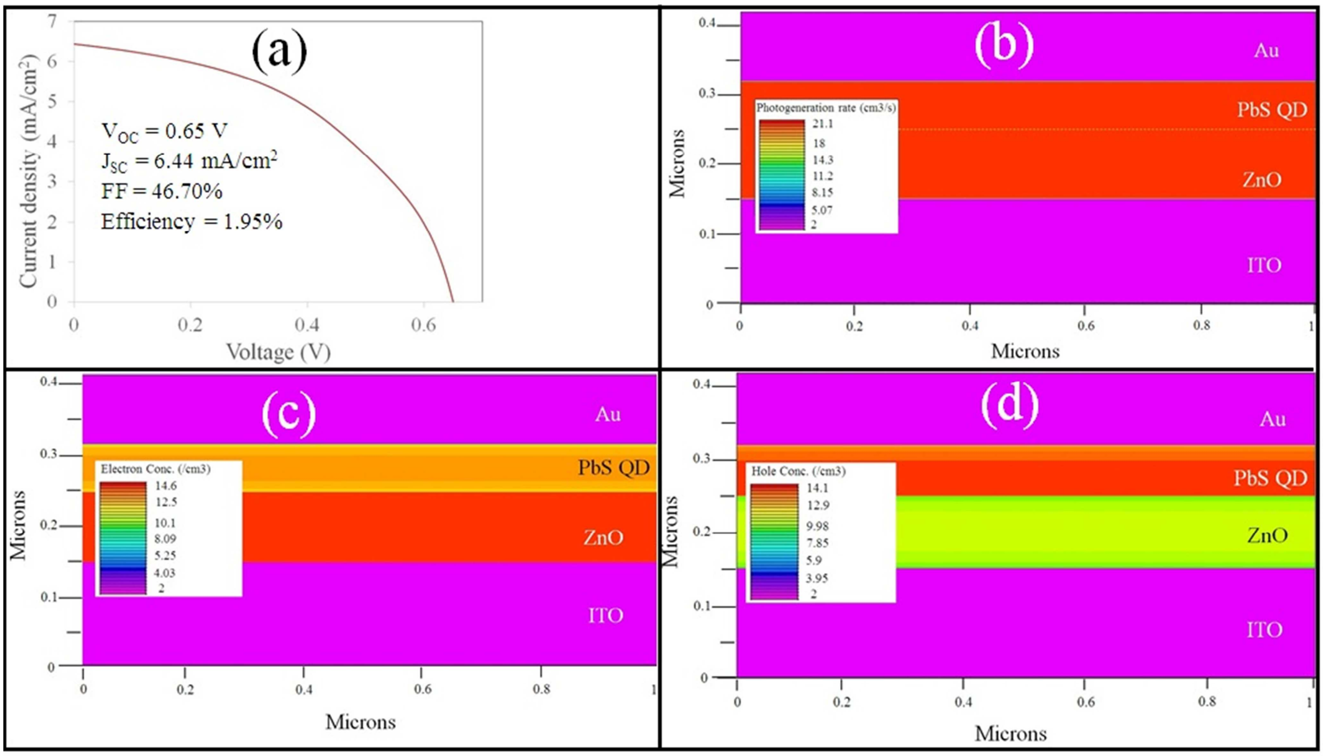


Figure 2. *(a) J-V curve and characteristics, (b) Photo-generation rate, (c) Electron concentration, (d) Hole concentration, in reference cell.*

Photo-generation (PG) rate diagram for reference device is shown in Figure 2(b). The maximum PG rate of 21.1 (/cm^3 s) was obtained in the PbS QD and ZnO layers, because they have band gaps of 1.3 and 3.3 eV, respectively.

The electron concentration is the number of electrons in the conduction band in material, and is shown in Figure 2(c). It was found that the maximum electron concentration of 14.6 (/cm^3) is related to ZnO-PbS interface. That means in this device, due to the existence of *surface defects*, photo excited electrons couldn't be injected efficiently into a large band gap background semiconductor (ZnO). A similar phenomenon is happening for holes, as shown in Figure 2(d).

2.2. Improving the Photovoltaic Performance

To improve the photovoltaic performance, staggered gap structure (type-II) of PbS/CdSe QDSCs for broad light absorption and efficient carrier extraction was studied. As shown in Figure 3(c), in staggered gap structure, the band gap of one semiconductor overlaps the other one. The minimal conduction band (CB) edge in the CdSe shell and maximal valence band (VB) edge in the PbS core, resulting in smaller band gap of for a broad absorption spectrum. The corresponding energy band gap of core-shell structure is determined by the CB edge of one semiconductor and the VB edge of the other semiconductor (CB2-VB1). The energy level positions of materials existing in both reference cell and PbS@CdSe solar cell are shown in Figure 3(a), (b), consistent with multiple literature reports [7-9]. The defect mediation effect of a CdSe shell on the PbS electronic structure is depicted in Figure 3(b).

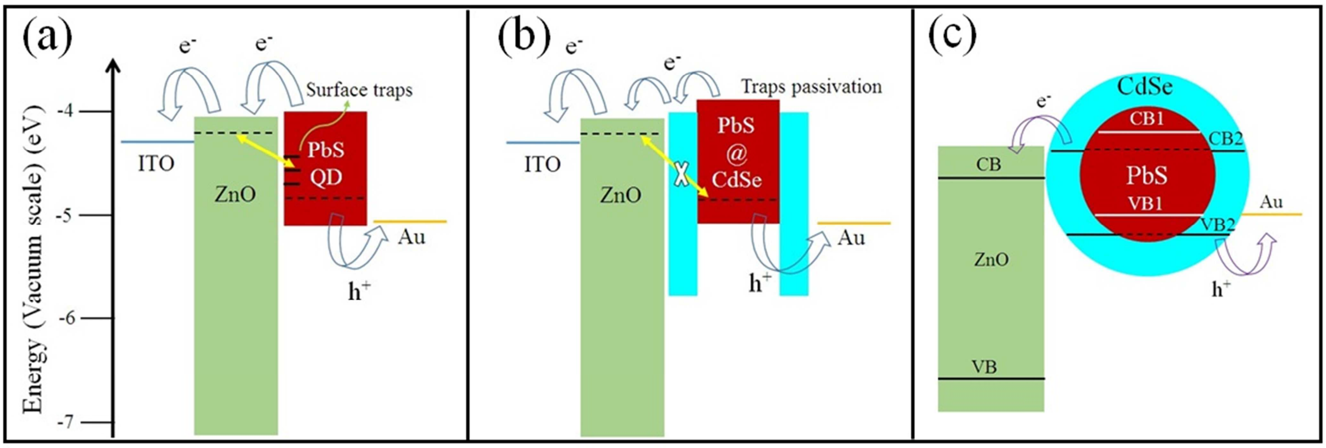


Figure 3. *Schematic representation of band alignment of (a) reference device, (b) the hetero-junction core-shell cell, and (c) type-II hetero-junction structure.*

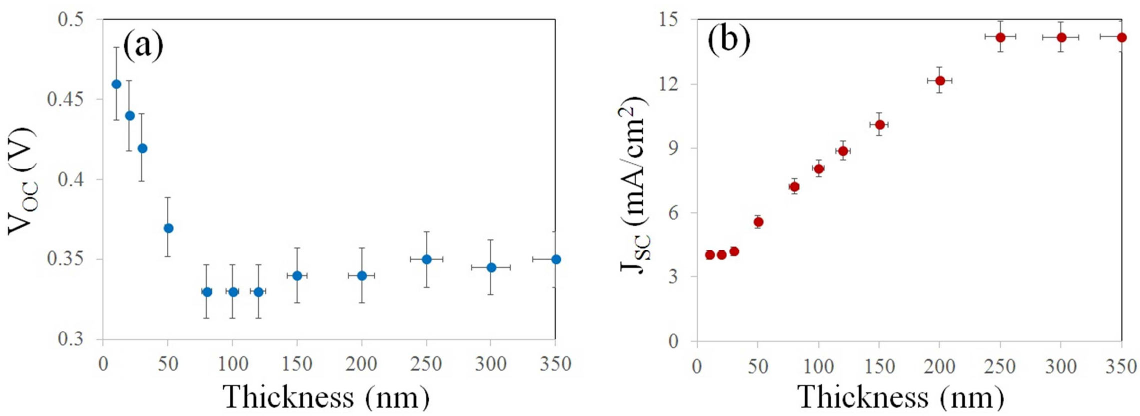
3. Result

To study the effect of thickness of core-shell layer on the performance of solar cells, devices with different thicknesses of core-shell layer were simulated under an illumination of one sun (AM 1.5 G, 100 mW/cm^2). The device performance statistics are listed in Table 1.

Table 1. *Photovoltaic properties of core-shell solar cell with different thicknesses of active layer.*

Layer thickness (nm)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	η (%)
10	0.460	4.03	71	1.36
20	0.440	4.04	70	1.26
30	0.420	4.21	65	1.16
50	0.370	5.58	50	1.06
80	0.330	7.23	57	1.40
100	0.330	8.08	64	1.70
120	0.330	8.90	67	2.01
150	0.340	10.13	69	2.37
200	0.340	12.18	71	2.99
250	0.350	14.22	71	3.50
300	0.345	14.20	70	3.46
350	0.350	14.22	71	3.50

Using the same layers of device, a series of core/shell with different thicknesses were simulated. Figure 4 shows 12 device performance metrics that demonstrate the effect of layer thickness on the photovoltaic properties.



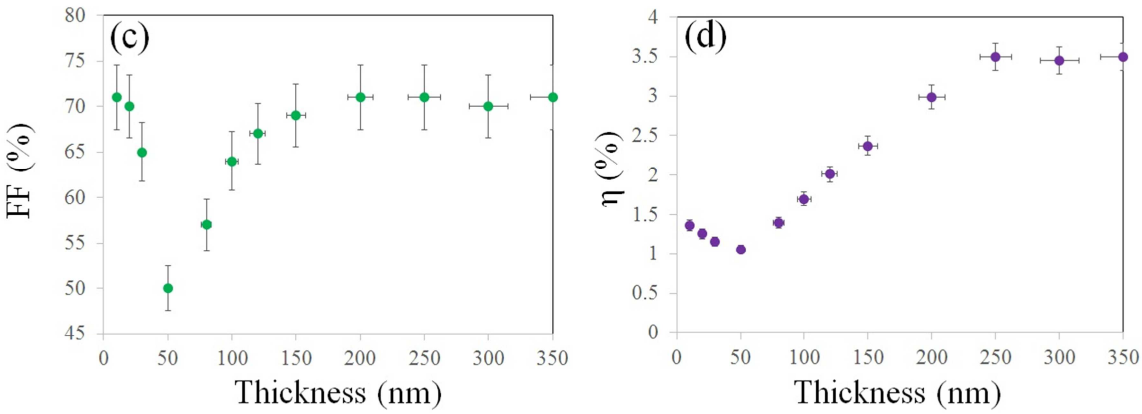


Figure 4. *(a) Open-circuit voltage, (b) Short-circuit current density, (c) Fill Factor, and (d) Power conversion efficiency versus thickness of core- shell absorber layer.*

External quantum efficiency (EQE) of reference device as a function of wavelength is shown in figure 5, which is around 70% peak (~ 60% average) and the photo-response extends to 1000 nm.

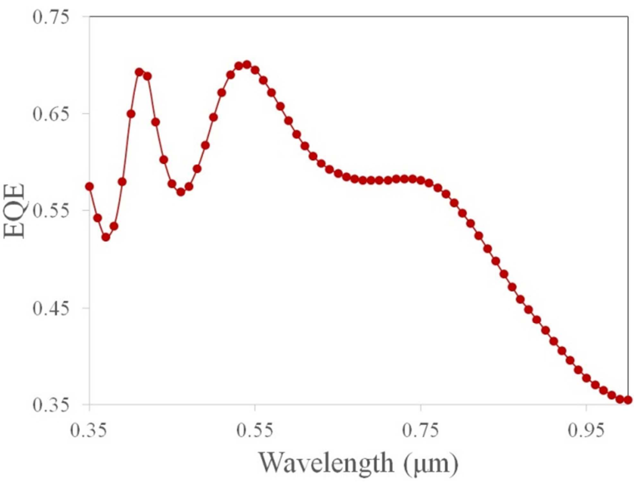


Figure 5. *The EQE spectrum of reference device with ITO/ZnO/PbS QD/Au structure.*

It could be concluded that photons in the range of 375-950 nm (corresponding to 3.30-1.3 eV) are converted and extracted more efficiently as light is absorbed in ZnO and PbS QD layers, respectively. The EQE peak at short wavelength region (375 nm) corresponds to the absorption by ZnO layer, while at long wavelength (~ 800 nm) corresponds to the absorption by active layer (PbS QD).

4. Discussion

These results show that increasing the thickness light absorber layer from 10 to 80 nm leads to increase in J_{SC} and decrease in V_{OC}, respectively. Decrease in V_{OC} refers to increase in surface recombination at the interface, while increase in J_{SC} relates to increasing light absorption and electron-hole pair separation.

For thicknesses thicker than 250 nm, the J_{SC} and V_{OC} are almost flat. That means the maximum charge carrier separation may occur through this thickness of layer. In this thickness, the power conversion efficiency reaches to its maximum value (3.5%).

It was reported that a reduction of surface trap density increases VOC by using density functional theory simulations [10]. It could be concluded that at 250 layer thickness, the surface passivation is complete. That is, in such thickness, each PbS core surface is fully bonded by CdSe shell. Thus, additional layer thickness does not lead to a substantial increase in passivation and VOC remains almost constant.

The photovoltaic characteristics reveals that although the short-circuit current (J_{SC}) is substantially lower for core-shell solar cell with thickness of less than 50 nm, but VOC of the non-shelled PbS device is higher than core-shell device by more than 0.19 V.

Moving from a PbS to a PbS@CdSe core-shell with 250 nm core-shell layer thickness resulted in a 7.78 mA/cm^2 change in J_{SC}, which confirms that this improvement originates from the core-shell passivation strategy.

In spite of the lower V_{OC} in core-shell structure, FF and J_{SC} are still large enough to produce a promising efficiency, which may result from an excellent passivation of interface defects.

5. Conclusion

In conclusion, the performance of PbS QDSSCs was improved by introducing a CdSe shell, and optimized the thickness of core-shell layer. The 250 nm core-shell layer enhanced the device JSC, FF, and η. These improvements was ascribed to the optimized passivation of interface traps of PbS by the CdSe shell layer, and additional photo generated carriers in the CdSe layer. Simulation findings in present work proves that type-II staggered structure could br served as highly efficient hetero structure for photovoltaic and optoelectronic devices.

References

[1] K. Szendrei, M. Speirs, W. Gomulya, D. Jarzab, M. Manca, O. V. Mikhnenko, M. Yarema, B. J. Kooi, W. Heiss, M. A. Loi, Adv. Funct. Mater. *22*, 1598-1605, (2012).

[2] Bo Hou, Yuljae Cho, Byung Sung Kim, John Hong, Jong Bae Park, Se Jin Ahn, Jung Inn Sohn, SeungNam Cha, and Jong Min Kim, Highly Monodispersed PbS Quantum Dots for Outstanding Cascaded-Junction Solar Cells, ACS Energy Lett. 1, 834-839, (2016).

[3] Weizhe Xu, Furui Tan, et al. Efficient PbS QD solar cell with an inverted structure, Solar Energy Materials & Solar Cells 159, 503-509, (2017).

[4] M. Kamruzzaman and J A. Zapien, Synthesis and characterization of ZnO/ZnSe NWs/PbS QDs solar cell, J Nanopart Res, 19: 125, (2017).

[5] A. J. Labelle, K. W. Chou, A. Amassian, E. H. Sargent, *Nat. Nanotechnol. 7*, 577-582, (2012).

[6] M. V. Kovalenko, R. D. Schaller, D. Jarzab, M. A. Loi, D. V. Talapin, *J. Am. Chem. Soc. 134*, 2457-2460, (2012).

[7] Darren C. J. Neo, Cheng Cheng, Samuel D. Stranks, Simon M. Fairclough, Judy S. Kim, Angus I. Kirkland, Jason M. Smith, Henry J. Snaith, Hazel E. Assender, and Andrew A. R. Watt, Influence of Shell Thickness and Surface Passivation on PbS/CdS Core/Shell Colloidal Quantum Dot Solar Cells, Chem. Mater. 26, 4004-4013, (2014).

[8] Andras G. Pattantyus-Abraham, Illan J. Kramer, Aaron R. Barkhouse, Xihua Wang, Gerasimos Konstantatos, Ratan Debnath, Larissa Levina, Ines Raabe, Mohammad K. Nazeeruddin, Michael Gratzel, and Edward H. Sargent, Depleted-Heterojunction Colloidal Quantum Dot Solar Cells, American Chemical Society, 4 (6), 3374-3380 (2010).

[9] Joseph M. Luther, Jianbo Gao, Matthew T. Lloyd, Octavi E. Semonin, Matthew C. Beard, and Arthur J. Nozik, Stability Assessment on a 3% Bilayer PbS/ZnO Quantum Dot Heterojunction Solar Cell, Adv. Mater. 22, 3704-3707, (2010).

[10] Yoon, W.; Boercker, J. E.; Lumb, M. P.; Placencia, D.; Foos, E. E.; Tischler, J. G. Enhanced Open-Circuit Voltage of PbS Nanocrystal Quantum Dot Solar Cells. Sci. Rep. 3, (2013).