



Performance Analysis of PbS Colloidal Quantum Dot Solar Cell at Different Absorption Coefficient

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ABSTRACT

This paper is based on the modelling of absorption model for PbS colloidal quantum dot solar cell using SCAPS. The main objective is to predict the best absorption coefficient (cm^{-1}) for the PbS colloidal quantum dot (CQD) at which the solar cell performance can be improved. In the present work, the modelling and simulation have been performed for the five different absorption model included in CQD layer and obtained different performance parameter such as open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), fill factor (FF), quantum efficiency (QE) and power conversion efficiency (PCE). The best absorption coefficient (cm^{-1}) is 10^5 having V_{oc} , J_{sc} , FF, QE and PCE (quantum efficiency) values are 1.64V, 7.6 mA/cm², 0.91%, 47.2% and 0.62% respectively. The quantum efficiency significantly changes with the absorption coefficient (cm^{-1}) for the 250nm to 1050nm wavelength range.

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1. Introduction

The incredible supply of solar energy is received by earth through the sun (Askari Mohammad Bagher, 2016). Solar power is a renewable resource that is freely available. A solar cell is a type of electrical device that uses the sun energy i.e. light and converts directly into the electricity. The conversion of sun energy (light) into electricity is caused by the phenomenon of photovoltaic effect, which is a chemical and physical phenomenon (Shruti Sharma et al., 2015). The solar cell material have some property in order to absorb sunlight. There are basically two configuration of solar cell. The conventional solar cells can use light absorbing material as one single layer or can use multiple physical configuration for various charge separation and absorption mechanism (Askari Mohammad Bagher et al., 2015). The solar can be categorized into first, second and third generation solar cells (Manjot Kaur and Harjit Singh, 2016). Polysilicon and monocrystal line silicon materials are included in the first generation solar cell. First generation solar cell are also known as traditional, conventional or wafer based solar cells (Kiran Ranabhat et al., 2016, Kiran Ranabhat et al., 2013). Second generation cells are thin film solar cell, that includes CdTe, CIGS and amorphous silicon. It avoid the use of silicon wafer and have lower consumption of material (Yongye Liang et al., 2010, Rasika Ganvir, 2016). Third generation solar cells made up of organic materials such as polymer or small molecules. Dye sensitized and perovskite cells are also used in the

third generation (Nandi Wu et al., 2017, A.B. Djuricic et al., 2017, Di Zhou et al., 2018).

Quantum dots which is working as the absorbing photovoltaic material used in quantum dot solar cell (QDSCs) (Lan X et al., 2016). In this paper, lead chalcogenide (PbS) CQD as the absorbing photovoltaic material is used (ZhenweiRen et al., 2017). Colloidal quantum dots (CQDs) used in photovoltaic and optoelectronic devices for wide application such as solar cells, photo detectors and light emitting diodes due to their low temperature fabrication, low cost, high stability and their peculiar photovoltaic and optoelectronic properties (Tianshuo Zhao et al., 2016). CQDs are also attracted much attention for their solution based processing which is advantageous for their integration into the variety of the solar cells (Chuang et al., 2014, Xiaoliang Zhang and Erik M. J. Johansson, 2017).

In this work, the solar cell CQD are constructed with the three different layer i.e. p-type CQDs as the absorbing layer, MZO (MgZnO) as the buffer layer and n-type metal oxide layer (such as ZnO). The absorption coefficient (cm^{-1}) is defined in the PbS CQD-TBAI layer and improved performance of the CQDs solar cell with respect to absorption coefficient is simulated. To enhance the quantum efficiency through selecting the best absorption coefficient, there is construction and comparison of different absorption model for PbS-TBAI CQD layer and calculated the V_{oc} , J_{sc} , FF, QE and PCE.

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2. Materials and Methods

2.1 A Single Solar Cell Model

A CQD solar cell device architecture with a buffer layer (BL) of MZO is shown in Figure 1 (Xiaoliang Zhang and Erik M. J. Johansson, 2017, G. H. Kim et al., 2015, M. Liu et al., 2016). The ZnO layer is firstly deposited on the surface of a cleaned FTO glass with a thickness of ~40 nm and subsequently there is a deposition of MZO layer with a thickness of ~20nm. The deposition of CQD is on the surface of MZO layer and this layer working as a light absorber layer in solar cell device. With the bilayer of tetrabutyl ammonium iodide (TBAI) and 1,2-ethanedithiol (EDT) performance of PbS QDs improved and result in higher signal to noise ratio (SNR), broader linear dynamic range (LDR), several times faster light response and many times higher detectivity (Zhenwei Ren et al., 2017). Finally, the device designing completed with the thermally deposition of an electrode that is Au on the top of the surface of the CQD-EDT layer as shown in figure 1 (Xiaoliang Zhang and Erik M. J. Johansson, 2017). The device become different and more efficient by the adding the absorption model in the PbS-TBAI material.



Figure 1: Architecture of single CQD solar cell device

2.2 Materials Parameter

The materials parameter used for the simulation is tabulated in following table 1 (Xiaoliang Zhang and Erik M. J. Johansson, 2017, G. H. Kim et al., 2015, M. Liu et al., 2016).

Table 1: Details of Material parameter in SCAPS simulation.

Part of these material parameter are taken from literature (Xiaoliang Zhang and Erik M. J. Johansson, 2017, G. H. Kim et al., 2015, M. Liu et al., 2016).

	PbS-EDT	PbS-TBAI	ZnO (or MZO)
Thickness (nm)	50	230	60(40+20)
Bandgap edge (eV)	1.2	1.2	3.2(or up shift)
Electron affinity (eV)	3.9	4.15	4.3
Permittivity (er)	20	20	66
CB/VB DOS (cm ⁻³)	10 ¹⁹	10 ¹⁹	10 ¹⁹
Electron mobility (cm ² /Vs)	2x10 ⁻⁴	2x10 ⁻²	5x10 ⁻²
Ndonor (cm ⁻³)	10 ¹⁴	10 ¹⁵	10 ¹⁷
Nacceptor (cm ⁻³)	10 ¹⁶	10 ¹⁵	0
Radiative recombination coefficient (cm ³ /s)	10 ⁻³		
EDT/TBAI defect (neutral)	Total density (integrated over all energies) (cm ⁻²): 10 ¹⁶		
Capture cross section (cm ²)	1.2x10 ⁻¹³	1.2x10 ⁻¹³	
Position below Ec (eV)	0.5	0.5	
Density (cm ⁻³)	10 ¹⁶	10 ¹⁷	
TBAI-ZnO interface defects (neutral)	Total density (integrated over all energies) (cm ⁻²): 10 ¹⁶		
Capture cross section (cm ²)	10 ⁻¹⁹		
Position above Ev (eV)	0.6		
Density (cm ⁻³)	10 ¹⁶		

G. H. Kim et al., 2015, M. Liu et al., 2016).

In these parameter there are two most important parameter which are added in this work. The first parameter is radiative recombination coefficient and second parameter is absorption coefficient. The current is converted from the p-contact hole current to the n-contact electron current in diode. It shows that somewhere in the diode recombination must take place. So the recombination should define at least one place (in a layer, at a contact or at an interface) in the diode.

The absorption coefficient (α) can be set from an experimental data file or from a model. The absorption coefficient for PbS CQD material is 10⁵ (cm⁻¹). The $\alpha(\lambda)$ can be measured using the following equation (Jaymin Ray et al., 2017);

$$\alpha(\lambda) = \left(A + \frac{B}{h\nu} \right) \sqrt{h\nu - E_g} \quad (1)$$

where α , $h\nu$ and E_g are absorption coefficient (cm⁻¹), photon energy (eV) and energy band gap (eV) respectively. A and B are wavelength dependent absorption constant.

3. Result and Discussion

In order to improve the system there are different calculation for different absorption coefficient to explore its performance under various operative conditions. In this work the model is simulated at five absorption coefficient (cm⁻¹) i.e. at 10³, 10⁴, 10⁵, 10⁶ and 10⁷ respectively which is added in PbS-CQD layer. The calculation is made under dark and light illumination. In the dark illumination calculation the working point voltage is zero. In the light illumination the simulation is done at the open circuit voltage (V_{oc}). At the five absorption coefficient (cm⁻¹) i.e. 10³, 10⁴, 10⁵, 10⁶ and 10⁷ there are different measurement which is tabulated in table 2.

Table 2: Different calculated value (V_{oc} , J_{sc} , FF and QE) for the different absorption file.

Absorption Coefficient	V_{oc} (V)	J_{sc} (mA/cm ²)	FF	QE (%)	PCE (%)
10 ³ (cm ⁻¹)	1.89	0.177	0.92	2.78	0.02
10 ⁴ (cm ⁻¹)	1.8	1.58	0.92	18.34	0.17
10 ⁵ (cm ⁻¹)	1.64	7.6	0.91	47.2	0.62
10 ⁶ (cm ⁻¹)	3.53	17.51	0.95	89.39	2.47
10 ⁷ (cm ⁻¹)	7.14	25.85	0.97	98.98	4.56

The first simulation of the system is with the 10³ absorption coefficient (cm⁻¹) in PbS-CQD layer and get the value of V_{oc} and J_{sc} 1.89V and 0.177 mA/cm² respectively. The voltage at which no current flows through the external circuit is known as open circuit voltage (V_{oc}) (Jizhong Yao et al., 2015). The calculation of FF from V_{oc} is done by the following equation (Nandi Wu et al., 2017):

$$FF = \frac{voc - \ln(voc + 0.72)}{voc + 1} \quad (2)$$

$$\text{In which, } voc = \frac{voc}{(mkB \frac{T}{q})}$$

Therefore, from the Eq.(2), the value of FF is 0.9284. The quantum efficiency graph for 10³ absorption coefficient (cm⁻¹) is plotted with open circuit voltage i.e. 1.89V.

The second simulation of the system is with the 10⁴ absorption coefficient (cm⁻¹) in PbS-CQD layer and get the value of V_{oc} , J_{sc} and FF 1.8V, 1.58 mA/cm² and 0.9256 respectively. Again the quantum efficiency graph for 10⁴ absorption coefficient (cm⁻¹) is plotted with the open circuit voltage of 1.8V (V_{oc}).

The third simulation with 10⁵ absorption coefficient (cm⁻¹) is consider. After the simulation, value of V_{oc} and J_{sc} are 1.64V and 7.6 mA/cm² respectively are obtained. The quantum efficiency is simulated with open circuit voltage of 1.64V. The FF at 10⁵ absorption coefficient (cm⁻¹) is 0.9198.

Fourth simulation is with 10⁶ absorption coefficient (cm⁻¹) and again after simulating, the value of V_{oc} and J_{sc} are 3.53V and 17.51 mA/cm² respectively are obtained. The FF at 10⁶ absorption coefficient (cm⁻¹) is 0.9569. The quantum efficiency graph for 10⁴ absorption coefficient (cm⁻¹) is plotted with open circuit voltage i.e. 3.53 V.

Fifth simulation is with 10⁷ absorption coefficient (cm⁻¹). After simulating, the value of V_{oc} and J_{sc} are 7.14V and 25.85 mA/cm² respectively are obtained. The FF at 10⁷ absorption coefficient (cm⁻¹) is 0.9761. The quantum efficiency graph for 10⁵ absorption coefficient (cm⁻¹) is plotted with open circuit voltage i.e. 7.14 V.

Figure 2 shows the comparison of different quantum efficiency with different absorption coefficient (cm^{-1}) i.e. 10^3 , 10^4 , 10^5 , 10^6 & 10^7 respectively with their corresponding V_{oc} .

When there is no connection of solar cell to the any load then there is no current flowing and voltage across the solar cell becomes maximum. This is known as open circuit voltage (V_{oc}). Changing the absorption coefficient the V_{oc} are also changed. Figure 3 shows the effect of V_{oc} at different absorption coefficient, there are five absorption coefficients (cm^{-1}) taken, which are 10^3 , 10^4 , 10^5 , 10^6 & 10^7 respectively.

The changes in J_{sc} over different absorption coefficient is summarizing in figure 4.

The fill factor is a measure of quality of solar cell essentially. The FF is also defined as the ratio of maximum power from actual solar cell to the maximum power to the ideal solar cell (A.B. Djurisic et al., 2017). The value of FF with different absorption coefficient $10^3, 10^4, 10^5, 10^6$ and 10^7 are different which are shown by figure 5.

The absorption of photon is more readily in the material which have the higher absorption coefficient, therefore electrons are excited into the conduction band. In this work, the power conversion efficiency (PCE) of the QDSCs is gradually increases from the lower absorption coefficient to the higher absorption coefficient and it shown in figure 6.

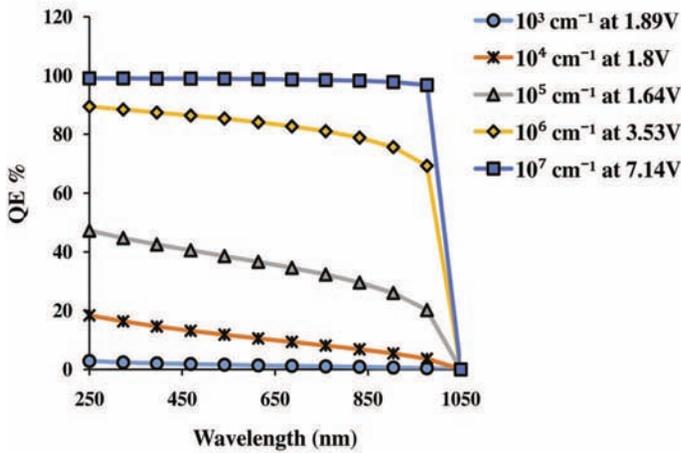


Figure 2: Comparison of different quantum efficiency with different absorption coefficient (cm^{-1}) i.e. 10^3 , 10^4 , 10^5 , 10^6 & 10^7 respectively with their corresponding V_{oc} .

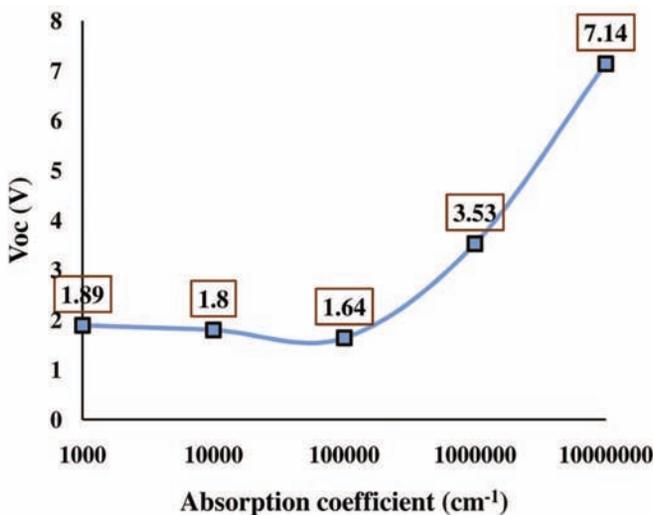


Figure 3: Measurement of V_{oc} with different absorption coefficient.

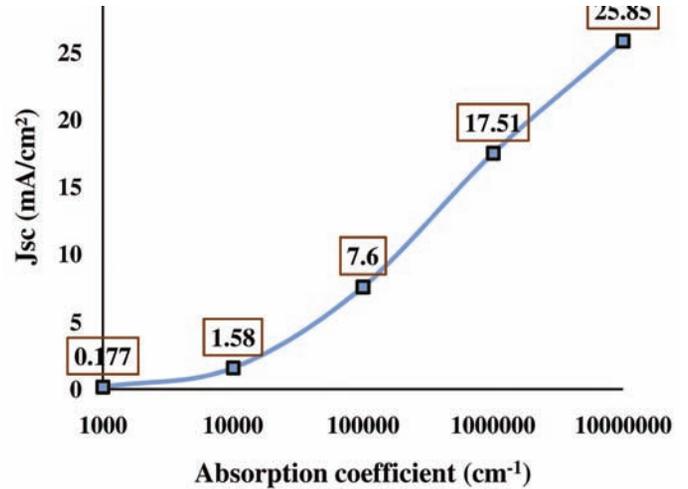


Figure 4: Measurement of J_{sc} with different absorption coefficient.

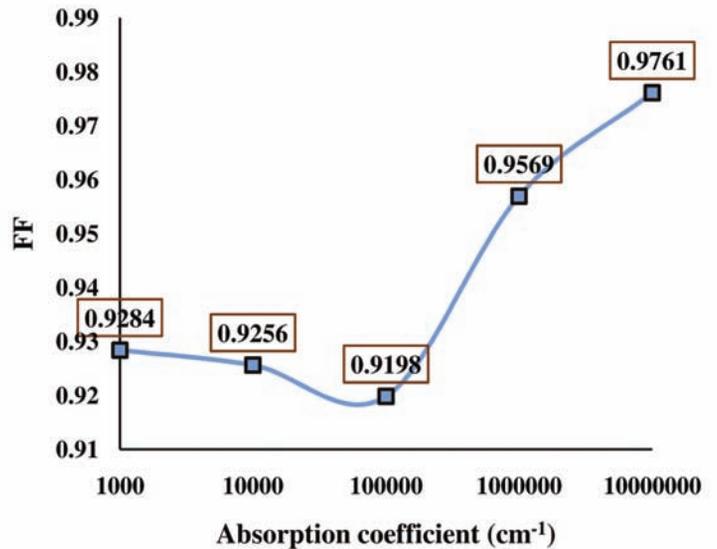


Figure 5: Measurement of FF with different absorption coefficient.

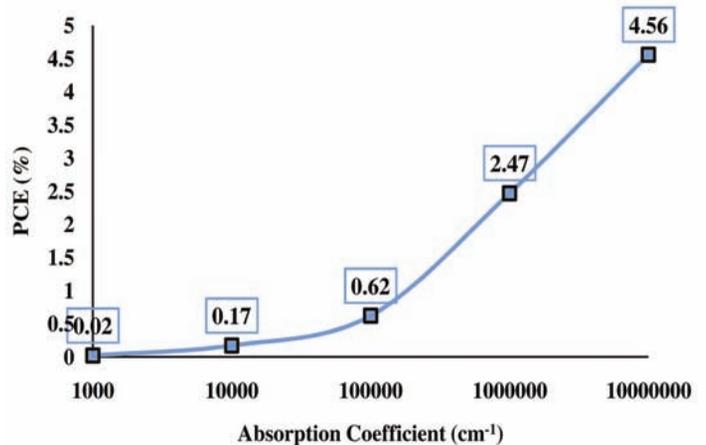


Figure 6: Measurement of PCE with different absorption coefficient

4. Conclusions

In this study, the improved performance parameter of solar cell have been calculated using the different absorption coefficient. The value of V_{oc} , J_{sc} , FF and QE vary with the different absorption model including in particular material or layer of solar cell. The different absorption model have been added in quantum dot layer of PbS-TBAI and shows their corresponding results. The best absorption coefficient (cm^{-1}) is 10^3 having V_{oc} , J_{sc} , FF and QE (quantum efficiency) values are 1.64 V, 7.6 mA/cm², 0.91 and 47.2%, respectively. By introducing the absorption model the efficiency of solar cell is improved significantly. In this work there are five absorption model with five absorption coefficient (cm^{-1}) i.e. 10^3 , 10^4 , 10^5 , 10^6 and 10^7 and simulating these value at different voltage. The quantum efficiency for 10^3 , 10^4 , 10^5 , 10^6 and 10^7 are 2.78%, 18.34%, 47.2%, 89.39% and 98.98% respectively.

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References

- [1] Askari Mohammad Bagher, (2016) "Solar Cell Quantum Dots", American Journal of Renewable and Sustainable Energy Vol. 2, No. 1, pp. 1-5
- [2] Shruti Sharma, Kamlesh Kumar Jain, Ashutosh Sharma, (2015), "Solar Cells: In Research and Applications-A Review", Materials Sciences and Applications, 6, 1145-1155
- [3] Askari Mohammad Bagher, Mirzaei Mahmoud AbadiVahid, Mirhabibi Mohsen, (2015) "Types of Solar Cells and Application", American Journal of Optics and Photonics; 3(5), 94-113
- [4] Manjot Kaur, Harjit Singh, , (2016), "A Review: Comparison Of Silicon Solar Cells And Thin Film Solar Cells", International Journal Of Core Engineering & Management (IJCEM), Vol. 3, Issue 2.
- [5] KiranRanabhat, LeeVPatrikeev, Aleksandra Antal, Kirill Andrianov, Valerii Lapshinsky Frumkin, Elena Sofronova, (2016), "An Introduction To Solar Cell Technology", Journal of Applied Engineering Science 14, 4, 405
- [6] Andrew Blakersa, NgweZina , Keith R. McIntoshb, Kean Fong, (2013), " High Efficiency Silicon Solar Cells", Energy Procedia, 33,1 – 10
- [7] Yongye Liang, ZhengXu, Jiangbin Xia, Szu-Ting Tsai, Yue Wu, Gang Li, Claire Ray, and Luping Yu, (2010), "For the Bright Future-Bulk Heterojunction Polymer Solar Cells with Power Conversion Efficiency of 7.4%", Adv. Mater., 22, E135–E138
- [8] Rasika Ganvir, (2016) "Modelling of the Nanowire CdsCdTe Device Design for Enhanced Quantum Efficiency in Window Absorber Type Solar Cells".
- [9] NandiWu, YiliangWu, Daniel Walter, Heping Shen,The Duong, Dale Grant, ChogBarugkin, Xiao Fu, Jun Peng, Thomas White, Kylie Catchpole, and Klaus Weber, (2017) "Identifying the Cause of Voltage and Fill Factor Losses in Perovskite Solar Cells by Using Luminescence Measurements", Energy Technol., 5, 1827–1835
- [10] A.B. Djuriscic, F.Z. Liu, H.W. Tam, M.K. Wong, A. Ng, C. Surya, W. Chen, Z.B. He, (2017), "Perovskite solar cells - An overview of critical issues", Progress in Quantum Electronics 53,1–37
- [11] Di Zhou, Tiantian Zhou, Yu Tian, Xiaolong Zhu, and Yafang Tu, (2018), "Perovskite-Based Solar Cells: Materials, Methods, and Future Perspectives", Journal of Nanomaterials, Vol. 2018, 1-15
- [12] Lan X, Vozny O, Kiami A, Garcia De Arquer FP, Abbas As, Kim Gh, Liu M, Yang Z, Walters G,xu J, Yuan M, Ning Z, Fan F, Kanjanaboos P, Kramer I, Zhitomirsky D, Lee P Perelgut A, Hoogland S, Sargent Eh, (2016), "Passivation Using Molecular Halides Increases Quantum Dot Solar Cell Performance", Adv Mater;28(2):299-304.
- [13] ZhenweiRen, Jiankun Sun, Hui Li, Peng Mao, Yuanzhi Wei, Xinhua Zhong, Jinsong Hu, Shiyong Yang, and Jizheng Wang, (2017), "Bilayer PbS Quantum Dots for High-Performance Photodetectors" Adv. Mater., 1702055
- [14] Tianshuo Zhao, Earl D. Goodwin,JiacenGuo, Han Wang, Benjamin T. Diroll, Christopher B. Murray, and Cherie R. Kagan, (2016), "Advanced Architecture for Colloidal PbS Quantum Dot Solar Cells Exploiting a CdSe Quantum Dot Buffer Layer", ACS Nano, 10, 9267"9273.
- [15] Chuang, C.-H. M.; Brown, P. R. Bulovic, V.,Bawendi, M. G., (2014), Improved Performance and Stability in Quantum Dot Solar Cells through Band Alignment Engineering. Nat. Mater., 13, 796"801
- [16] Xiaoliang Zhang, and Erik M. J. Johansson, (2017), "Reduction of Charge Recombination in PbS Colloidal Quantum Dot Solar Cells at the Quantum Dot/ ZnO Interface by Inserting a MgZnO Buffer Layer",J. Mater Chem. A, 5, 303-310.
- [17] Jaymin Ray, Tapas K. Chaudhuri, Chetan Panchal, Kinjal Patel, Keyur Patel, Gopal Bhatt, Priya Suryavanshi, (2017), " PbS-ZnO Solar Cell: A Numerical Simulation", Journal of nano electronics and physics, J. Nano- Electron. Phys. 9, 03041.
- [18] G. H. Kim, F. P. Garcia de Arquer, Y. J. Yoon, X. Lan, M. Liu, O. Voznyy, Z. Yang, F. Fan, A. H. Ip, P. Kanjanaboos, S. Hoogland, J. Y. Kim, and E. H. Sargent, (2015), "High-Efficiency Colloidal Quantum Dot Photovoltaics via Robust Self-Assembled Monolayers", Nano Lett., 3, 7691-7696.
- [19] M. Liu, F. P. de Arquer, Y Li , X. Lan , G.H. Kim , O. Voznyy , L. K. Jagadamma, A. S. Abbas, S. Hoogland, Z. Lu, J. Y. Kim, A. Amassian, and E. H. Sargent, (2016), "Double-Sided Junctions Enable High-Performance Colloidal-Quantum-Dot Photovoltaics", Advanced Materials, 28(21), 4142–4148
- [20] Jizhong Yao, Thomas Kirchartz, Michelle S. Vezie, Mark A. Faist, Wei Gong, Zhicai He, Hongbin Wu, Joel Troughton, Trystan Watson, Daniel Bryant, and Jenny Nelson, (2015), "Quantifying Losses in Open-Circuit Voltage in Solution-Processable Solar Cells", Phys. Rev. Applied 4, 014020