Numerical development of lead-free Cs_2TiI_6 -based perovskite solar cell via SCAPS-1D

Ilyas Chabri^{1,*}, Ali Oubelkacem¹, and Youness Benhouria¹

¹Laboratory of Physics of Materials and Modeling of Systems, (LP2MS), Physics Department, Faculty of Science, University Moulay Ismail, Meknes, Morocco

Abstract. Because of the toxicity and stability concerns, commercialization of lead-based perovskite solar cells (PSCs) is limited. Solar cells made entirely of Ti-based all-inorganic perovskite could be a viable answer to these issues. This paper is a theoretical paper on a perovskite solar cell (PSC) based on Cs_2TiI_6 using all-inorganic charge transport materials. We proposed a high performance perovskite solar cell (PSC) according to variables such as charge transport materials and its optimal thicknesses, absorber thickness, absorber defect density and interface defect density and working temperature. The optimal absorber thickness, Hole transport layer (HTL) thickness, and Electron transport layer (ETL) thickness are 500 nm, 50 nm, and 10 nm, respectively. After analyzing the other factors, we ended up with a high-performance PSC with a power conversion efficiency of 22.5% at room temperature and 22.84% at 270 K. These results are useful for the conception and manufacture of PSCs.

1 Introduction

Organic-inorganic perovskite materials have been extensively explored in recent years as an alternative to silicon-based solar cells for improving device efficiency, and it are a potential alternative to silicon-based solar cells because of its lower manufacturing costs [1,2]. Since the 2012 breakthroughs [3,4], it is now generally agreed that the halide perovskite solar cells could have a significant practical influence in the future generation solar cells. The active material of a typical perovskite solar cell was an organic-inorganic halide material [5,6]. Jena et al. developed the perovskite solar cell (PSC) by employing an organic-inorganic lead halide as an absorber instead of an organic dye [7]. From 2009 to 2019, the PCE (power conversion efficiency) of a typical organic-inorganic hybrid PSC (perovskite solar cell) has risen from 3.8% to over 25%. Despite the excellent optoelectronic properties of organic-inorganic hybrid PSCs, they display three major problems. For starters, it reduce the shelf life of perovskite compounds. Second, the presence of organic cations creates instability, and third, they use a lead (Pb)-based absorber, which is environmentally damaging [8]. As a result, all inorganic lead-free halide-based PSCs are now introduced [9]. As with organic-inorganic hybrid absorber, organic charge transport become unstable in oxygen, sunlight, and humidity [10,11]. Chen and his colleagues developed Cs_2TiBr_6 thin film Perovskites with a 3.28 % solar efficiency [12].

Because of its potential light harvesting properties, acceptable bandgap, good optical absorption, high stability, and benign defect property, Cs_2TiI_6 absorber material is shown to be a suitable alternate. The Cs_2TiI_6 absorber can be more resistant to environmental stress and have better tolerance [12,13]. Ahmed et al. reported an FTO/ SnO_2 / Cs_2TiBr_6 / MoO_3 /Au structure, with a stable PCE up to 11.49% [14]. Ahmad and his colleagues suggested a unique perovskite solar cell configuration of Au/ CdTe / Cs_2TiI_6 / TiO_2 /ITO, which has a PCE of 15.06 % [15].

In this study, we propose an all-inorganic PSC with a new combination of FTO/ ZnO / Cs_2TiI_6 / MoO_3 /Au using (SCAPS 1D-3.3.10). We analyzed the effects of various inorganic charge transport materials to find the optimum material for Cs_2TiI_6 -based PSC, e.g., p- MoO_3 , p-CuI, p-NiO, n- TiO_2 , n- SnO_2 , n- ZnO , n- CdS as HTL (Hole Transport Layer) and ETL (Electron Transport Layer) and optimized its thicknesses for achieving optimum performance. We also studied the effect of defect density of Cs_2TiI_6 , defect density of the interface, and the effect of operating temperature on device performance. Upon comparing the performance parameters, e.g., short circuit J_{sc} (current density), V_{oc} (open-circuit voltage), PCE (power conversion efficiency), and FF (Fill Factor), we have obtained an optimized high-performance PSC with a novel combination of FTO/ ZnO / Cs_2TiI_6 / MoO_3 /Au, that may aid in designing eco-friendly Ti-based perovskite solar cell for future technologies.

* Corresponding author: i.chabri@umi.ac.ma

2 Theoretical simulation

FTO/ETL/perovskite/HTL/Au is a unidimensional n-i-p planar heterojunction composition in our modeled PSC structure (Fig. 1). In this structure, we used inorganic lead-free Cs_2TiBr_6 as PAL (perovskite active layer), inorganic n- TiO_2 , n- SnO_2 , n- ZnO , and n- CdS as ETL (electron transport layer), and inorganic p- MoO_3 , p- CuI , and p- NiO as HTL (hole transport layer). For validation of our simulation, we first simulated the $\text{FTO}/\text{TiO}_2/\text{Cs}_2\text{TiBr}_6$ (200 nm)/P3HT/Au structure using the SCAPS 1D simulation software and then compared it to the experimental results [12]. HTL and ETL thicknesses of 30 nm are determined by calibrating simulation data with experimental data.

Fig. 1. Schematic of the simulated n-i-p perovskite solar cell

Table 1. Input parameters for each layer of the PSC structure

	FTO	TiO_2	Cs_2TiBr_6	P3HT
Thickness, d (nm)	500	30	200	30
Band gap, E_g (eV)	3.5	3.2	1.8	2
Electron affinity, χ (eV)	4	4.1	4	3.2
Permittivity, ϵ_r	9	9	10	3
Effective density states at CB, N_c (cm^{-3})	$2.2\text{E}+18$	$2.2\text{E}+18$	$6\text{E}+19$	$1\text{E}+20$
Effective density states at VB, N_v (cm^{-3})	$1.8\text{E}+19$	$1\text{E}+19$	$2.14\text{E}+19$	$1\text{E}+20$
Electron mobility, μ_n ($\text{cm}^2/\text{V s}$)	20	20	0.236	0.0001
Hole mobility, μ_p ($\text{cm}^2/\text{V s}$)	10	10	0.171	0.0001
Density of n-type doping, N_D (cm^{-3})	$1\text{E}+19$	$1\text{E}+18$	$3\text{E}+19$	0
Density of p-type doping, N_A (cm^{-3})	0	0	$3\text{E}+18$	$1\text{E}+16$
Defect density, N_t (cm^{-3})	-	$1\text{E}+15$	$4.17\text{E}+15$	$1\text{E}+15$
Capture cross-section electrons (cm^2)	-	$2\text{E}-14$	$1\text{E}-15$	$1\text{E}-15$
Capture cross-section holes (cm^2)	-	$2\text{E}-14$	$1\text{E}-15$	$1\text{E}-15$
Reference	[16]	[12],[17]	[12]	[12,16]

FTO and Au have work functions of 4.4 eV and 5.1 eV, respectively. We used the following settings for all defect layers: At 300K, the thermal velocity of electrons and holes is 10^7 cm/s, the energy distribution is Gaussian, the characteristic energy is 0.1 eV, and the energy level relative to the reference is 0.6 eV [18]. We provided absorber/ETL and absorber/HTL interface defects with hole capture cross section of 10^{-18} cm^2 and 10^{-19} cm^2 , electron-capture cross section of 10^{-19} cm^2 and 10^{-18} cm^2 respectively, and interface defect density of 10^{13} cm^{-3} . We took a constant illumination of 1000 W/m^2 at AM 1.5G, a continuous temperature of 300 K, a series resistance of 1 $\Omega\text{-cm}^2$, and a shunt resistance of 4200 $\Omega\text{-cm}^2$ to perform the simulation.

Table 2. Comparison between simulated and experimental Cs_2TiBr_6 based solar cells using P3HT as HTM

Device Architecture	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	PCE (%)
(Experiment) [12]	3.87	0.89	59.5	2.05
(Simulation)	3.78	0.9	50.01	1.71

Fig. 2 depicts the energy band diagram and J-V plots of the simulated $\text{FTO}/\text{TiO}_2/\text{Cs}_2\text{TiBr}_6/\text{P3HT}/\text{Au}$ structure. Table 2 shows the performance comparison between the simulated and experimental structure. The simulation results are clearly in agreement with the relevant experimental results. This also means that the simulation parameters are nearly identical to those of a real device.

Fig. 2. J-V curve for $\text{FTO}/\text{TiO}_2/\text{Cs}_2\text{TiBr}_6/\text{P3HT}$

3 Results and discussion

In this paper, analyzing several HTMs (Hole Transport Materials) and ETMs (Electron Transport Materials) by optimizing its thicknesses and, also by optimizing the density of PAL defects and interface defects, we propose a new structure FTO/ZnO/Cs₂TiI₆/MoO₃/Au.

3.1 HTL optimization

Instead of using organic P3HT as an HTM, we now select the most suited HTM and calculate its optimal thickness using inorganic CuI, MoO₃, and NiO. Table 3 shows the input values for several HTMs.

Table 3. Parameter settings for several HTMs, ETMs and for the PSC structure's absorber

	p-CuI	p-NiO	p-MoO ₃	Cs ₂ TiI ₆	n-SnO ₂	n-ZnO	n-CdS
Thickness, d (nm)	30	30	30	200	30	30	30
Band gap, E _g (eV)	3.1	3.8	3	1.80	3.5	3.3	2.4
Electron affinity, χ (eV)	2.1	1.46	2.5	4.20	4	4.1	4.18
Permittivity, ϵ_r	6.5	10.7	12.5	18.0	9	9	10
Effective density states at CB, N _c (cm ⁻³)	2.8E+19	2.8E+19	2.2E+18	1.0E+19	2.2E+17	2.2E+18	2.2E+18
Effective density states at VB, N _v (cm ⁻³)	1E+19	1E+19	1.8E+19	1.0E+19	2.2E+16	1.9E+19	1.9E+19
Electron mobility, μ_n (cm ² /V s)	100	12	25	4.4	20	100	100
Density of p-type doping, N _A (cm ⁻³)	43.9	2.8	100	2.5	10	25	25
Density of n-type doping, N _D (cm ⁻³)	0	0	0	1E+19	1E+18	1E+18	1E+18
Density of p-type doping, N _A (cm ⁻³)	1E+18	1E+18	1E+18	1E+19	0	0	0
Defect density, N _t (cm ⁻³)	1E+15	1E+15	1E+15	1E+15	1E+15	1E+15	1E+15
Capture cross-section electrons (cm ²)	1E-15	1E-15	1E-15	1E-15	2E-14	2E-14	2E-14
Capture cross-section holes (cm ²)	1E-15	1E-15	1E-15	1E-15	2E-14	2E-14	2E-14
Reference	[19]	[19]	[20]	[15,21]	[17]	[17]	[22]

The measurements for several HTMs are shown in table 4, and fig 3 shows the corresponding J-V characteristics for each HTM employed in the device. When compared to the performances of other HTMs, MoO₃ has better J-V characteristics, a higher V_{oc}, and a higher PCE.

Fig. 3. J-V characteristics curve for several HTLs

Table 4. Performance parameters of several HTLs

Hole Transport Material	J _{sc} (mA/cm ²)	V _{oc} (V)	FF (%)	PCE (%)
MoO ₃	11.53	0.97	83.88	9.4
CuI	11.53	0.69	80.76	6.42
NiO	11.52	0.75	81.92	7.08

Fig. 4. Energy level of Cs₂TiI₆ and HTMs

The Valance Band Offset (VBO) for all HTMs is negative, as seen in Fig. 4. When VBO is negative, there is no barrier to photo-generated holes flowing toward the back electrode, hence J_{sc} is nearly constant. J_{sc} is found to be 11.52 mA/cm² for NiO, 11.53 mA/cm² for CuI and

MoO₃. However, the increase in negative VBO causes an increase in interface recombination, which reduces V_{oc} [23]. We find V_{oc} is 0.97 V, 0.69 V, and 0.75 V for MoO₃, CuI, and NiO respectively. For MoO₃, CuI, and NiO, the V_{oc} is 0.97 V, 0.69 V, and 0.75 V, respectively. When it is increased, negative VBO decreases FF from 83.88 % to 81.92 %. MoO₃ has the highest PCE = 9.4 % because it has the lowest negative VBO, i.e. best band alignment with Cs₂TiI₆. PCE declines to 7.08 % when negative VBO increases in NiO. CuI, on the other hand, has the largest negative VBO, indicating poor band alignment, and lowest PCE of 6.42 % [23].

Fig. 5. PCE for several HTLs

The structure of MoO₃ has the best PCE, as shown in Fig. 5, so we picked MoO₃ to optimize the thickness. We changed the HTL thickness from 20 nm to 50 nm to optimize the HTL thickness taking in mind the regular feasibility of the perovskite solar cell construction process [24], and its effect is shown in Fig. 6. It can be found that with the increase in the HTL thickness, the values of J_{sc} decreases gradually. V_{oc} increases when the thickness is smaller than 35 nm and then it remained almost unchanged. The FF and PCE of the device first increase when the HTL thickness is less than 50 nm and then decrease slightly with further increasing the HTL thickness. This is because when the HTL is too thin, it may lead to low shunt resistance and current leakage, thus resulting in a low FF [25]. However, when the HTL is too thick, the series resistance will increase, leading to a reduction in FF. The structure using MoO₃ as HTM provides the best performance at 50 nm having V_{oc} □ 0.97 V, J_{sc} = 11.54 mA/cm², FF = 84.06%, and PCE = 9.46 %. Therefore, we select MoO₃ as the optimum HTM for Cs₂TiI₆ based PSC with an optimized thickness of 50 nm.

Fig. 6. HTL thickness optimization curve for MoO₃

3.2 Absorber thickness optimization

We have optimized the absorber thickness by using optimized MoO₃ as HTL. We have varied the absorber thickness from 300-520 nm using inorganic TiO₂, SnO₂, ZnO, and CdS as ETMs underneath the perovskite. Tables 1 and 3 provide the input parameters of the ETMs. Fig. 7 displays the optimization of the absorber thickness for different ETMs. It shows that the use of TiO₂ and ZnO provides both the best results than other ETMs, with a PCE of 12.01%, but using ZnO gives a better J_{sc} than using TiO₂. The other parameters; V_{oc} and FF are almost the same for all ETMs. So we chose ZnO as ETL, with optimal absorber thickness of 500 nm. The reason for this better PCE of ZnO can be elicited from Fig. 8.

Fig. 7. PCE curve against thickness variation of the Cs₂TiI₆ absorber for different ETMs.

Table 5. Output parameters for ETMs of the PSC structure

Electron Transport Material	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
ZnO	16.402363	0.9805	74.68	12.01
TiO ₂	16.402336	0.9805	74.68	12.01
CdS	16.415707	0.9804	74.55	12.00
SnO ₂	16.301709	0.9804	74.75	11.95

Fig. 8. Energy level diagram of the absorber and different ETMs

In Fig. 8, the conduction band offset (CBO) is negative for all ETMs. When CBO is negative, V_{oc} decreases monotonically. The negative CBO being very small there is no effect on the value of V_{oc} and FF [14]. According to literature, all the ETMs have a good band alignment with the absorber. So we should have obtained a constant J_{sc} [23].

However, we obtain J_{sc} 16.415707 mA/cm² for CdS, 16.402336 mA/cm² for TiO₂, 16.402363 mA/cm² for ZnO and, 16.301709 mA/cm² for SnO₂ due to the variation in its quantum efficiency (QE) which is shown in Fig. 9. As J_{sc} varies, the PCE of structure using different ETMs also varies.

Fig. 9. Quantum efficiency curves for various ETMs at optimal absorber thickness.

From Fig. 9, we find the CdS, TiO₂, SnO₂, and ZnO exhibit as much as 98.75 %, 98.72 %, 98.69%, and 98.72 % QE respectively in the visible range. Therefore, ZnO possesses J_{sc} of 16.402363 mA/cm² and thus the best PCE. Therefore, we select the optimized Perovskite Active Layer (PAL) thickness to be 500 nm for ZnO as ETL.

3.3 ETL thickness optimization

We optimized the ZnO thickness by varying it from 10 nm to 55 nm as ETL using the optimal HTL and PAL thicknesses. As shown in Fig. 10, there was no significant improvement in the output parameters when the ETL thickness was varied. As a result, we choose the optimized thickness of 10 nm with the highest PCE 12.02 %, V_{oc} 0.9805 V, J_{sc} 16.402430 mA/cm², and FF 74.71%.

Fig. 10. Variations in J_{sc} and FF as a function of ETL thickness

3.4 Absorber defect density optimization

We have studied the impacts of defect density by varying it from 10^{11} cm^{-3} to 10^{16} cm^{-3} using selected ETM and HTM, as well as optimal HTL, PAL, and ETL thicknesses. The J-V curves at various defect densities are seen in Fig. 11. The J_{sc} of PSC degrades from 16.50 mA/cm^2 for 10^{12} cm^{-3} to 16.26 mA/cm^2 for 10^{16} cm^{-3} . The increase in the recombination rate as defect density increases is the source of this degradation [26]. When the defect density is less than 10^{12} cm^{-3} , however, it remains almost constant. As a result, we chose a defect density of 10^{12} cm^{-3} , with a V_{oc} of 0.9886 V , and J_{sc} of 16.50 mA/cm^2 .

Fig. 11. J-V curve comparison for various absorber defect densities

3.5 Optimization of the defect density at the interface

J-V characteristics for different defect densities at the interfaces for values between 10^4 cm^{-3} and 10^9 cm^{-3} are shown in Fig. 12. V_{oc} saturates at defect densities below 10^5 cm^{-3} , as shown in this diagram. V_{oc} , on the other hand, decreases from 1.63 V to 1.4 V above 10^5 cm^{-3} to 10^9 cm^{-3} . As a result, at 10^5 cm^{-3} , we choose the optimum interface defect with V_{oc} of 1.63 V , J_{sc} of 16.50 mA/cm^2 , FF of 83.42% and PCE of 22.50% .

Fig. 12. Comparison of J-V curve for different interface defects

3.6 Optimized device

We achieved a high performance PSC with a new combination of FTO/ZnO/CsTiI₆/MoO₃/Au after optimizing HTL, PAL, and ETL. The new structure's schematic is shown in Figure 13.

Fig. 13. The optimized novel structure FTO/ZnO/Cs₂TiI₆/MoO₃/Au

Fig. 14. (a) J-V characteristics curve, (b) QE curve, for optimized FTO/ZnO/Cs₂TiI₆/MoO₃/Au structure

The J-V characteristics curve and the QE curve for the optimized device are shown in Fig.14. The device offers a PCE of 22.5%, J_{sc} of 16.5 mA/cm², V_{oc} of 1.63 V, and FF of 83.42% with a 99.28% QE at 360 nm, in the visible range. Table 6 compares the performance of different lead-free PSC studies. It can be seen that our device produces comparatively promising results, it's eco-friendly because it is made entirely of inorganic Ti-based perovskite materials, and that it is expected to be highly stable in the environment due to the use of all inorganic charge transport layers.

Table 6. Performance of several lead-free PSC

Absorber	PCE	Ref
CsSnI ₃	4.81	[27]
CsSnBr ₃	3.04	[26]
CsSnCl ₃	9.66	[28]
CsSnBr ₃	10.46	[28]
CsGeI ₃	4.94	[29]
CsGeBr ₃	4.92	[29]
CsGeCl ₃	2.57	[28]
CsSn _{0.5} Ge _{0.5} I ₃	7.11	[30]
CsSnIBr ₂	3.2	[31]
CsSnI ₃	2.3	[32]
Cs ₂ TiBr ₆	11.49	[14]
Cs ₂ TiI ₆	15.06	[15]
Cs₂TiI₆	22.5	This work

3.8 Working Temperature effect

To understand the effect of temperature on our new device, and the suitable temperature to get the best PCE, we changed the working temperature from 270 K to 360 K. Fig. 16 shows that as the working temperature rises from 270K to 360 K, the V_{oc} decreases from 1.6585 V to 1.5790 V. This is due to

the fact that when the temperature rises, the saturation current and recombination rate increase. Additionally, due of the thermal generation of carriers and the reduction of the band gap, J_{sc} increases from 16.503854 mA/cm² to 16.504397 mA/cm² [33]. The FF decreases from 83.43 % to 81.63 % as the rate of increase in J_{sc} is less than the rate of decrease in V_{oc} , and the PCE reduces from 22.84 % to 21.27 %. The overall performance of the PSC degrades when PCE decreases [34]. So the device gives a better performance for 270K, it can be used especially in cold regions.

Fig. 15. Output parameters variations for various working temperatures.

4 Conclusion

FTO/ZnO/Cs₂TiI₆/MoO₃/Au has been presented as a new PSC configuration. We presented a high-performance PSC with a PCE of 22.5 % at ambient temperature and 22.84 % at 270 K based on factors such as charge transport materials and thickness, absorber thickness, absorber defect density, and interface defect density. For a temperature of 270K, the device performs better, making it ideal for usage in cold areas. The results indicate that Cs₂TiI₆ could be useful as an absorber perovskite in highly efficient lead-free inorganic perovskite solar cell technology.

References

1. M. A. Green, Y. Hishikawa, E. D. Dunlop, D. H. Levi, J. Hohl-Ebinger, M. Yoshita, A. W. Y. Ho-Baillie, *Prog. Photovoltaics Res. Appl.* **27**, 1 (2019)
2. W. Gao, P. Li, J. Chen, C. Ran, Z. Wu, *Adv. Mater. Interfaces* **6**, 24 (2019)
3. I. Chung, B. Lee, J. He, R. P. H. Chang, M. G. Kanatzidis, *Nature* **485**, 7399 (2012)
4. M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami, H. J. Snaith, *Science* **338**, 6107 (2012).
5. M. I. Ahmed, A. Habib, S. S. Javaid, *Inter. J. of Phot.*, 1-13 (2015)
6. W. Ke and M. G. Kanatzidis, *Nat. Commun.* **10**, 1 (2019)
7. A. K. Jena, A. Kulkarni, T. Miyasaka, *Chem. Rev.* **119**, 5 (2019)
8. F. Giustino, H. J. Snaith, *ACS Energy Lett.* **1**, 1233-1240 (2016)
9. I. Chung, J. H. Song, J. Im, J. Androulakis, C. D. Malliakas, H. Li, A. J. Freeman, J. T. Kenney, M. G. Kanatzidis, *J.A.C.S.* **134**, 20 (2012)
10. B. V. Lotsch, *Angew. Chemie - Int. Ed.* **53**, 3 (2014)
11. L. Calió, S. Kazim, M. Grätzel, S. Ahmad, *Angew. Chemie - Int. Ed.* **55**, 47 (2016)
12. M. Chen, M. G. Ju, A. D. Carl, Y. Zong, R. L. Grimm, J. Gu, X. C. Zeng, Y. Zhou, N. P. Padture, *Joule* **2**, 3 (2018)
13. M. G. Ju, M. Chen, Y. Zhou, H. F. Garces, J. Dai, L. Ma, N. P. Padture, X. C. Zeng, *ACS Energy Lett.* **3**, 2 (2018)
14. S. Ahmed, F. Jannat, M. A. K. Khan, M. A. Alim, *Optik* **225**, p. 165765 (2021)
15. O. Ahmad, A. Rashid, M. W. Ahmed, M. F. Nasir, I. Qasim, *Opt. Mater.* **117**, p. 111105 (2021)
16. E. Karimi, S. M. B. Ghorashi, *Optik* **130**, 650-658 (2017)
17. N. Lakhdar, A. Hima, *Opt. Mater.* **99**, p. 109517 (2020)
18. F. Belarbi, W. Rahal, D. Rached, S. benghabrit, M. Adnane, *Optik* **216**, p. 164743, (2020)
19. S. Pitchaiya, M. Natarajan, A. Santhanam, V. Asokan, A. Yuvapragasam, V. Madurai Ramakrishnan, S.E. Palanisamy, S. Sundaram, D. Velaauthapillai, *Arab. J. Chem.* **13**, 1 (2020)
20. Raghvendra, R. R. Kumar, S. K. Pandey, *Superlattices Microstruct.* **135**, p. 106273 (2019)
21. K. Chakraborty, M. G. Choudhury, S. Paul, **194**, 886-892 (2019)
22. M.M. Salah, K.M. Hassan, M. Abouelatta, and A. Shaker, *Optik* **178**, 958-963 (2019)
23. T. Minemoto, M. Murata, *Sol. Energy Mater. Sol. Cells* **133**, 8-14 (2015)
24. M. Shahiduzzaman, K. Yamamoto, Y. Furumoto, T. Kuwabara, K. Takahashi, T. Taima, *Chem. Lett.* **44**, 12 (2015)
25. L. Lin, L. Jiang, P. Li, Y. Qiu, Q. Yan, J. Photonics Energy **9**, 2 (2019)
26. T. B. Song, T. Yokoyama, C. C. Stoumpos, J. L. Logsdon, D. H. Cao, M. R. Wasielewski, S. Aramaki, M. G. Kanatzidis, *J.A.C.S.* **139**, 2 (2017)
27. T. B. Song, T. Yokoyama, S. Aramaki, M. G. Kanatzidis, *ACS Energy Lett.* **2**, 4 (2017)
28. L. J. Chen, C. R. Lee, Y. J. Chuang, Z. H. Wu, C. Chen, *J. Phys. Chem. Lett.* **7**, 24 (2016)
29. L. J. Chen, *RSC Adv.* **8**, 33 (2018)
30. M. Chen, M. G. Ju, H. F. Garces, A. D. Carl, Luis K. Ono, Z. Hawash, Y. Zhang, T. Shen, Y. Qi, R. L. Grimm, D. Pacifici, X. C. Zeng, Y. Zhou, N. P. Padture, *Nat. Commun.* **10**, 1 (2019)
31. W. Li, J. Li, J. Li, J. Fan, Y. Mai, L. Wang, *J. Mater. Chem. A* **4**, 43 (2016)
32. P. Zhu, C. Chen, S. Gu, R. Lin, J. Zhu, *Sol. RRL* **2**, 4 (2018)
33. M. A. Green, *Sol. Energy* **28**, 5 (1982)
34. W. Abdelaziz, A. Shaker, M. Abouelatta, A. Zekry, *Opt. Mater.* **91**, 239-245 (2019)