

RESEARCH PAPER

## High Efficient Perovskite Solar Cells Base on Niobium Doped TiO<sub>2</sub> as a Buffer Layer

Ardeshir Baktash<sup>1</sup>, Omid Amiri<sup>2\*</sup> and Mohsen Saadat<sup>3</sup>

<sup>1</sup> Centre for Theoretical and Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, QLD, 4072, Australia

<sup>2</sup> Chemistry Department, college of science, University of Raparin, Rania, Kurdistan Region, Iraq

<sup>3</sup> Department of Physics, University of Sistan and Baluchestan, Zahedan, Iran

### ARTICLE INFO

#### Article History:

Received 02 October 2019

Accepted 04 December 2019

Published 01 January 2020

#### Keywords:

Buffer layer

Niobium doped TiO<sub>2</sub>

Operating temperature

Perovskite solar cell

### ABSTRACT

Here, the effect of lightly Niobium doped TiO<sub>2</sub> layer on the performance of perovskite solar cells has been studied by using solar cell capacitance simulator (SCAPS). *In addition*, the effects of Niobium concentration, buffer film thickness and operating temperature on the performance of the perovskite solar cell are investigated. For doping level of 3.0 mol% into the TiO<sub>2</sub> layer, cell efficiency of 18.26% with V<sub>oc</sub> of 0.96 V, J<sub>sc</sub> of 22.45 mA/cm<sup>2</sup> and FF of 84.25% has been achieved. Calculations show that thickness widening of Nb-doped TiO<sub>2</sub> layer would decrease the efficiency and Voc of the cells. Increase in operating temperature from 300 K to 400 K would weaken the performance of the perovskite solar cell with both pure and Nb-doped TiO<sub>2</sub> layers. However, the cell with Nb-doped TiO<sub>2</sub> layer shows higher stability than the cell with pure TiO<sub>2</sub> buffer at higher temperatures.

### How to cite this article

Baktash A, Amiri O, Saadat M. High Efficient Perovskite Solar Cells Base on Niobium Doped TiO<sub>2</sub> as a Buffer Layer . J Nanostruct, 2020; 10(1): 119-127 DOI: 10.22052/JNS.2020.01.013

### INTRODUCTION

Due to the exhaustion of traditional energy sources and serious need for the energy, replacement of new and clean energy is a vital task for scientists. In recent years, solar energy due to its availability and abundance is being considered as a replacement for energy. During last five years, perovskite solar cell has absorbed scientist's attention from all parts of the world [1-7] and recently power conversion efficiency of close to 20% is reported [8, 9]. As a very important component for perovskite solar cells, wide band gap materials such as TiO<sub>2</sub> for their unique characteristics such as wide range of applications, controllable framework compositions and tunable pore sizes have attracted scientists [10-13]. Up

until now for application in dye sensitized solar cells, TiO<sub>2</sub> with different morphologies such as nanoparticles [14, 15], nanowires [16, 17], nanosheets [18], nanotubes [19, 20], spheres [21, 22] and some other mesoscopic structures [23-27] has been used. Another way to improve characteristics of TiO<sub>2</sub> as an electrode is doping. For this purpose, TiO<sub>2</sub> can be n-type doped to improve charge collection and electron transport properties. One of the elements that were used as a dopant with different concentrations (up to a doping level of 20 mol%) to enhance TiO<sub>2</sub> performance is Niobium (Nb) [28-32]. To date, few researches on application of Nb-doped TiO<sub>2</sub> have been done to improve the conversion efficiency

\* Corresponding Author Email: MAIL

of dye-sensitized solar cells (DSSCs) [30, 33]. To the best of our knowledge, however, there is no experimental or theoretical study for application of Nb- doped TiO<sub>2</sub> in perovskite solar cell. To control the junction characteristics and enhance the charge transport properties of TiO<sub>2</sub> electrode, Nikolay and co-workers work on lightly doped (from 0.5 to 3 mol% Nb) TiO<sub>2</sub> [33] and an increasing in the photocurrent of DSSCs with lightly doped (from 2.5 to 10 mol% Nb) TiO<sub>2</sub> were concluded by Lu and co-workers [30].

Buffer layer plays an important role in cell's efficiency, so choosing a suitable buffer layer is very important for creation of an efficient perovskite solar cell [34]. The band gap [33], stability [35], and charge transport property [36] can be tuned by doping different concentrations of Nb into the TiO<sub>2</sub> structure.

In this study, our aim is to show that application of Nb-doped TiO<sub>2</sub> could improve the efficiency of Provskite solar cell. As experiment has shown before, Lightly Nb-doped TiO<sub>2</sub> will result in widening band gap [33]. In this work the effect of band gap widening, effects of operating temperature and thickness variation of Nb-doped TiO<sub>2</sub> as a buffer layer on performance of Provskite solar cells are investigated. For this purpose, we considered a doping level of 1.5, 2.5 and 3 mol%. For base electronic properties of simulated pure and doped TiO<sub>2</sub>, experimental results and parameters are used [33, 39].

**COMPUTATIONAL METHOD**

In this work, SCAPS version 3.2.01(a Solar Cell Capacitance Simulator) software which is a one dimensional solar cell simulation program is used. This software is developed at Department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium [37]. The simulated perovskite solar cell has layer configuration with transparent conductive oxide (TCO)/ blocking

Table 1. Definition of electronic properties

Parameter	Definition
$\chi$	Electron Affinity
$\epsilon_r$	Relative permittivity
$\mu_n(\text{cm}^2/\text{Vs})$	Electron band mobility
$\mu_p(\text{cm}^2/\text{Vs})$	Hole band mobility
$N_A(\text{cm}^{-3})$	Acceptor concentration
$N_D(\text{cm}^{-3})$	Donor concentration
$N_t(\text{cm}^{-2})$	Defect Density

layer (TiO<sub>2</sub>)/ absorber/ and hole transport material (HTM) layers. The considered materials for the mentioned layers are fluorine doped SnO<sub>2</sub> (SnO<sub>2</sub>:F), pure and doped TiO<sub>2</sub>, CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> and spiro-OMeTAD, respectively. For TiO<sub>2</sub>, the effect of the Niobium dopant with the concentrations of 1.5, 2.5 and 3 mol% into TiO<sub>2</sub> is considered [33] and accordingly the electron affinity of the layer are varied too. The descriptions of base parameters are available in Table 1, and Table 2 which shows the base parameter set for different layers of the simulation that have been used in this study. The thicknesses of layers are chosen based on experimental works on perovskite solar cell. To consider interface recombination, the interface layers INT1 and INT2 were defined from reference [38]. In this study, to obtain carrier diffusion lengths ( $L_n$  and  $L_p$ ) of 1  $\mu\text{m}$  that is similar to that of for experimental work, the value of defect parameters for all layers are considered identical and defect density for absorber is assumed equal to  $N_t = 2.5 \times 10^{13} \text{cm}^{-3}$  [40].

**RESULTS AND DISCUSSION**

*Effect of doping concentration*

To simulate the effect of doping concentration into the buffer layer of perovskite solar cell, we considered the effect of Niobium dopant on the energy band gap of the TiO<sub>2</sub> layer. The data for band gap energy that are used in simulations

Table 2. Base Parameters for simulated solar cell

Parameters	TCO	TiO <sub>2</sub>	INT1	Absorber	INT2	HTM
Thickness(nm)	500	100	10	330	10	350
$E_g(\text{ev})$	3.5	3.05[33]	1.55	1.55 [44]	1.55	3 [42]
$\chi(\text{ev})$	4	4.21[xx]	3.9	3.9[45]	3.90	2.45 [42]
$\epsilon_r$	10	10	6.5	6.5 [38]	6.5	3 [43]
$\mu_n(\text{cm}^2/\text{Vs})$	15	15 [39]	2.0	2.0 [2]	2.0	$2 \times 10^{-4}$ [42]
$\mu_p(\text{cm}^2/\text{Vs})$	10	10 [39]	2.0	2.0 [2]	2.0	$2 \times 10^{-4}$ [42]
$N_D(\text{cm}^{-3})$	$2 \times 10^{19}$	$10^{18}$ [39]	$10^{13}$	$10^{13}$	$10^{13}$	-
$N_A(\text{cm}^{-3})$	-	-	-	-	-	$2 \times 10^{18}$ [41]
$N_t(\text{cm}^{-2})$	$10^{15}$	$10^{16}$	$10^{17}$	$2.5 \times 10^{13}$	$10^{17}$	$10^{15}$



Table 3. The energy band gap for different concentrations of Nb into TiO<sub>2</sub> film.

Percentage of Niobium (% mol)	Bang Gap Energy (ev)
Pure	3.05
1.5%	3.06
2.5%	3.12
3.0%	3.18

are chosen from experimental results [33]. The amount of Niobium into the TiO<sub>2</sub> layer and the energy band gap of the pure and doped layers are available in Table. 3.

Fig. 1 shows the fill factor (FF) and efficiency (η) for different doping concentrations. As it can be seen from the Fig. 1, cell efficiency and FF for doped samples are improved. The calculated cell's efficiency for pure cell is 15.52% and for 1.5, 2.5, and 3 mol% Nb-doped cells are 15.71%, 17.39% and 18.26%, respectively. The value of FF increased from 71.43% for pure TiO<sub>2</sub> to 84.25% for 3.0 mol% Nb- doped layer. Also, FF for 1.5 and 2.5 mol% Nb-doped are 79.09% and 83.77%, respectively. As it can be seen from table 3, adding Niobium as a defect into TiO<sub>2</sub>, caused the band gap widening for doped TiO<sub>2</sub> layer. This can be explained by the difference in band gap energy of anatase (with E<sub>g</sub> = 3.2 ev) and rutile (with E<sub>g</sub> = 3.0 ev) phases. The use of Niobium into the TiO<sub>2</sub> structure facilitates the formation of anatase phase and prevents the formation of rutile phase [33-36]. The shift in the conduction band minimum position toward the LUMO of the absorber may enhance the electron injection from the absorber to the conduction band

of TiO<sub>2</sub>. Also, another reason for improvement in cell's performance is existence of oxygen vacancies into the structure and on the surface of TiO<sub>2</sub> that is independent from the band gap energy. Oxygen vacancies on the surface of and inside TiO<sub>2</sub>, give p-type characteristics to the structure. Utilization of Niobium into the TiO<sub>2</sub>, because of its tendency for attracting extra oxygen, Niobium reduces the oxygen vacancies and strengthens the n-type characteristics of the layer.

Fig. 2 shows open circuit voltage (V<sub>oc</sub>) and short circuit current density (J<sub>sc</sub>) of the cells with different Niobium doping levels. By doping Nb into the TiO<sub>2</sub> structure, minimum conduction band level of TiO<sub>2</sub>, because of band gap widening, moves toward the LUMO level of the absorber. Closeness of minimum conduction band of TiO<sub>2</sub> to LUMO level of the absorber facilitates electron injection from the absorber into the TiO<sub>2</sub> layer and consequently improves the J<sub>sc</sub> of the cell. Higher carrier concentrations at TCO layer and HTM layer Improve V<sub>oc</sub> too. However, calculations of our simulation (Fig. 2) show a rapid strange decline in V<sub>oc</sub> from pure TiO<sub>2</sub> layer to 1.5 mol% Nb-doped sample. On the other hand, comparing pure and doped cells, a rapid and irrational rise for FF (From 71.43% for pure layer to 79.09% for doped layer) is seen too.

*Effect of Buffer Thickness*

In this section, the effect of the thickness of the Nb-doped TiO<sub>2</sub> layer on the performance of the perovskite solar cell is investigated. The Thickness

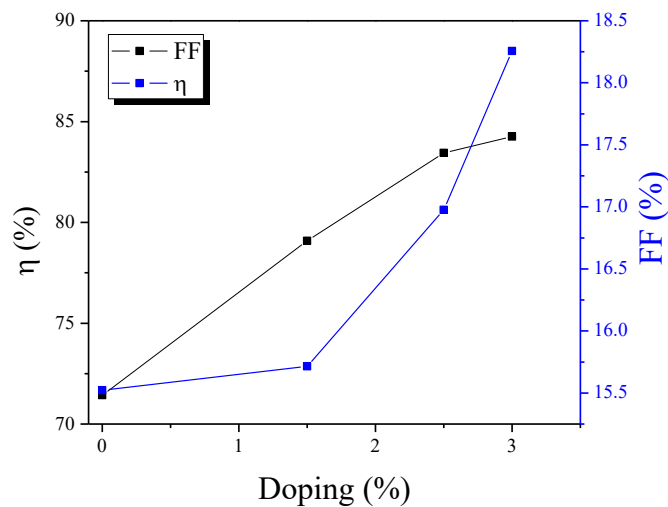


Fig. 1. Cell's efficiency and fill factor for different doping levels.



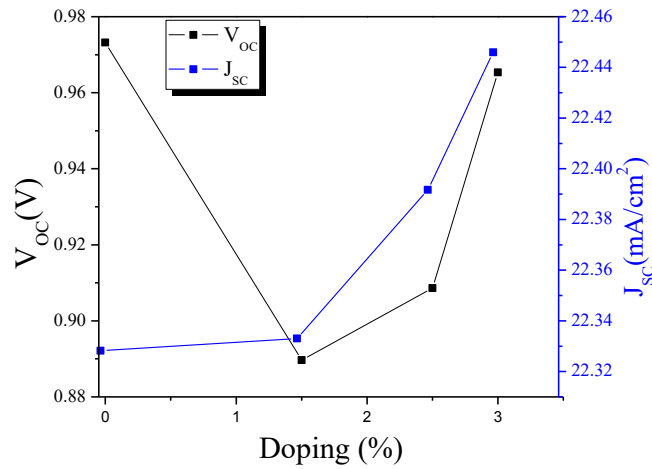


Fig. 2. Open circuit voltage ( $V_{oc}$ ) and short circuit current density ( $J_{sc}$ ) for different doping levels.

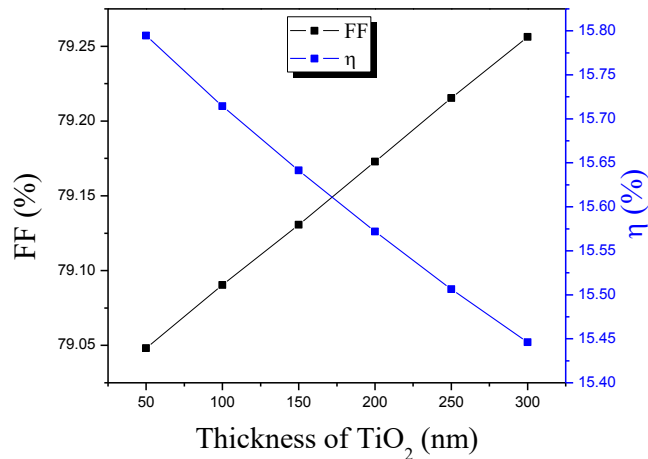


Fig. 3. Impact of thickness on the  $\eta$  and the FF of the perovskite solar cell.

of this layer as a buffer layer was considered 100 nm in order to study the effect of dopant on cell's performance. To study the effect of doped buffer's thickness on the cell, the thickness of 1.5 mol% Nb-doped layer is changed from 50nm to 300 nm in this simulation. The results for efficiency and FF have been shown in Fig. 3. Based on the information from Fig. 3, increase in thickness of the Nb-doped TiO<sub>2</sub> layer has a negative impact on the cells efficiency. However, the FF of the simulated cell is improved.

Fig. 4 demonstrates the results for  $V_{oc}$  and  $J_{sc}$ . It has been shown in Fig. 4 that by increasing thickness of the doped buffer layer, the  $J_{sc}$  of the cell goes toward the lower current density values. Possible reason is that photon loss is happening when the thickness is increasing. In fact, each photon is

carrying energy and when the thickness of the layer is increased, the numbers of absorbed photons by the layer are increased too. Accordingly the number of photons that have been transferred from the buffer layer to the absorber would decrease too. Therefore, reduction in the number of photons inside the absorber layer would cause the  $J_{sc}$  to fall down and consequently reduce the efficiency.

Spectral of solar cell with variable thickness of Nb-doped TiO<sub>2</sub> buffer layer are shown in Fig. 5. From Fig. 5, it can be found that by enlarging the thickness, the incident photon to electron efficiency (IPCE) of the cell is being reduced (especially for short wavelengths). So, thicker buffer layer would cause for the absorption in short wavelengths and consequently the loss in absorption edge would happen.

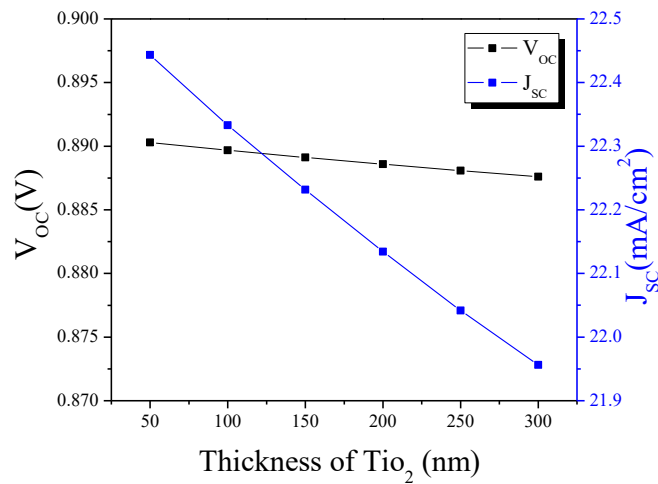


Fig. 4. Impact of the thickness on the V<sub>oc</sub> and the J<sub>sc</sub> of the perovskite solar cell.

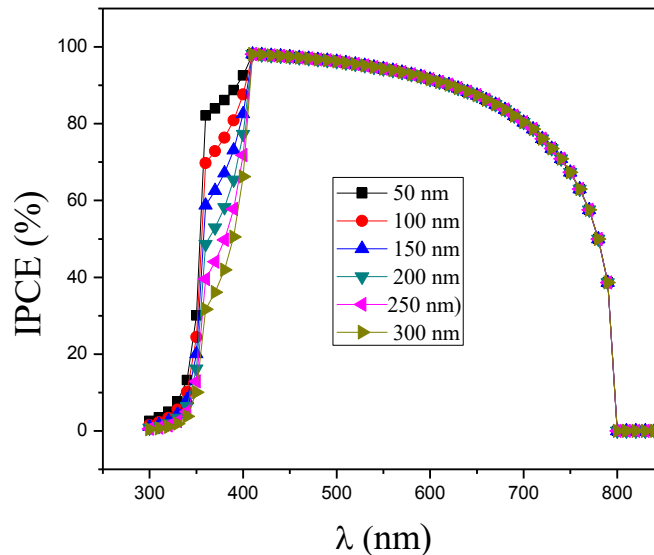


Fig. 5. Quantum Efficiency diagram for the cell with different buffer thicknesses.

*Effect of Temperature*

Temperature plays a vital role in the performance of solar cells. The variation of temperature could have intense influence on the efficiency of solar cell. In this study, up to now, all the calculations were done at 300 K. In this section, our aim is to study the effect of the temperature on the performance of the perovskite solar cell with Nb- doped TiO<sub>2</sub> buffer layer. For this purpose, the operating temperature has been changed from 300 K to 325, 350, 375 and 400 K. Fig. 6 illustrate that how the temperature variation could affect the efficiency and fill factor of the cell.

As it can be found from Fig. 6, when the operating temperature is increased from 300K to 400K, the efficiency of the cell is dramatically reduced from 18.26% to 14.07%.

Actually, temperature could affect Physical parameters such as the electron and hole mobility as well as carrier concentration and band gap of the layers. Higher temperature can also lead to the production of more electrons into the conduction band that leads to the higher short circuit current density (J<sub>sc</sub>). On the other hand, the band gap energy at higher temperatures would reduce and this would increase the recombination rate of

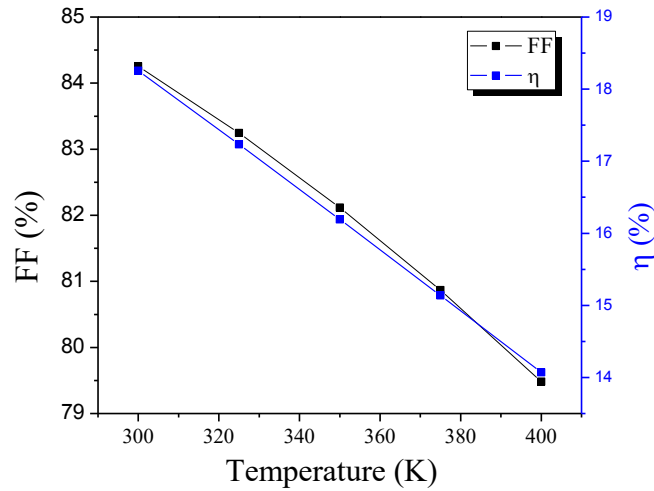


Fig. 6. Effect of temperature on FF and η of perovskite cell with Nb-doped TiO<sub>2</sub> buffer layer.

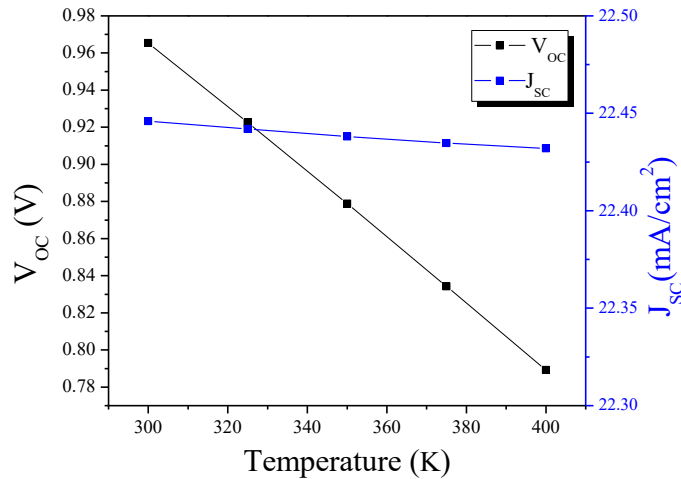


Fig. 7. Effect of temperature on V<sub>oc</sub> and J<sub>sc</sub> of perovskite cell with Nb-doped TiO<sub>2</sub> buffer layer.

mobile electrons and holes between the valance band and the conduction band which finally leads to the reduction in J<sub>sc</sub>. Also, V<sub>oc</sub> decreases at higher temperatures, whereas it increases with increasing in band gap. The results from our simulation (Fig. 7) have proven the experimental results. For the perovskite simulated cell, from 300K to 400K the V<sub>oc</sub> decreased from 0.965V to 0.79V, while the short circuit current density is not significantly changed.

The efficiency of the Nb-doped TiO<sub>2</sub> perovskite solar cell by increasing the operating temperature from 300 K to 400K has been reduced by 22.9%.

The effect of the temperature on perovskite solar cell with pure TiO<sub>2</sub> layer has been studied too. The results in Fig. 8 shows that the efficiency of the cell with pure buffer layer is reduce too. By

an increase in temperature from 300 K to 400 K, the efficiency of the cell declined from 15.52% to 11.47%. The efficiency of the cell for 325, 350 and 375 K are 14.49%, 13.48%, and 12.48%, respectively.

For the cell with pure buffer layer, reduction in efficiency with increase in operating temperature would occur faster than that of for the solar cell with Nb-doped TiO<sub>2</sub> buffer layer. Therefore, at higher temperatures, perovskite solar cell with Nb-doped TiO<sub>2</sub> buffer is more stable than the cell with pure TiO<sub>2</sub> buffer layer. The results for the impact of the temperature on the efficiency of doped and pure buffer layers are shown in Fig. 9. The reduction rate in efficiency for pure perovskite solar cell is 26.09%, while the rate for the cell with Nb-doped buffer is 22.9%.

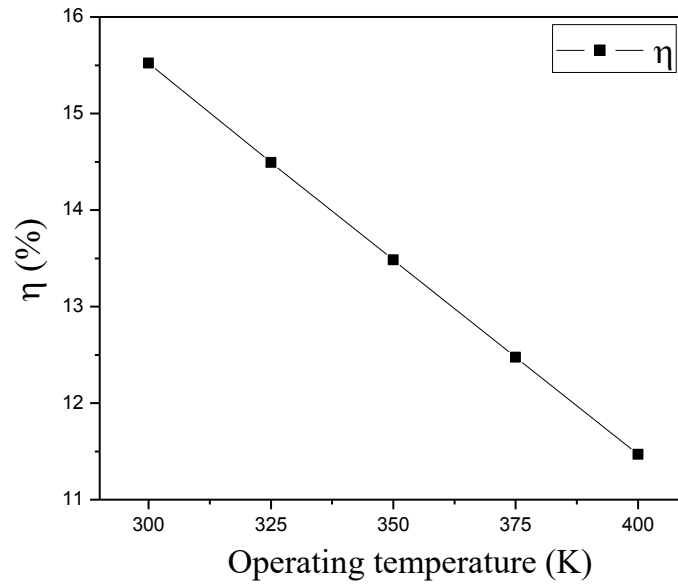


Fig. 8. Effect of temperature on FF and η of perovskite cell with pure TiO<sub>2</sub> buffer layer.

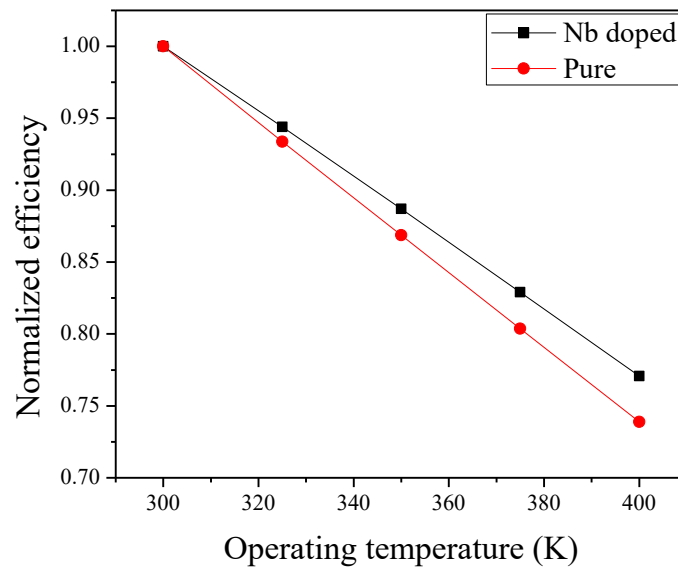


Fig. 9. Comparison of the pure TiO<sub>2</sub> and Nb-doped TiO<sub>2</sub> buffer layers at different operating temperatures (300K- 400K).

### CONCLUSION

Effect of Niobium dopant concentration into the TiO<sub>2</sub> buffer layer and its effect on the performance of the perovskite solar cell are studied. The cell's efficiency increased from 15.52% to 18.26% with doping level of 3.0 mol%. Also, the effect of thickness on doped TiO<sub>2</sub> buffer layer and effect of operating temperature on the performance of the perovskite solar cell with doped and pure buffer layers are investigated too.

Optimum thickness for the cell with doped buffer layer is around 50nm to 100 nm. In general the operating temperature has negative effect on cell's performance. The efficiency of the cell with pure and doped buffer layers decreased from 15.52% to 11.47% (with 26.09% reduction) and 18.26% to 14.07% (with 22.9% declination), respectively. Therefore, the cell with doped buffer layer shows better stability at higher operating temperatures.

## ACKNOWLEDGEMENTS

The authors would like to thank Professor Marc Burgelman, Department of Electronics and Information Systems, University of Gent for the development of the SCAPS Software package and allowing its use.

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

## REFERENCES

1. Etgar L, Gao P, Xue Z, Peng Q, Chandiran AK, Liu B, et al. Mesoscopic CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/TiO<sub>2</sub> Heterojunction Solar Cells. *Journal of the American Chemical Society*. 2012;134(42):17396-9.
2. Lee MM, Teuscher J, Miyasaka T, Murakami TN, Snaith HJ. Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites. *Science*. 2012;338(6107):643-7.
3. Burschka J, Pellet N, Moon S-J, Humphry-Baker R, Gao P, Nazeeruddin MK, et al. Sequential deposition as a route to high-performance perovskite-sensitized solar cells. *Nature*. 2013;499(7458):316-9.
4. Docampo P, Ball JM, Darwich M, Eperon GE, Snaith HJ. Efficient organometal trihalide perovskite planar-heterojunction solar cells on flexible polymer substrates. *Nature Communications*. 2013;4(1).
5. Stranks SD, Eperon GE, Grancini G, Menelaou C, Alcocer MJP, Leijtens T, et al. Electron-Hole Diffusion Lengths Exceeding 1 Micrometer in an Organometal Trihalide Perovskite Absorber. *Science*. 2013;342(6156):341-4.
6. Laban WA, Etgar L. Depleted hole conductor-free lead halide iodide heterojunction solar cells. *Energy & Environmental Science*. 2013;6(11):3249.
7. Mei A, Li X, Liu L, Ku Z, Liu T, Rong Y, et al. A hole-conductor-free, fully printable mesoscopic perovskite solar cell with high stability. *Science*. 2014;345(6194):295-8.
8. Zhou H, Chen Q, Li G, Luo S, Song Tb, Duan HS, et al. Interface engineering of highly efficient perovskite solar cells. *Science*. 2014;345(6196):542-6.
9. Jeon NJ, Noh JH, Yang WS, Kim YC, Ryu S, Seo J, et al. Compositional engineering of perovskite materials for high-performance solar cells. *Nature*. 2015;517(7535):476-80.
10. Wang Z-S, Kawauchi H, Kashima T, Arakawa H. Significant influence of TiO<sub>2</sub> photoelectrode morphology on the energy conversion efficiency of N719 dye-sensitized solar cell. *Coordination Chemistry Reviews*. 2004;248(13-14):1381-9.
11. Amiri O, Salavati-Niasari M. High efficiency dye-sensitized solar cells (9.3%) by using a new compact layer: Decrease series resistance and increase shunt resistance. *Materials Letters*. 2015;160:24-7.
12. Shin J-H, Moon JH. Bilayer Inverse Opal TiO<sub>2</sub> Electrodes for Dye-Sensitized Solar Cells via Post-Treatment. *Langmuir*. 2011;27(10):6311-5.
13. Li W, Wu Z, Wang J, Elzatahry AA, Zhao D. A Perspective on Mesoporous TiO<sub>2</sub> Materials. *Chemistry of Materials*. 2013;26(1):287-98.
14. Nakade S, Saito Y, Kubo W, Kitamura T, Wada Y, Yanagida S. Influence of TiO<sub>2</sub> Nanoparticle Size on Electron Diffusion and Recombination in Dye-Sensitized TiO<sub>2</sub> Solar Cells. *The Journal of Physical Chemistry B*. 2003;107(33):8607-11.
15. Yu J, Fan J, Lv K. Anatase TiO<sub>2</sub> nanosheets with exposed (001) facets: improved photoelectric conversion efficiency in dye-sensitized solar cells. *Nanoscale*. 2010;2(10):2144.
16. Feng X, Shankar K, Varghese OK, Paulose M, Latempa TJ, Grimes CA. Vertically Aligned Single Crystal TiO<sub>2</sub> Nanowire Arrays Grown Directly on Transparent Conducting Oxide Coated Glass: Synthesis Details and Applications. *Nano Letters*. 2008;8(11):3781-6.
17. Sun M, Fu W, Yang H, Sui Y, Zhao B, Yin G, et al. One-step synthesis of coaxial Ag/TiO<sub>2</sub> nanowire arrays on transparent conducting substrates: Enhanced electron collection in dye-sensitized solar cells. *Electrochemistry Communications*. 2011;13(12):1324-7.
18. Lv K, Xiang Q, Yu J. Effect of calcination temperature on morphology and photocatalytic activity of anatase TiO<sub>2</sub> nanosheets with exposed {001} facets. *Applied Catalysis B: Environmental*. 2011;104(3-4):275-81.
19. Mor GK, Shankar K, Paulose M, Varghese OK, Grimes CA. Use of Highly-Ordered TiO<sub>2</sub> Nanotube Arrays in Dye-Sensitized Solar Cells. *Nano Letters*. 2006;6(2):215-8.
20. Guo M, Xie K, Lin J, Yong Z, Yip CT, Zhou L, et al. Design and coupling of multifunctional TiO<sub>2</sub> nanotube photonic crystal to nanocrystalline titania layer as semi-transparent photoanode for dye-sensitized solar cell. *Energy & Environmental Science*. 2012;5(12):9881.
21. Yu J, Fan J, Zhao L. Dye-sensitized solar cells based on hollow anatase TiO<sub>2</sub> spheres prepared by self-transformation method. *Electrochimica Acta*. 2010;55(3):597-602.
22. Xiang P, Li X, Wang H, Liu G, Shu T, Zhou Z, et al. Mesoporous nitrogen-doped TiO<sub>2</sub> sphere applied for quasi-solid-state dye-sensitized solar cell. *Nanoscale Research Letters*. 2011;6(1):606.
23. Cheng B, Le Y, Yu J. Preparation and enhanced photocatalytic activity of Ag@TiO<sub>2</sub> core-shell nanocomposite nanowires. *Journal of Hazardous Materials*. 2010;177(1-3):971-7.
24. Hung P-L, Wen M-H, Hung K-H, Bow J-S, Wang H-W, Han JCC, et al. 3D Electrodes for Dye-Sensitized Solar Cells: Synthesis of ITO Nanowire Arrays Inside the TiO<sub>2</sub> Nanotubes. *Journal of the Chinese Chemical Society*. 2010;57(5B):1157-61.
25. Jin M, Kim SS, Yoon M, Li Z, Lee YY, Kim JM. Mesoporous Inverse Opal TiO<sub>2</sub> Film as Light Scattering Layer for Dye-Sensitized Solar Cell. *Journal of Nanoscience and Nanotechnology*. 2012;12(1):815-21.
26. King JS, Graugnard E, Summers CJ. TiO<sub>2</sub> Inverse Opals Fabricated Using Low-Temperature Atomic Layer Deposition. *Advanced Materials*. 2005;17(8):1010-3.
27. Stott SJ, Mortimer RJ, Dann SE, Oyama M, Marken F. Electrochemical properties of core-shell TiO<sub>2</sub>-TiO<sub>2</sub> nanoparticle films immobilized at ITO electrode surfaces. *Phys Chem Chem Phys*. 2006;8(46):5437-43.
28. Furubayashi Y, Hitosugi T, Yamamoto Y, Inaba K, Kinoda G, Hirose Y, et al. A transparent metal: Nb-doped anatase TiO<sub>2</sub>. *Applied Physics Letters*. 2005;86(25):252101.
29. Mattsson A, Leideborg M, Larsson K, Westin G, Österlund L. Adsorption and Solar Light Decomposition of Acetone on Anatase TiO<sub>2</sub> and Niobium Doped TiO<sub>2</sub> Thin Films. *The Journal of Physical Chemistry B*. 2006;110(3):1210-20.
30. Lü X, Mou X, Wu J, Zhang D, Zhang L, Huang F, et al.



- Improved-Performance Dye-Sensitized Solar Cells Using Nb-Doped TiO<sub>2</sub> Electrodes: Efficient Electron Injection and Transfer. *Advanced Functional Materials*. 2010;20(3):509-15.
31. Tenczek-Zajac A, Radecka M, Rekas M. Photoelectrochemical properties of Nb-doped titanium dioxide. *Physica B: Condensed Matter*. 2007;399(1):55-9.
32. Di Valentin C, Pacchioni G, Selloni A. Reduced and n-Type Doped TiO<sub>2</sub>: Nature of Ti<sup>3+</sup> Species. *The Journal of Physical Chemistry C*. 2009;113(48):20543-52.
33. Nikolay T, Larina L, Shevaleevskiy O, Ahn BT. Electronic structure study of lightly Nb-doped TiO<sub>2</sub> electrode for dye-sensitized solar cells. *Energy & Environmental Science*. 2011;4(4):1480.
34. Son D-Y, Im J-H, Kim H-S, Park N-G. 11% Efficient Perovskite Solar Cell Based on ZnO Nanorods: An Effective Charge Collection System. *The Journal of Physical Chemistry C*. 2014;118(30):16567-73.
35. Han X, Song K, Lu L, Deng Q, Xia X, Shao G. Limitation and extrapolation correction of the GGA + U formalism: a case study of Nb-doped anatase TiO<sub>2</sub>. *Journal of Materials Chemistry C*. 2013;1(23):3736.
36. Burgelman M, Nollet P, Degraeve S. Modelling polycrystalline semiconductor solar cells. *Thin Solid Films*. 2000;361-362:527-32.
37. Minemoto T, Murata M. Theoretical analysis on effect of band offsets in perovskite solar cells. *Solar Energy Materials and Solar Cells*. 2015;133:8-14.