Extracting optimal preparation parameters of TiO$_2$ electron transmission layer in perovskite solar cell for increasing efficiency of the cell

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Abstract

In this research, a thin film of titanium dioxide was prepared as electron transporting layer to be used in perovskite solar cell simulation. The thin film TiO$_2$ was prepared under different lab conditions such as changing the chamber pressure from $2.0 \times 10^{-2}$ to $4.0 \times 10^{-2}$ mbar and changing the power of deposition device from 200 to 240 watts for different thickness ranging from 30 to 150 nm. Radio frequency magnetron sputtering method has been used to fabricate the layers under the mentioned laboratory conditions. Then, the band gap energy of the thin films was calculated by Tauc’s plot method. It was shown that the bands gap energy which is one of the contributing factors in solar cell characteristics, such as short-circuit current, open-circuit voltage, fill factor and solar cell efficiency, highly depends on laboratory conditions of preparing the thin film and it changes with changes in deposition parameters of the device. The simulated solar cells were considered as ZnO: Al / TiO$_2$ compact layer/ CH$_3$NH$_3$SnI$_3$ / Cu/ Au. Investigation on the effects of preparation conditions of TiO$_2$ on properties of the cell and perovskite solar cell efficiency was carried out using experimental data related to TiO$_2$ and extraction of data of other layers from authentic articles using comsol multiphysics software. In comparison with other preparation conditions, the prepared layer with 30 nm thickness under 240 watts device power and $3.5 \times 10^{-2}$ mbar chamber pressure had the best possible results. In this condition, perovskite solar cell characteristics obtained $I_{sc} = 22.368 mA$, $V_{oc} = 1.02 V$, % FF = 80.522 and % PCE = 18.37.

Introduction

Economic crises and other problems like fossil fuels decline and their destructive effects on the environment as well as the rise of energy consumption due to world population increase [1] have made scientists to find appropriate solutions to solve global energy and its environmental impact problem [2, 3]. Developed countries and developing countries are using renewable energy sources like sunlight, wind, water, etc. to provide clean energy sources and consequently decrease detrimental environmental hazards, greenhouse gasses, and global warming [4]. The only solution to these problems is to use renewable energy sources. Nowadays, the strategy of the world’s countries is to use renewable energies especially solar photovoltaic energy [5]. Solar energy is one of the renewable sources; this endless energy source has the potential to solve most of the mentioned problems [6]. Solar cells can solve human’s energy needs by receiving sunlight and converting it into electrical energy. This energy can be used in different industries. The naming of different solar cells is based on their semi-conductor materials. These materials should have specific characteristics to absorb the sunlight. Some kinds of solar cells have been made of different compounds like silicon solar cells [7], cadmium-telluride [8], gallium arsenide [9], hybrid solar cells composed of semi-conductor organic a non - organic materials [10], bio-hybrid solar cells [11, 12], and recently perovskite solar cells [13] that is the purpose of this article. Inclusion of lead as a feature of perovskite material is a common concern. Tin-based perovskite absorbents like CH$_3$NH$_3$SnI$_3$ have been reported with lower power efficiency [14, 15]. In their structure, generally, solar cells have that they have been made of different layers to convert luminous energy to electrical energy. Semi-conductor nano-materials are promising options for the economic and environment friendly system having copious chemical and catalyst non-toxic energy sources without any secondary pollution. There are many semi-conductor compounds which can be used as anti-reflection coating in solar cells, the most important of them are SiO$_2$ [16], ZnS [17], MgF$_2$ [18], ZnO [19], and TiO$_2$ [19]. Titanium dioxide is one the most highly used anti-reflection materials. Its natural stability is titanium oxide [20]. Titanium dioxide can be prepared in three main phases of brookite, anatase, and rutile [21]. This material has a wide range of application in the paint industry, paper industry, plastic, glaze, glass industry, cosmetic products, water refinery (as catalyst) [22, 23], isolators, sensors, etc. Titanium dioxide is the most appropriate candidate to be used in solar cells due to having peculiar physical-chemical properties such as high stability in the vast environment around in high acidity [24], high refractive index [25, 26] and the very low edge of conduction band to energy balances of light absorbent layers [27]. In general, titanium dioxide is used as electron transporting layer in solar cells. For instance, since the conduction edge of titanium dioxide in solar cells sensitive

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to pigment is a little bit smaller than the energy of excited state of most of the sensitive pigments, an electron can be injected efficiently. Moreover, having high refractive index, titanium dioxide prevents recombination before reproduction by an oxidative electrolyte [28]. This material is a good candidate for using solar cells. Because of its high refractive index [29], titanium dioxide can be used as a white pigment or transparency regulator in powder form [30]. Recently, it has been shown that, to increase light trapping capacity in perovskite solar cells, TiO₂ can be prepared in form of nano-tube or nano-particles [31] or nano-bar and nano-particle through the hydrothermal method. It’s been shown that perovskite solar cell efficiency obtained 12.2% [32]. Currently, photovoltaic cells with heterojunctions are being seriously investigated because they are a promising route toward converting solar energy with high efficiency and low cost [33-36]. There has been considerable growth in the development of perovskite solar cells since 2008 [37]. The efficiency of perovskite solar cell increased from 3.1% in 2009 to 3.8% in 2011 [38], 6.5% in 2012 [39] to 9.7% [40] and 10.9% [41]. Then, with relatively rapid growth, the efficiency reached to 15.3% in 2013 [42, 43]. In 2015, the chemical technology research institute of South Korea (KRICT) reported the efficiency of solid-state perovskite solar cells 17.9%. More recently, perovskite solar cell efficiency has enhanced approximately to 22.1% [44, 45] for a cell with a cross-sectional area less than 0.1cm². This study investigated the effect of lab conditions on preparation of titanium dioxide layer as one of the most highly used layers in different solar cells especially perovskite. This layer was prepared experimentally under different lab conditions like chamber pressure change and device power change using radio frequency magnetron sputtering method. Then, the effect of lab conditions on preparation of titanium dioxide layer on perovskite solar cell parameters such as short-circuit current, open-circuit voltage, fill factor, and solar cell efficiency was investigated. Thus, the required information of other layers was selected from valid sources, then simulation was performed using comsol multiphysics software.

Materials and methods

This study used radio frequency magnetron sputtering device model MSS – MDAU 160 from an injection of Argon neutral gas with 99.99% purity. Titanium dioxide tablet had a thickness of 3 mm, a diameter of 76.2 mm and purity of 99.99%. The fixed value of 5 cm was selected as the target distance to substrate for deposition. The normal glass substrate of (2 cm × 5 cm) was used for deposition. In this research, the effects of lab conditions of the preparation of titanium dioxide for different thicknesses in fixed deposition pressure and power as well as a fixed thickness under different deposition pressure and power are examined using radio frequency magnetron sputtering method.

Sample preparation

Lab conditions and deposition process

First, all substrates were washed with distilled water for 15 minutes. Then, the substrates were washed several times with acetone and placed in alcohol for 10 minutes to remove all impurities. Before starting the main deposition on substrates, to purify the vacuum chamber, the initial pressure inside the chamber was reached to 3.0×10⁻⁵ mbar to minimize the pollution inside the environment. After adjusting the device and formation of plasma for deposition, a deposition was carried out tentatively for 10 minutes to remove all possible impurities on the target tablet. After these stages and ensuring the minimization of the chamber pollution and substrate, a plasma was formed for deposition by regulating the initial power of 500 watts and a chamber pressure of 3.0×10⁻⁵ mbar and deposition of different lab conditions was completed. During the deposition process, the temperature inside the chamber was kept fixed for 58°C. Then, using Argon gas, five thicknesses of 30, 75, 60, 90, 105 nm were deposited with power 240 watts and 3.5×10⁻² mbar chamber pressure as shown in the table (1). In the next step, by selecting the fixed thickness of 30 nm, this thickness was deposited once with the fixed 220 watts power under different pressures inside the chamber as shown in the table (2).

The next time, the chamber pressure kept fixed 3.5×10⁻² mbar and deposition were carried out with different powers as shown in the table (3). Then, to specify coefficient absorption and using it determine bands gap energy, the layers were lighted by Perkins Elmer model Lambda 45. A sample of a substrate without coating was placed in the device and its absorption rate became zero for further accurate measurements of substrates with coating. Lighting the prepared layers was completed in wavelength of the visible light spectrum of (320-900) nm. Laboratory samples made are shown in figure (1).

Table 1 Deposition under fixed power & pressure of device for different thicknesses

| Thickness (nm) | Power (watts) | Pressure (mbar) |
|---------------|--------------|----------------|
| 30            | 500          | 3.0×10⁻⁵       |
| 75            | 240          | 3.5×10⁻²       |
| 60            |              |                |
| 90            |              |                |
| 105           |              |                |

Table 2 Deposition under fixed power of device for fixed thicknesses 30 nm under different chamber pressure.

| Power (watts) | Pressure (mbar) | Thickness (nm) |
|--------------|-----------------|----------------|
| 220          | 3.0×10⁻⁵        | 30             |
|              | 3.5×10⁻²        | 75             |
|              |                  | 60             |
|              |                  | 90             |
|              |                  | 105            |

Table 3 Deposition under fixed chamber pressure for 30 nm layer under different powers of device
Characterization

Determining band gap energy

There are different methods such as Beer-Lambert law [46] and Tauc’s plot [47] for calculating bands gap energy. This research used Tauc’s plot method for measuring bands gap energy. Coefficient absorption (equation 1) can be described based on a function of Photon energy (eV) and used to calculate bands gap energy:

\[ \alpha h \nu = A (Eg - h \nu)^n \]  

(1)

Where fixed h is Planck’s constant, v is frequency, n is the numerical value which is dependent on transition nature having values of 1/2, 2, and 3/2 for direct, indirect and forbidden transition. Regarding that TiO₂ is a semi-conductor or direct band gap transition, the value of 1/2 was considered for n [48]. Therefore, with drawing \((\alpha h \nu)^2\) versus \(h \nu\) and extrapolation of the linear area of the curve in \(\alpha=0\), direct bands gap energy for titanium dioxide is calculated.

Fig. 2  Tauc’s plot for the thin film prepared TiO₂ a) different thicknesses, b) under different pressures, c) Different powers

The final results of extraction of bands gap energy of the prepared layers under different conditions using figures (2- a, 2-b and 2-c) are shown in table (4).

Table 4  The extracted band gap energy related to TiO₂ compact layer.

Methodology

Computational simulation is a method of studying and analyzing the behavior of a real device by a hypothetical system using a computer program. Simulation is based on mathematical model that describes the system. For years, it’s been confirmed that numerical simulation method of solar cell device is a valid instrument for studying and understanding properties of solar cell devices like optical, electrical and mechanical properties [49]. Numerical simulation has been used for studying the performance of the solar cell for 40 years [50]. With development of these numerical models, a clear understanding of the mechanism of solar cells has been obtained which has led considerably to improvement and development of the performance and efficiency of the device. Comsol multiphysics software is a complete set of simulation which can solve differential equations of non-linear systems by partial derivatives through FEM method in one, two, and three-dimensional space. This is a numerical method for approximate solution of partial differential equations using numerical methods like Euler method. Comsol multiphysics software can examine thin film systems and photonic structures properly. This study designs and investigates tin-based perovskite solar cell efficiency using experimental results and previous studies simultaneously through simulation in comsol multiphysics software.

Device structure

According to figure (3), tin-based perovskite solar cell is considered as flat heterojunction, TiO₂ is the electron transporting material, CH₃NH₃SnI₃ is the absorbent layer and Cul is hole transporting material. ZnO: Al and Au are the front and back contact respectively.

Fig. 3  a) Schematic structure and b) perovskite solar cell energy diagram CH₃NH₃SnI₃

The parameters used in simulation

The parameters used in simulation of different layers were meticulously selected from experimental data of this study and previous studies. The data related to TiO₂ like different thicknesses and bands gap energy measured under deposition conditions in the first section of this study were entered into the simulation. Table (5) shows the simulation parameters.

Table 5  The selected parameters for simulation process in AM1.5G.

In this simulation, the recombination process was considered Shockley-Reed-Hall recombination [60] and doped impurities assumed \(10^{17}\) (1/cm³). After the completion of simulation and extraction of data from I-V curve using \(\text{FF=}(\text{Imp} \times \text{Vmp})/(\text{Isc} \times \text{Voc})\) and \(\text{PCE=}(\text{FF} \times \text{Isc} \times \text{Voc})/\text{Pin}\) where \(\text{Imp}\) and \(\text{Vmp}\) are voltage and current in maximum power and \(\text{Isc}\) and \(\text{Voc}\) are open-circuit voltage and short-circuit voltage and \(\text{Pin}\) is the power of the incident light to solar cell surface, the fill factor and perovskite solar cell efficiency can be calculated. The cross section of the perovskite solar cell is considered to be 2cm² and comsol multiphysics software considers the connection model to be an ideal ohmic and the ideal ohmic connection equation have been used [61]. Graphs are down using MATLAB Software. The I-V curves were extracted by combining the data related to prepare TiO₂ layer under different physical conditions experimentally and the data of table (4) in comsol multiphysics software. Using these
Different thicknesses of the prepared layers under fixed power and pressure

The prepared layers TiO$_2$ with 30nm thickness under fixed power and different pressures of chamber

As can be seen from figure (4), the I-V diagram is quite sensitive to changes in the thickness of the TiO$_2$ layer. As the thickness increases, the short-circuit current decreases. But there is no change in the open-circuit voltage. I-V curves and perovskite solar cell parameters for 30 nm thickness under different pressures of chamber are shown in figure (5) and table (7), respectively.

The prepared layers TiO$_2$ with 30nm thickness under the fixed pressure and different powers device

I-V curves and perovskite solar cell parameters for 30 nm thickness under different powers of chamber are shown in figure (6) and table (8), respectively.

The dependence of photovoltaic performance on thickness of the TiO$_2$ thin film

Figure (8-a) shows that $I_{sc}$ significantly depends on the change of the thin film thickness and it decreases with the increase of thickness. In 30 to 105 nm range, $I_{sc}$ changes from 22.37(mA) to 19.64(mA) and the current declines 12% approximately.

This behavior can be explained in this way: there are two ways for transporting charge from perovskite to side current, one of them via TiO$_2$ and the other one via perovskite itself [62, 63]. In structures having an approximate thickness of 1 µm (like the selected structure in this article), regarding the lower conduction band of TiO$_2$ in comparison to lower perovskite’s unoccupied molecular orbital, the rate of TiO$_2$ is much lower than perovskite electron transport. Therefore, the capacity of electron transport from compact layer shows higher dependence on thickness [63, 64] and the other reason can be related to increase of thickness so that pair electron-hole are produced and recombined before reaching the contacts. $V_{oc}$ decreased slightly with an increase of thickness which can be disregarded. In other words, $V_{oc}$ is to some extent independent of the compact layer thickness [64] With the change of $I_{sc}$, fill factor and consequently the perovskite solar cell TiO$_2$ acts as an anti-reflector layer in solar cells and transparency of TiO$_2$ thin film is of paramount importance. This layer should be as thin as possible to decline its
The thickness of the layer allows more light to pass and reach a perovskite absorbent layer for production of the pair electron-hole. The series resistance is proportionate to a thickness so that the less the thickness the less the series resistance and the more the current. The increase of the thickness increases the TiO₂ layer’s series resistance which thin film is of paramount importance. This layer should be as thin as possible to decline its resistance against the current. The thickness of the layer allows more light to pass and reach a perovskite absorbent layer for production of the pair electron-hole. The series resistance is proportionate to a thickness so that the less the thickness the less the series resistance and the more the current. The increase of the thickness increases the TiO₂ layer’s series resistance which leads to a decrease in I<sub>sc</sub> current and decreases the efficiency in consequence. The electron transporting layer impacts on the performance of solar cell: the resistance should be as low as much as possible and the thickness should be as thin as possible. Therefore, to transport the electron and the hole, the edge of conduction band of TiO₂ should be under perovskite’s conduction band and its valance should be under perovskite’s valance band. According to figure (8-b), V<sub>oc</sub> has not changed, (1.02), which it can be concluded that during shining the rate of production and recombination of electrons and holes almost remains fixed and V<sub>oc</sub> does not change as a result. In addition to the mentioned factors, there is a peculiar relationship between V<sub>oc</sub> and contributing factors including energetic disorder, charge transfer states, donor-acceptor interface, micro-structure, carrier density, etc. Each of which having a special importance in V<sub>oc</sub>. Other parameters like electrode work function, morphology, light intensity, density of state (DOS) recombination, temperature, and defect state and crystallinity impact on open-circuit voltage of organic solar cells with heterogeneous junction directly or indirectly. The amount on the effect of each of these factors can be considered separately [65]. According to figures (8-a) and (8-b), the rate of efficiency solar cell (% PCE) as shown in figure (8-d), change is similar to I<sub>sc</sub> showing that the efficiency is all dependent on short current circuit. It should be noted that the change of fill factor as shown in figure (8-c) needs more investigations. The fill factor depends on the short-circuit current and the open-circuit voltage. For example, open-circuit voltage depends on various factors such as morphology, electrodes work function, light intensity, recombination and etc. [64]. In this paper, only the effect of physical conditions on the fabrication of the titanium dioxide layer is investigated. Therefore, the effect of other factors on the fill factor should be investigated, which requires more investigations.

The effect of pressure on the band gap energy of TiO₂ prepared at constant thickness and power

The dependence of photovoltaic performance on construction of TiO₂ thin film in different pressures

Figure (10-a) shows that I<sub>sc</sub> depends slightly on the change of chamber’s pressure in making of the thin film so that with the increase of the chamber pressure from 0.02 to 0.04 mbar, it changes and increases from 22.356 mA to 22.364 mA. In other words, with the increase of the chamber pressure, a slight increase about 0.04% happens which can be disregarded and it can be said that I<sub>sc</sub> is almost independent of the chamber pressure during the layer making. The approximate fixed state of short-circuit current means that the series resistance is almost fixed under different conditions of the layer making and the capacity of electron transport of this layer has almost not changed. In general, V<sub>oc</sub> is resulted from the splitting of quasi-fermi levels and the hole caused by shining.

\[
V_{oc} = \frac{1}{q} (E_{FN} - E_{FP})
\]

(2)

Where q is elementary charge and E<sub>FN</sub> and E<sub>FP</sub> are respectively electron and hole quasi-fermi energy levels [65]. Under open-circuit conditions, when switching off the source of light shining, the charge carriers caused by light are not produced, and naturally due to recombination phenomenon, the number of electrons and holes decreases and V<sub>oc</sub> declines theoretically [66]. Regarding that V<sub>oc</sub> remains fixed, (1.02), according to figure (10-b), it can be concluded that during shining the rate of production and recombination of electrons and holes almost remains fixed and V<sub>oc</sub> does not change as a result. Regarding the reliance of FF as shown in figure (10-c), on short-circuit current and open-circuit voltage and fixity of I<sub>sc</sub> and V<sub>oc</sub>, this parameter also remained fixed. Regarding the reliance of solar cell efficiency on I<sub>sc</sub>, V<sub>oc</sub> and FF, the efficiency changes with the change in I<sub>sc</sub>, V<sub>oc</sub> and % FF. Since V<sub>oc</sub> and FF are fixed and independent of the chamber pressure, as shown in figure (10-a) and (10-b), it is all clear that the solar cell efficiency (% PCE) as shown in figure (10-d), has changed slightly with I<sub>sc</sub> change. Since the change is very subtle. This means that according to table 8, this change is something around 0.038%, which is very small.

It can be concluded that efficiency of the simulated perovskite solar cell is almost independent of the changes in chamber’s pressure in making of compact layer of titanium dioxide.

The effect of pressure on bands gap energy of TiO₂ compact layer bands gap as a function of chamber’s pressure.

Using table (4), the change of bands gap energy versus different chamber pressures is drawn and the effect of pressure on bands gap energy is shown in figure 9.

Fig. 8 Compact layer (CL) thickness-dependent variation in (a) Isc, (b) Voc, (c) % FF, and (d) % PCE.

Fig 9 TiO₂ compact layer bands gap energy as a function of chamber’s pressure.

Fig. 10 Compact layer (CL) pressure-dependent variation in a) Isc, b) Voc, c) % FF, and d) % PCE
The effect of device deposition power on the band gap energy of TiO₂ prepared at constant thickness and pressure

According to table (4) and figure (7, 9 and 11), the rate of bands gap change is (3.618 to 3.687) eV, which shows that bands gap energy highly depends on the conditions under which the process is carried out [67]. Titanium dioxide’s bands gap energy deposited through DC magnetron sputtering method under different powers and pressures in (3.20-3.28) eV limit which is in line with the results of this study [68]. The bands gap energy of thin film of titanium dioxide with mixed phase has been reported in (3.58 to 3.75) eV limit [69] which is in line with bands gap energy of this study in (3.576-3.687) eV.

The dependence of photovoltaic performance on TiO₂ thin film in different deposition power

Figure (12-a) shows that Iₜₑ depends on the change of deposition power of the device and with an increase of the power, in 200 to 240 watts, Iₜₑ current changes from 14.899(mA) to 22.368 (mA) and an approximate current increase of 33% happens. In other words, the series resistance decreases with the increase of the power and the current increases as a consequence. According to figure (12-b), Vₜₑ remain fixed, (1.02), showing that the change in deposition power has no effect on the open-circuit voltage. Regarding the fixity of Vₜₑ, the change trend of % FF as shown in figure (12-c), has an ascending pattern with an increase of power. With the reliance of this parameter on Iₜₑ, its change trend is almost proportionate to short-circuit current having an ascending trend with an increase of power. Finally, the efficiency of perovskite solar cell (%) PCE as shown in figure (12-d) increases with power increase so that it reaches to its highest rate of 18.371% in 240 watts.

Conclusion

The simulation technique of a solar cell for investigating its parameters like Iₜₑ, Vₜₑ, % FF, % PCE is very useful and low cost. In this study, thin layer of TiO₂ was prepared under different lab conditions like thickness, changing deposition power of the device and changing chamber pressure using radio frequency magnetron sputtering method and its effects on optical parameters of bands gap energy of TiO₂ thin layer was investigated. In the next step, a tin-based perovskite solar cell was simulated by COMSOL multiphysics software followed by analysis of the effect of the preparation conditions of TiO₂ electron transporting layer on the performance and efficiency of the solar cell. The tin-based perovskite solar cell is important since tin is not toxic and is easily accessible with low cost. The results of the simulation showed that the 30 nm layer under 240 watts power and 3.5×10⁻² mbar pressure was the most appropriate layer for trapping light. In this prepared layer, the highest efficiency was % PCE = 18.371 and other parameters obtained Iₜₑ = 22.368 mA, Vₜₑ = 1.02 mV, % FF = 80.522.

Declaration of competing interest

1.Availability of data and materials (not applicable) and the reason is the disagreement of all the authors of the article.
2.The author(s) declare(s) that they have no known competing financial interests.
3.funding (not applicable)

Parameters Using table (4), the change of bands gap energy versus different deposition powers are drawn and the effect of bands gap energy power is shown in figure 11.

Fig. 11 TiO₂ compact layer bands gap energy as a function of deposition power.

Fig. 12 compact layer (CL) Power-dependent variation in a) Isc, b) Voc, c) % FF, and d) % PCE

References

1. Kulkarni, S.H., Anil, T.R.: Rural Electrification through Renewable Energy Sources: An Overview of Challenges and Prospects. International Journal of Engineering Research. 3, 384 (2014)
2. Stone, J.L.: unlimited electrical energy from the sun. Physics Today. 2780, 1990 (1999)
3. Stone, J.L.: unlimited electrical energy from the sun. Photovoltaics. 4, 9 (1993)
4. Herzog, A.V, Lipman, T.E., Kammen, D.M.: Perspective and Overview of Life Support systems and Sustainable Development Perspective and Overview of Life Support systems and Sustainable Development, (University of California, Berkeley), 2001.
5. Sommerfeld, J., Buys, I., Vine, D.: Residential consumers’ experiences in the adoption and use of solar PV. Energy Policy. 105, 10 (2017)
6. Lior, N.: Sustainable energy development: The present (2009) situation and possible paths to the future Energy. 35, 3976 (2010)
50. Lee, C., Elstathiadis, H., Raynolds, J.E., Haldar, P.: Two-dimensional computer modeling of single junction a-Si: H solar cells. In Photovoltaic Specialists Conference (PVSC) 34th IEEE (2009)

51. Hodes, G.: Perovskite-based solar cells. Applied physics Science. 342, 317 (2013)

52. Chen, Q.-Y., Huang, Y., Huang, P.-R., Ma, T., Cao, C., He, Y.: Electro negativity explanation on the efficiency-enhancing mechanism of the hybrid inorganic–organic perovskite ABX3 from first principles study. China Physics B. 25, 027104 (2015)

53. Xosrovshvili, G., Gorji, N.E.: Numerical analysis of TiO2/Cu2ZnSnS4 nanstructured PV using SCAPS1D. Journal of Modern Optics, 60, 939 (2013)

54. Lin, P., Lin, L., Yu, J., Cheng, S., Lu, P., Zheng, Q.: Numerical Simulation of Cu2ZnSnS4 Based Solar Cells with In2S3 Buffer Layers by SCAPS-1D. Journal of Applied Science and Engineering. 17, 383 (2014)

55. Wu, H., Wang, L.-S.: A study of nickel monoxide (NiO), nickel dioxide (NiO2), and Ni(O2)Ni(OO) complex by anion photoelectron spectroscopy. The Journal of Chemical Physics. 107, 1621 (1998)

56. Madelung, O.: Semiconductors Data Handbook. (third ed. Springer), 1-247 (2004)

57. Fonas, S.: Solar Cell Device Physics (second ed Academic Press) 1-381 (2010)

58. Stoumpos, C.C., Malliakas, C.D., Kanatzidis, M.G.: Semiconducting tin and lead iodide perovskites with organic cations: phase transitions, high mobilities, and near-infrared photoluminescent properties. Inorganic chemistry. 52, 9019 (2013)

59. Chen, D., Wang, Y., Lin, Z., Huang, J., Chen, X., Pan, D., Huang, F.: Growth strategy and physical properties of the high mobility p-type CuI crystal. Crystal Growth & Design. 10, 2057 (2010)

60. Yin, W.J., Shi, T.T., Yan, Y.F.: Unique properties of halide perovskites as possible origins of the superior solar cell performance. Advance Materials. 26, 4653 (2014)

61. Sze, S.M., Ng, K.K.: Physics of semiconductor devices, (Third edition). Wiley (2007)

62. Roati, V., Colella, S., Lerario, G., Marco, L.D., Rizzo, A., Listorti, A.: Investigating charge dynamics in halide perovskite-sensitized mesostructured solar cells. Energy and Environmental Science. 6, 1889 (2014)

63. Marchioro, A., Teuscher, J., Friedrich, D., Kunst, M., van de Krol, R., Moehl, T., Grätzel, M., Moser, J.-E.: Unravelling the mechanism of photoinduced charge transfer processes in lead iodide perovskite solar cells. Nature Photonics, 8, 250 (2014)

64. Wang, X., Fang, Y., He, L., Wang, Q., Wu, T.: Influence of compact TiO2 layer on the photovoltaic characteristics of the organometal halide perovskite-based solar cells. Materials Science in Semiconductor Processing. 27, 569 (2014)

65. Elumalai, N.K., Uddin, A.: Open circuit voltage of organics solar cells: An in-depth review. Energy Environmental. Science. 9, 391 (2016)

66. Li, Ch., Lv, L., Qin, L., Zhu, L. Teng, F., Lou, Zh., Deng, Zh., Hu, Y., Cui, Q., Hou, Y.: Investigation on the Overshoot of Transient Open-Circuit Voltage in Methylammonium Lead Iodide Perovskite Solar Cells. Materials. 11, (2018)

67. Poddar, N.P., Mukherjee, S.K.: Characterization of TiO2thin films deposited by using dc magnetron sputtering. Carbon–Sci. Tech. 8, 1 (2016)

68. Singh, P., Kaur, D.: Room temperature growth of nanocrystalline anatase TiO2 thin films by dc magnetron sputtering. Physica B: Condensed Matter. 405, 1258 (2010)

69. Nair, P.B., Justin victor, V.B., Daniel, G.P., Joy, K., Ramakrishnan, V., Thomas, P.V.: Effect of RF power and sputtering pressure on the structural and optical properties of TiO2 thin films prepared by RF magnetron sputtering. Applied Surface Science. 257, 10869 (2011)