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Ministry of Higher Education and Scientific Research

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Faculty of technology



THEME :

Inslight into novel HTL and ETL materials and architectures for perovskite solar cells with efficiency using scaps-1D

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شكر وعرفان :

الحمد لله الذي أمر بشكره ووعد من شكره بالمزيد ونشهد أن لا اله إلا الله هو المبدئ والمعيد، ونشهد أن محمدا عبده ورسوله الذي بعث بالقرآن المجيد،

اللهم صل عليه وعلى آله وصحبه أجمعين.

والحمد لله الذي وفقنا لإنجاز هذا العمل المتواضع، وما توفيقنا إلا بالله عليه توكلنا وعليه فليتوكل المتوكلون.

" من لا يشكر الناس لا يشكر الله"

نتقدم بأحر تشكراتنا إلى الأستاذة المشرفة د.رابحي سلمى و الأستاذ د.بنعطاالله محمد لقبولهم الإشراف على هذه المذكرة، وعلى ملاحظاتهم النيرة و تشجيعاتهم القيمة التي ساعدتنا في إعداد بحثنا هذا.

الى كل أهلنا وأصدقائنا جازاهم الله خيرا.

إلى كل من ساهم و لو بكلمة طيبة في إعداد هذا العمل المتواضع سائلين المولى تبارك و تعالى ان يجزيهم عنا و عن الآمة الإسلامية كل الخير إنه ولي ذلك و القادر عليه.

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ABSTRACT

In this project, we aim to perform modeling and numerical simulation of a solar cell using the SCAPS-1D simulation program. The studied solar cell has an N-I-P type structure, with its active layer based on a hybrid (organic-inorganic) triple cations materials (($\mathbf{FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}}$). This semiconductor has demonstrated its efficiency in the field of photovoltaic. The objective of this study is primarily focused on improving the performance of the solar cell, specifically enhancing the reproducibility and stability of perovskite solar cells, as they tend to degrade rapidly. To achieve this, we have proposed the use of novel such as **Se/Te,Cu_2O, D-PBTTT-14,** ZrS_2, and WS_2 as Holes transport layer (HTL) and Electrons transport layer (ETL) respectively and varying the thickness of the active layer to obtain the optimal parameters that ensure the proper functioning of the cell. The electrical behavior of 3D PVK-based solar cells is a crucial aspect to analyze and enhance in order to improve their overall performance.

Keywords: SCAPS-1, triple cations, hybrid, perovskite, photovoltaics, ETL, HTL.

Résumé :

Dans ce projet, nous visons à effectuer la modélisation et la simulation numérique d'une cellule solaire en utilisant le programme de simulation SCAPS-1D. La cellule solaire étudiée a une structure de type N-I-P, avec sa couche active basée sur un triple cations hybride (organique-inorganique) $((FAPbI3)_{0,77}(MAPbBr3)_{0,14}(CsPbI3)_{0,09})$. Ce semi-conducteur a démontré son efficacité dans le domaine du photovoltaïque. L'objectif de cette étude est principalement axé sur l'amélioration des performances de la cellule solaire, en particulier l'amélioration de la reproductibilité et de la stabilité des cellules solaires pérovskite, car ils ont tendance à se dégrader rapidement. Pour y parvenir, nous avons proposé l'utilisation de nouveaux produits tels que Se/Te,Cu_2O, D-PBTTT-14, ZrS_2 et WS2 comme couche de transport des trous (HTL) et couche de transport des électrons (ETL) respectivement et la variation de l'épaisseur de la couche active pour obtenir les paramètres optimaux qui assurent le bon fonctionnement de la cellule. Le comportement électrique des cellules solaires 3D à base de PVK est un aspect crucial à analyser et à améliorer afin d'améliorer leurs performances globales.

Mots clés: SCAPS-1, triple cations, hybride, pérovskite, photovoltaïque, ETL, HTL,Cellules solaires.

ملخص

في هذا المشروع، نهدف إلى إجراء نمذجة ومحاكاة عددية لخلية شمسية باستخدام برنامج المحاكاة .SCAPS-1D تحتوي الخلية الشمسية المدروسة على هيكل نوعN-I-P ، وطبقتها النشطة تعتمد على مواد الكاتيونات الثلاثية (عضوي - غير عضوي يسمى $(FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09}$) وقد أثبت هاته المواد كفاءتها في مجال الطاقة الشمسية. تتمحور هدف هذه الدراسة في التركيز بشكل أساسي على تحسين أداء الخلية الشمسية، وتحسين خصائص إعادة إنتاجية واستقرار خلايا البيروفسكيت، حيث تتحلل بسرعة. لتحقيق ذلك، اقترحنا استخدام Se/Te,Cu_2O D-PBTTT-14 ZrS_2 WS_2 كطبقات نقل الشحنة ETL وHTL على التوالي) وتغيير سمك الطبقة النشطة للحصول على المعلمات الأمثل التي تضمن العمل السليم للخلية.

الكلمات المفتاحية: HTL، ETL، هجين، بيروفسكيت، الطاقة الشمسية،الخلية اللشمسية، SCAPS-1

GENERAL INTRODUCTION:

GENERAL INTRODUCTION:

Perovskite solar cells are known in the world of photovoltaics, since they have reached very quickly high yields and using simple and inexpensive deposition methods. This rapid progress in a short time is an unprecedented phenomenon, which is revolutionizing research on solar cells.

Since 20, hybrid halogenated perovskites, including lead iodide methylammonium $CH_3NH_3PbI_3$, has established itself as a very promising absorber for solar cells, demonstrating in a short time remarkable performances. But solar cells based on methylammonium lead iodide suffer instability and degradation, its gradation leads to the diffusion of Pb and the latter is a toxic material that has a negative impact on the environment.

One promising solution to overcome these problems is to mix the methylammonium with the formamidine by incoperating the Cesium aui known by their perfomance on the stability of the perovskite. Thus the perovskite solarcell based on $(FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09}$ will be studied in this work.

In this work, the numerical modeling of the solar cell based on 3D PVK, using SCAPS-1D is studied. Organic and inorganic materials such as Se/Te,Cu_2O, D-PBTTT-14 and two other inorganic materials ZrS_2 and WS_2 were used as (ETL) electron transport layers. A study of the effect of the thickness of the active layer will be implemented. We will also follow the evolution of the performance of the perovskite solar cell according to the temperature increase.

This Memoire is divided into three chapters; a chapter dealing with generalities on photovoltaic cells, in particular the halogenated hybrid perovskite cells. The second chapter is co-written to the simumation. This Memoire is then concluded with a genaral conclusion.

Chapter I:

State of Art about Perovskite Solar Cell

I.1 Introduction:

Photovoltaic energy results from the direct transformation of sunlightin electrical energy by means of cells generally based on crystalline silicon whichremains the most technologically and industrially advanced sector, in fact siliconand one of the most abundant elements on earth in the form of non-toxic silica.For definition the word "photovoltaic " comes from the Greek " photo " which means light and "voltaic" which originates from the name of an Italian physicist AlessandroVolta (1754 -1827) who contributed much to the discovery of electricity, then thephotovoltaic literally means light electricity[1][2].

I.2 Photovoltaic effect:

In 1839, a French physicist, Alexandre-Edmund Becquerel, discovered the creation of tension when he wasexperiment with an electrolytic cell composed of two metal electrodes placed in an electrical conductor solution[3] Electricity generation increases when exposed to light. This effect is known as photovoltaic. His discovery laid the foundation for solar cell technology. The photovoltaic effect is the backbone of cell technology. The PV effect was first studied in solids such as selenium in 1870. It was expensive and less efficiency (1% to 2%)[4] In the 1940s and early 1950s, the Czochralski method was developed to obtain Silicon crystal. With the use of this method, crystalline silicon solar cells were manufactured that had efficiency up to 11%[5].

In photovoltaic effect, when light is incident on a PN junction (N-type semiconductor region facingsunlight), photons incidents those that have an energy equivalent to that of the semiconductor energy gapare absorbed by producing electrons and holes as load carriers (Figure I1).These electrons and holes are separated due to the built-in potential. This developed voltage is measured .This DC voltage is converted into AC voltage to operate different household appliances or it is used for industry.

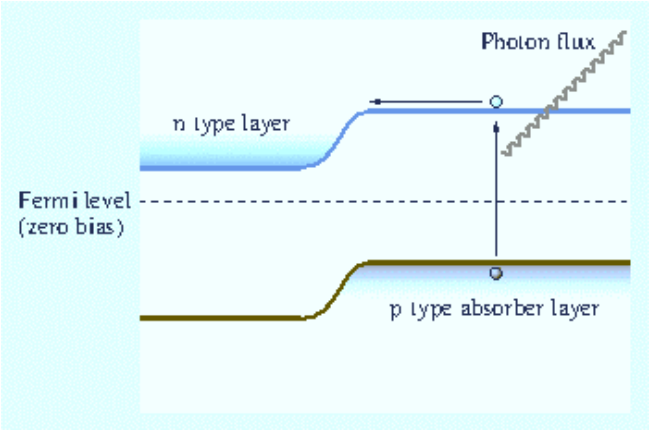


Figure I1. A PN junction showing absorption of incidence photon, generation of electron and hole and diffusion of electron towards junction[6]

I.3 Solar cell generations:

I.3.1 First generation solar cells :

These are solar cells based on crystalline Si wafers. Manufactured from Crystalline Si, thus most costlytechnique of obtaining pure Silicon crystal is involved in this technology. These solar cells are usedworldwide and these have highest commercial efficiency[7]. About 80% solar cell market is based onsingle crystalline solar cells. It was reported by Zhao et al (1998) that polycrystalline solar cells havinghoneycomb like structure have efficiency of about 19.8%. Polycrystalline solar cells are less efficient ascompared to the crystalline solar cells.

- Single crystalline solar cells
- Polycrystalline solar cells

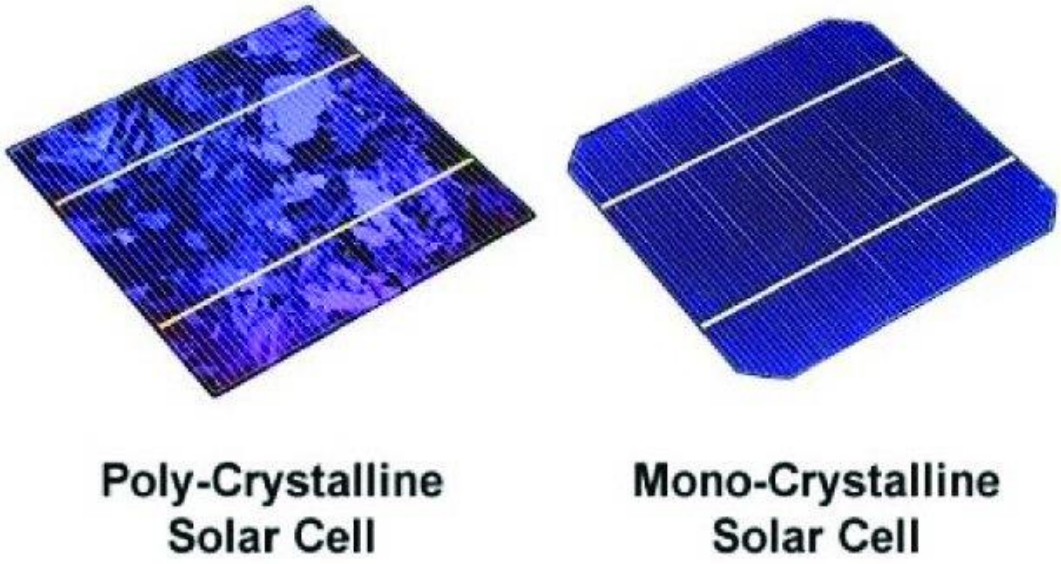


Figure I2. Silicon solar cells

I.3.2 Second generation solar cell Technology (Thin film solar cell technology):

Si crystal wafer technology is costly as it uses mostly pure crystalline Si. Obtaining pure Si is a complex and costly process. Cost of solar cells can be reduced if thin films of Si (1μm) can be deposited. Very little amount of Silicon is used by thin film technology as compared to wafer based technology. R. Chittick developed amorphous Si deposited thin films first[8]. Then his co-workers published a report on first systematic and explenatory study on plasma enhanced chemical vapour deposition technique.

I.3.3 Third generation solar cell technology :

Third generation PV cell technology refers to single junction solar cell which can overcome Shockley–Queisser limit of 31–41% power efficiency. C-Si solar cells (First generation) and thin film solar cells are having some limitations for achieving higher efficiency and to be established as Photovoltaic technology to fulfil all conditions as per golden triangle. Third generation solar cell technology consists of the following types of solar cells:

- CZTS solar cells including materials CZTSe and CZTSSe
- Dye sensitized solar cells
- Quantum Dot solar cells
- Perovskite solar cells
- Organic solar cells

To increase efficiency of solar cell, it is needed to absorb all photons in incident sunlight. A single junction solar cell will not solve this purpose. Thus multi-junction solar cell is considered as a solution to this problem.

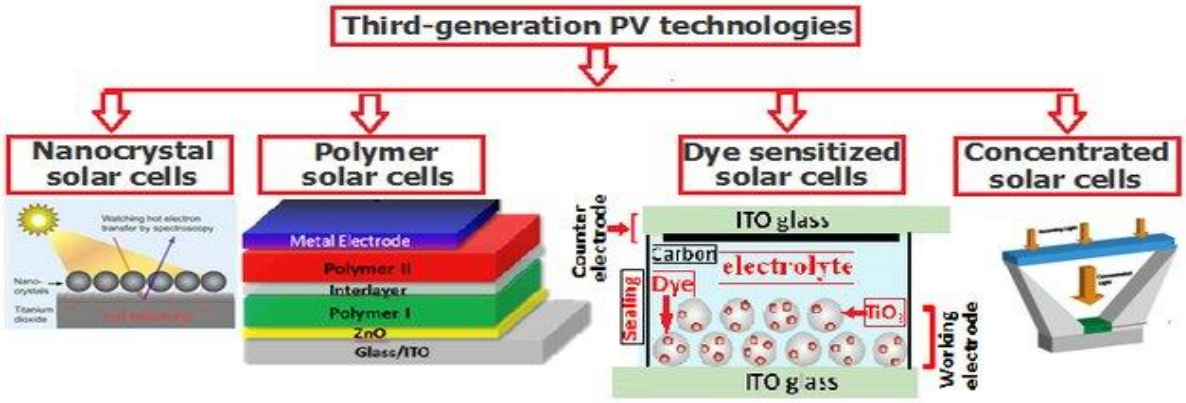


Figure I3. Third-generation PV technologies[9]

I.4 Perovskite solar cell:

I.4.1 Strecture of perovskite:

Perovskite is the name given to mineral $CaTiO_3$, after a Russian mineralogist, L.A. Perovski and type of all compounds which crystallize in same structure of ABX_3, where A and B are cations and X is the anion species.

The two most common architectures of a planarperovskite solar cell are the so called n-i-p and p-i-n.(As shown in Fig. I4)

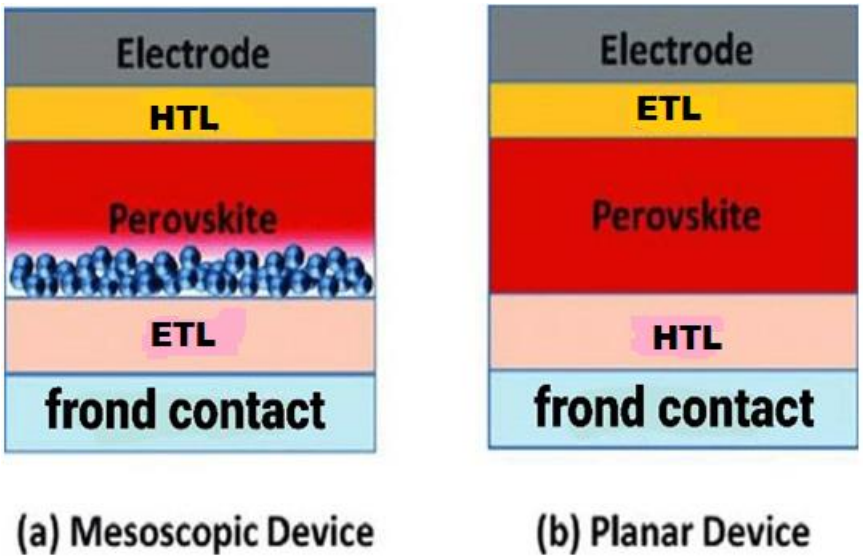


Figure I4. n-i-p and p-i-n Planar device architecture for Perovskite solar cell

For perovskite solar cells, they can be grouped into two main categories: N-I-P-type structural devices and P-I-N-type structural devices, as shown in . The difference comes from the chronological order in which the different layers of the PV system are deposited.

Effect of environmental factors like moisture and oxygen can become less damaging due to encapsulation of PSC.

The N-I-P type structure begins with the ETL (N), continues with the perovskite layer (I) and ends with the HTL (P); the P-I-N type structure being its reverse counterpart. In both cases, the roles of these layers remain the same: the perovskite layer generates the load carriers (electrons and holes) which are then transferred to the corresponding transport layers, i.e. electrons to the ETL and holes to the HTL, to be collected by the electrodes (respectively, cathode and anode).

I.5 Solar cell parameters :

The conversion of sunlight into electricity is determined by various parameters of a solar cell. To understand these parameters, we need to take a look at the I – V Curve as shown in **figure I 5** below. The curve has been plotted based on the data in **table I 1**.

Table I 1. Various parameters of a solar cell :

Amp [A]	Volts [V]	Watts [A*V=W]
0	V_{oc}=11.4	0
0.2	11.06	2.21
0.4	10.59	4.24
0.5	10.24	5.12
0.6	9.54	5.72
0.61	9.39	5.73
I_M=0.62	V_M=9.27	P_M=5.75
0.63	9.08	5.72
0.64	8.72	5.58
I_{sc}=0.65	0	0

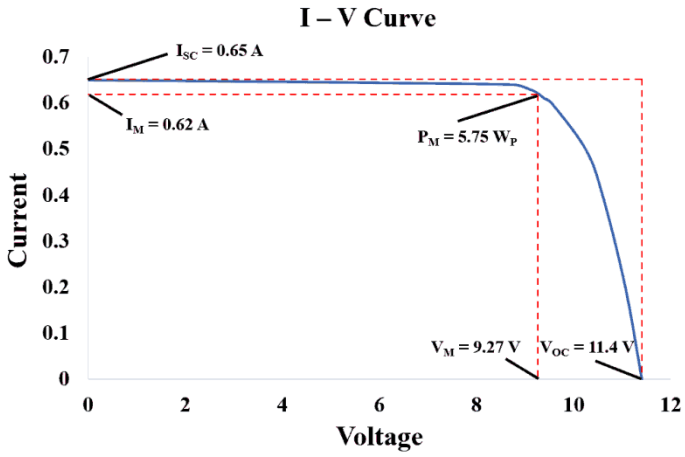


Figure I5 . I – V Curve.

The cell parameters are given by manufacturers at the STC (Standard Test Condition). Under STC the corresponding solar radiation is equal to 1000 W/m2 and the cell operating temperature is equal to 25ºC. The solar cell parameters are as follows:

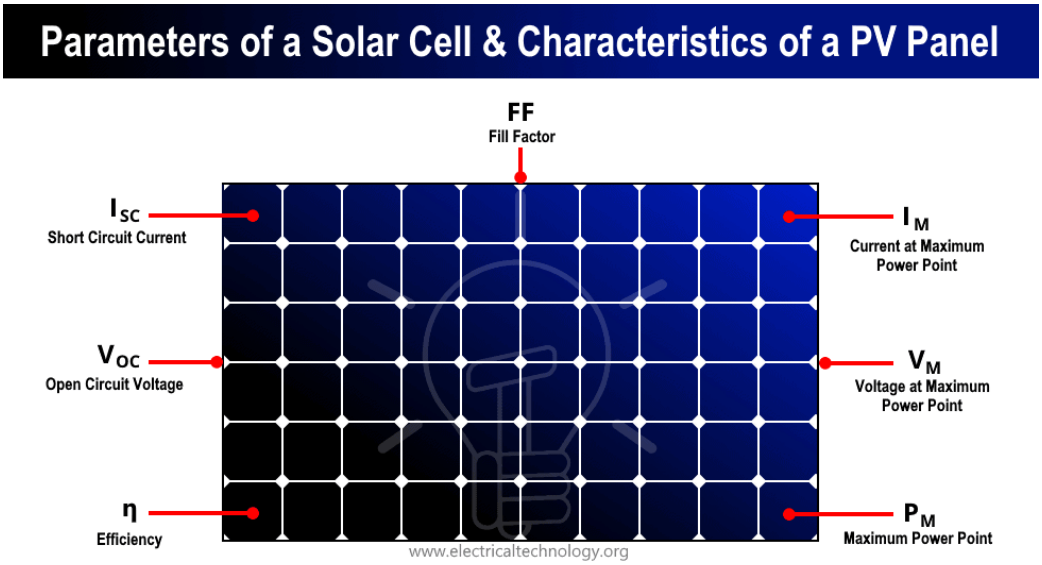


Figure I6. Parameters of a solar cell & Characteristics of a PV Panel

- **Short Circuit Current (ISC):**

Short circuit current is the maximum current produced by the solar cell, it is measured in ampere (A) or milli-ampere (mA). As can be seen from table 1 and figure 2 that the open-circuit voltage is zero when the cell is producing maximum current (I_{SC} = 0.65 A).

The value of short circuit depends on cell area, solar radiation on falling on cell, cell technology, etc. Sometimes the manufacturers give the current density rather than the value of the current. The current density is denoted by "J" and the short circuit current density is denoted by "J_{SC}". The short circuit current density is obtained by dividing the short circuit current by the area of the solar cells as follow:

$$J_{SC} = I_{SC} / A$$

Let's take an example, a solar cell has a current density of 40 mA/cm^2 at STC and an area of 200 cm^2. Then the short circuit current can be determined as follows;

$$I_{SC} = Jsc \times Area = 40\ mA/cm^2 \times 200\ cm^2 = 8000\ mA = 8\ A$$

- **Open circuit voltage (V_{oc}) :**

Open circuit voltage is the maximum voltage that the cell can produce under open-circuit conditions. It is measured in volt (V) or milli-volt (mV). As can be seen from table 1 and figure 2 that the short circuit current is equal to zero when the cell produces maximum voltage. The value of V_{OC} depends on cell technology and the operating temperature of the cell.

- **Maximum Power Point (P_M) :**

Maximum power point represents the maximum power that a solar cell can produce at the STC (i.e. solar radiance of 1000 W/m^2 and cell operating temperature of 25^{o}C). It is measured in W_{Peak} or simply W_P. Other than STC the solar cell has P_M at different values of radiance and cell operating temperature.

The cell can operate at different current and voltage combinations. But it can only produce maximum power P_M at a particular voltage and current combination. As shown in figure 2 the maximum power point is at the knee of the I – V curve and is the product of I_M and V

$$P_M = I_M \times V_M = 0.62 \times 9.27 = 5.75\ W_P$$

- **Current at Maximum Power Point (I_M) :**

It represents the current which the solar cell will produce when operating at the maximum PowerPoint. It is denoted by I_M and can be seen in figure 3 that its value is always less than the short circuit current (I_{SC}). It is measured in ampere (A) or milli-ampere (mA).

- **The Voltage at Maximum Power Point (V_M) :**

It represents the voltage that the solar cell will produce when operating at the maximum PowerPoint. It is denoted by V_M and can be seen in figure 3 that its value is always less than the open-circuit voltage (V_{OC}). It is measured in volts (V) or millivolts (mV).

- **Fill Factor (FF) :**

It represents the area covered by I_M – V_M rectangle with the area covered by I_{SC} – V_{OC} rectangle as by dotted lines in figure 3. The fill factor represents the squareness of the I – V curve. It is represented in terms of the percentage (%), the higher the fill factor in percent the better is the cell.

$$FF = P_M / (I_{SC} \times V_{OC})$$

Based on the data in table 1 and figure 2 we can determine the fill factor as follows;

$$FF = [5.75 / (0.65 \times 11.4)] \times 100 = 77.59\ \%$$

Represented in percentage by multiplying it by 100.

- ***Efficiency (η) :***

A solar cell efficiency is defined as the maximum output power (P_M) divided by the input power (P_{IN}). It is measured in percentage (%), which indicates that this percentage of input sunlight power is converted to electrical power. The input power is power density. Therefore, to calculate efficiency multiply P_{IN} at STC by area. The efficiency can be calculated as follows :

$$\eta = P_M / (P_{IN} \times \text{Area})$$

If the given area of the cell is 0.01 m^2, P_M = 5.75 W_P then the efficiency at standard test condition can be given as :

$$\eta = [5.75\ W_P / (1000\ W/m^2 \times 0.01\ m^2)] = 57.5\ \%$$

Represented in percentage by multiplying it by 100.

Chapter II: Theoretical Simulation

II.1 Introduction:

In this chapter, we will discuss an essential step in the new product R&D process.

With the development of the computer tool, numerical simulation software and their calculation code dedicated to the field of application (Finite element calculation for thermal, fluidic, mechanical resistance, etc.), have become the cheapest and fastest alternative to real trials to develop new products, optimize an existing design or opt for a technological choice over another by arguing with a simulation report. The development of photovoltaic panel cells is no exception to the rule, numerical simulation tools have been created to reduce the cost of real-life test companions and allow the choice of semi-materialdriver with the comparison criteria mentioned in the previous chapter.

II.2 SCAPS-1D Software Overview

SCAPS-1D acronym for «Solar Cell Capacitance Simulator one Dimension» is a program developed at the University of Gent in Belgium with Windows/CVI National Instruments by Marc Burgelman et al. This program is designed specifically for the simulation of photonic devices such as CdTe and CIGS cells.This software has several advantages, Some of the key benefits of SCAPS-1D include:

- High speed of execution;
- Ease of exporting results (results obtained are in text format);
- The ability to introduce seven semiconductor layers,
- The possibility of introducing interfaces and taking into account the phenomenon of recombination and the levels of defects in it.

SCAPS 1D explores fundamental properties such as:

- ✓ the I_{SC} short circuit current,
- ✓ the open circuit voltage V_{OC},
- ✓ the current density Jc,
- ✓ the voltage characteristics I-V,
- ✓ capacity-frequency (C - f),
- ✓ the efficiency of the power conversion of the device η,
- ✓ quantum efficiency QE,
- ✓ the filling factor FF.

In the SCAPS-1D Start Panel (see **Figure II 1**), there are several sections, numbered from 1 to 6.

Section 1 shows that the problem box defines a complete solar cell structure containing several layers and physical properties. In section 2, the action box is used to define the parameters of the I-V characteristic scale, the parameters of the quantum efficiency scale (QE or IPCE), the parameters of the capacitance-voltage scale (C - V) and the capacitance-frequency (C - f). In section 3, the illumination box allows you to select the light and dark conditions for the simulation and the required spectrum file. In section 4, the work point box is used to define the working temperature and to describe parasitic resistances, such as series and bypass resistances. Section 5 allows for single calculations, batch calculations and curve fit calculations. Recording and script configuration options are also available. Finally, in section 6, the "Calculation Results" box gives the options to check the results of the simulated device, such as the energy band (EB), I-V, QE characteristics, etc.

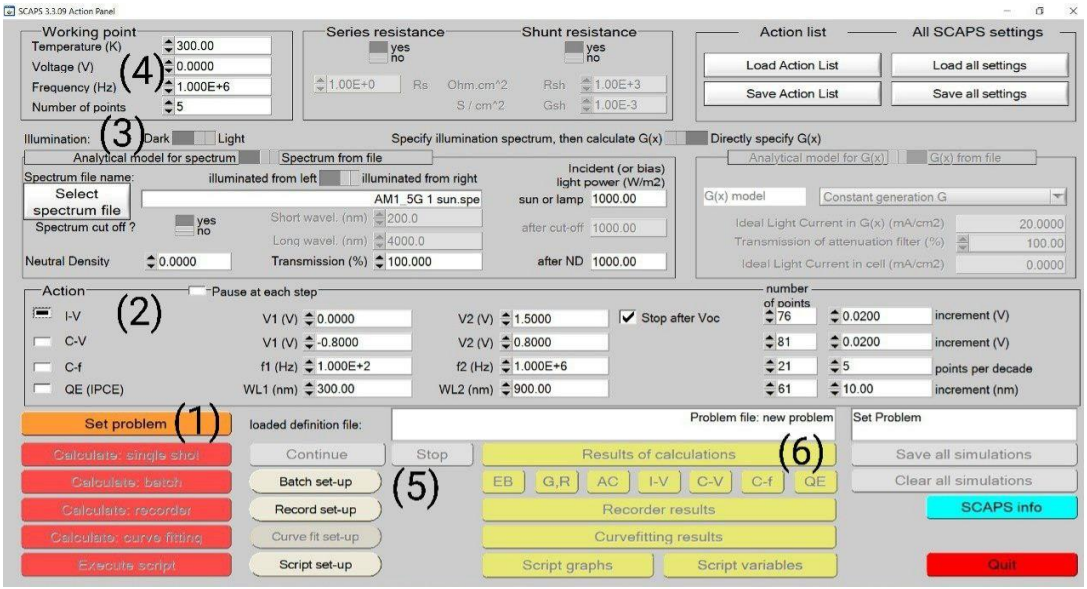


Figure II 1.*SCAPS-1D Software Startup Control Panel* ***[1]***

Starting the construction of the solar cell structure by clicking on section one, **Figure II 2** , shows three different sections that are available and offer options to build the desired solar cell structure with/without the interface layer.

Section 1 helps us define the different layers to complete the structure of the device, including the front and rear contact. Section 3 presents the constructed device, and there are other options for selecting the light illumination and the applied voltage sides using either the front contact side or the rear contact side. Section 3 allows you to create a new structure file or load the available file and save the required device structure file.

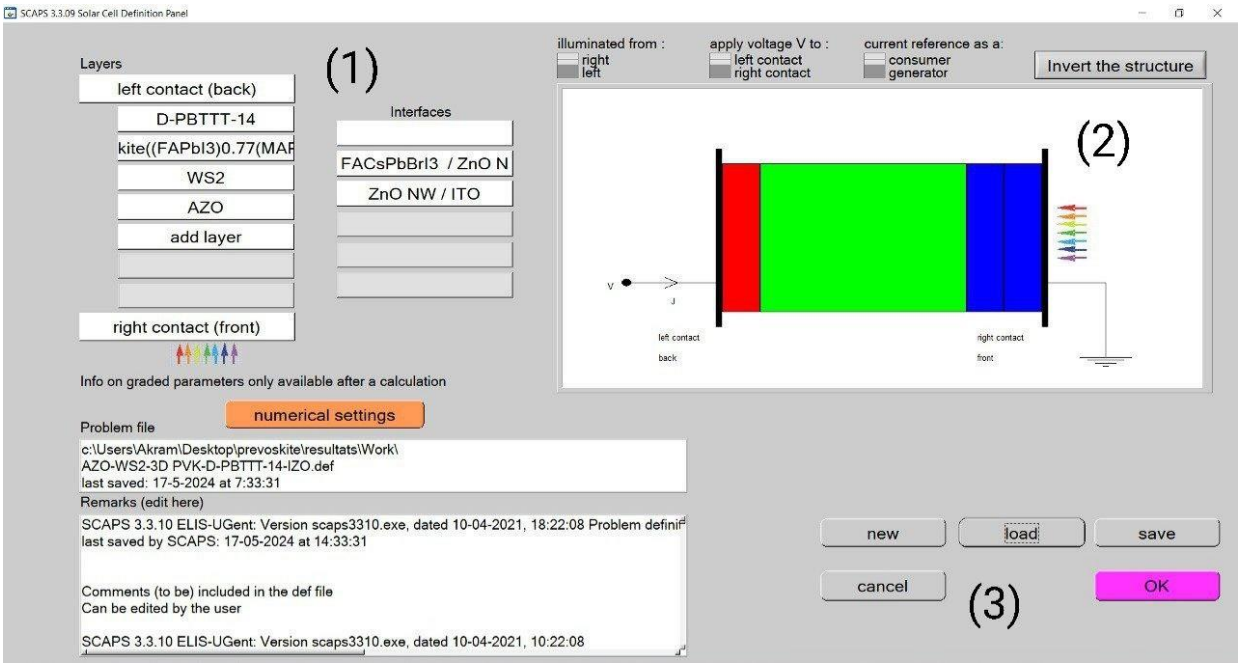


Figure II 2. SCAPS-1D solar cell definition panel with perovskite structure

Figure II 3.shows the Material and Defect Definition Panel, which defines the physical parameters of each layer, such as Eg (gap energy), χ(electronic affinity), ε(dielectric constant), NC (conductivity band state density), NV (valence band state density), μN (electron mobility), μP (hole mobility), NA (donor dopant concentration), ND (donor dopant concentration), etc..

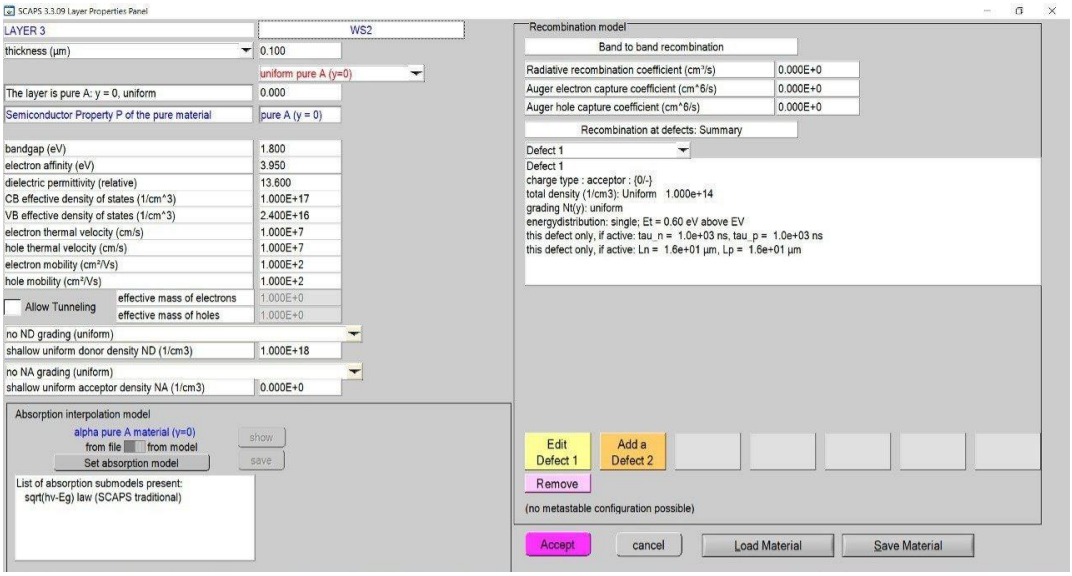


Figure II 3. Layer Physical Properties Definition Panel

II.2.1Structure of Solar cells:

The performance of perovskite-based photovoltaic cells depends on several parameters, such as the cell architecture, the materials used for contacts, the active layer, the interfacial layers for the transport of ETL electrons and for the transport of HTL holes as well as the techniques and conditions of manufacture **[2]**

In our work we considered $((FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09})$ as active layer and WS_2 as hole transport material (ETL) with D-PBTTT-14 as electron transport material (HTL).

The solar cell to be built is of type P-I-N. The numerical simulation is carried out using the simulation software SCAPS-1D to analyze the effect of different parameters such as thickness, doping, defects and temperatureon the efficiency of the structures of the perovskites solar cell.

III.2.2 Parameters and properties of the cell to be studied:

Table II 1 shows the parameters of the layers that build the perovskites solar cells; we will use these parameters to simulate the short-circuit current, open circuit voltage, fill factor and cell efficiency in this cell.

Table II 1 : Parameters used for simulating perovskite solar cell structures **[3]**

	Front contact	**3D PVK**	**Back contact**	**ETL**		**HTL**	
Parameters	**AZO**	**$(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$**	**IZO**	**WS_2**	**ZrS_2**	**D-PBTTT-14**	**Se/Te:Cu_2O**
Thickness (nm)	100	550	/				100
E_g (eV)	3.10	1.5	/	1.8	2.5	2.16	1.88
χ (eV)	4.1	3.9	/	3.95	4.1	3.2	3.53
ε_r	9.00	10	/	13.6	16.4	10	7.11
N_c (cm^{-3})	1.1×10^{17}	2.7×10^{18}	/	1×10^{17}	2.2×10^{18}	2.8×10^{19}	2.02×10^{17}
N_v(cm^{-3})	1.0×10^{18}	3.9×10^{18}	/	2.4×10^{16}	1.8×10^{19}	1.0×10^{19}	1.17×10^{19}
μ_n ($cm^2V^{-1}s^{-1}$)	100	10	/	100	2.3×10^{3}	2.83×10^{-3}	1297
μ_p ($cm^2V^{-1}s^{-1}$)	25	10	/	100	1.3×10^{3}	2.83×10^{-3}	1297

N_D (cm^{-3})	1.0×10^{15}	1.0×10^{9}	/	1×10^{18}	1×10^{15}	0	0
N_A (cm^{-3})	0	1.0×10^{9}	/	0	0	1×10^{18}	3.0×10^{18}
N_t (cm^{-3})	1.0×10^{10}	1.0×10^{14}	/	1×10^{14}	1×10^{15}	1×10^{14}	1.0×10^{15}
Work Function (eV)	4.19 -		/				
Reference	[1]	[2]	[3]	[4]	[5]	[6]	[7]

Chapter III : Results and Discussions

III.1 Introduction :

In this chapter we will present and discuss our simulation results of the perovskite solar cell based on $CH_3NH_3SnI_3$. For these solar cells the most used component as an active layer is $CH_3NH_3PbI_3$, which is referred to as MAPI, or lead iodide methylammonium. While MAPI-based perovskites is toxic because of the presence of Pb, which can destabilize the further commercialization of these cells.

One of the alternative soulutioons is a perovskite material that contains the tin Sn aulieu of Pb it is the iodide of tin methylammonium ($CH_3NH_3SnI_3$ or MASI). Many researchers have started to devolve $CH_3NH_3SnI_3$-based cells and what we have been trying to do is also us.

The tin exists in nature and it has almost the same electronic properties as the Pb. In addition, Sn-based perovskites have good absorption to visilble light and high mobilities of loads which leads to high solar cell performance. Transport layers and architecture also play an important role in the performance of solar cells.

III.2 The simulated structure :

Layers of the simulated soliared cell ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$) are stacked under the N-I-P structure. This structure starts with the ETL (N), continues with the perovskite layer (I) and ends with the HTL (P).

In our case, the material of the N layer is 'WS_2' tungsten sulphide; the active layer I is perovskite ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$) and the material the last layer P is a conductive polymer D-PBTTT-14. These materials have good electronic properties, with regard to ETL, WS_2 has optical and electronic properties appreciated in the field of electronics. For HTL, the most commonly used material in perovskite photovoltaics is D-PBTTT-14 , because it is simple to implement and efficient in cells. Thus it is particularly used in the case of perovskite cell development in the N-I-P type structure.

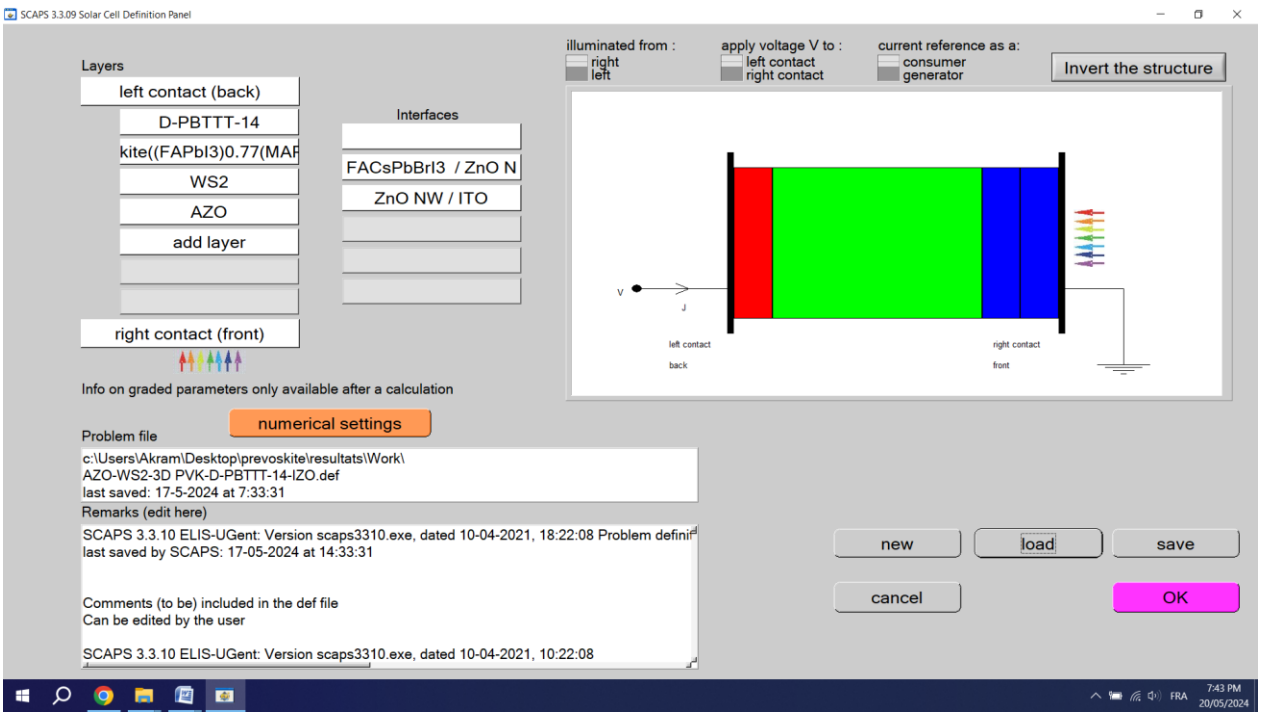


Figure III7 :the structure of the solar cell simulated by scaps

III.3 Simulation of solar cells :

After selecting the materials of the layers N, I, P with their properties we need them for the SCAPS; we modeled solar cells Perovskites. The cells are illuminated by a single face (front face of the HTL side), and we calculated for the very first time the characteristic density of the current-voltage (J-V). Table 2 and 3 shows the current-voltage characteristic (J-V) of this cell under an illumination by the solar spectrum AM 1.5 and a power density of 1000w/m².

Table III 1: ETL the photovoltaic characteristics of perovskites solar cells using WS_2 as an ETL:

ETL (WS2)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
AZO/WS2/3D PVK/D-PBTTT-14	1.18	25.81	80.62	24.54
AZO/WS2/2D PVK/D-PBTTT-14	1.53	7.24	85.55	9.46
AZO/WS2/3D PVK/Se-Te,Cu_2O	1.18	25.83	84.57	25.77
AZO/WS2/2D PVK/Se-Te,Cu_2O	1.55	7.31	85.77	9.71

Table III 02:the photovoltaic characteristics of perovskite solar cells using ZrS_2 as an ETL

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
AZO/ZrS_2/3D PVK/D-PBTTT-14	1.18	25.99	80.49	24.65
AZO/ZrS_2/2D PVK/D-PBTTT-14	1.25	2.35	85.94	2.54
AZO/ZrS2/3D PVK/Se-Te,Cu_2O	1.18	26.01	84.46	25.91
AZO/ZrS_2/2D PVK/Se-Te,Cu_2O	1.26	2.35	86.56	2.57

Based on these results, two of them have completed very high ECPs: AZO/ZrS_2/3D PVK/Se-Te,Cu_2O and AZO/WS_2/3D PVK/Se-Te,Cu_2O, but we will focus on one currency: AZO/WS2/3D PVK/D-PBTTT-14. Figure01 shows the photovoltaic characteristic of AZO/WS_2/3D PVK/D-PBTTT-14, where V_{OC}=1.18 V, J_{SC} =25.81mA/cm^2, FF= 80.62%, PCE =24.54%. omparing these parameters with other considered solar cells they are considered very good parameters, but despite this we will try to optimize the photovoltaic parameters of this currency. .

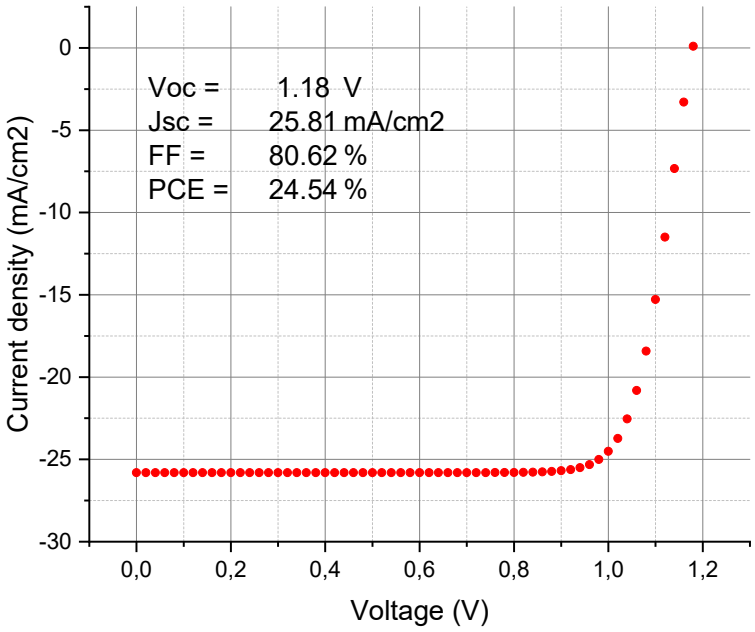


Figure III 2. J-V characteristics of the 3D PVK-based solar cell using the photovoltaic parameters obtained from simulation for **AZO/WS_2/3D PVK/D-PBTTT-14 device**

We will try to improve the yield obtained (19%) by optimizing one of the technological parameters, namely the thickness of the active layer ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$). Thus, we will simulate the effect of temperature on the complete solar cell.

III.3.1 The effect of the thickness of the active layer on the photovoltaic parameter:

We varied the thickness of the active layer ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$) from 100 nm to 800 nm by a 50 nm increments. At each thickness we extracted J_{SC} short-circuit current density, V_{OC} open-circuit voltage, form factor FF, and output η(eta), these performances are presented in **Table III3**.

Table III 3: The differences photovoltaic performances of the solar cell as a function of the thickness of the active layer:

Thikness (µm)	**Voc (V)**	**Jsc (mA/cm^2)**	**FF (%)**	**PCE (%)**
0,1	1,25	15,75	83,09	16,34
0,15	1,23	18,21	82,68	18,57
0,2	1,22	20,1	82,29	20,22
0,25	1,21	21,56	81,94	21,45
0,3	1,21	22,71	81,65	22,37
0,35	1,2	23,62	81,4	23,06
0,4	1,19	24,35	81,17	23,59
0,45	1,19	24,94	80,97	24
0,5	1,18	25,42	80,79	24,31
0,55	1,18	25,81	80,62	24,54
0,6	1,18	26,14	80,47	24,72
0,65	1,17	26,41	80,33	24,85
0,7	1,17	26,64	80,2	24,95
0,75	1,16	26,84	80,08	25,03
0,8	1,16	27	79,97	25,08

To better visualize the effect of the thickness on the performance of this photovoltaic cell, we traced the four performances according to the thickness. Figure 03 shows these performances (V_{oc}, J_{sc}, FF and PCE).

Figure 03 a shows the open circuit voltage as a function of active layer thickness ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$). We observe that this tension decreases with the thickness. This gradual decrease of the open circuit voltage with the increase of the layer thickness, goes from 1.25 V to 1.16 V.

In the second performance, Figure 03 also shows the evolution of the current density Jsc as a function of the thickness of the active layer. A steady increase in the short-circuit current is observed as the layer thickness increases from 15.75 mA/cm^2 to 27.00 mA/cm^2 in the range from 100 nm to 800 nm.

The filling factor FF (%) is shown in Figure 03. We observe a decrease in the filling factor, from 16.34% to 25.08%.

Now we come to the performance of the solar cell. As already mentioned, PCE efficiency is a measure of the overall efficiency of a solar cell to convert light energy into electrical energy. The results presented in Figure 03 dmshow a significant increase in efficiency with the increase in layer thickness, from 16.34% to 25.08%.

In summary, these results indicate a correlation between the active layer thickness of $(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$ and the performance of the global perovskite solar cell (see Figure 03). Higher thickness promotes higher values of open circuit voltage, short circuit current density and overall efficiency. The correct result is obtained for a 750nm thick ($(FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09}$) active layer thickness. At this thickness:

- 24.54% efficiency means that the solar cell efficiently converts 24.54% of the received solar energy into usable electricity. Such a high efficiency is considered excellent for a solar cell, as most commercial solar cells have lower yields, usually between 15% and 22%.
- Open circuit voltage (V_{oc}) of 1.18 V is also considered good. This means that more maximum power is available, which is beneficial for many applications.
- Filling factor (FF) of 80.62% is considered a good figure. This indicates that the solar cell efficiently uses 71% of its maximum voltage to provide electricity.

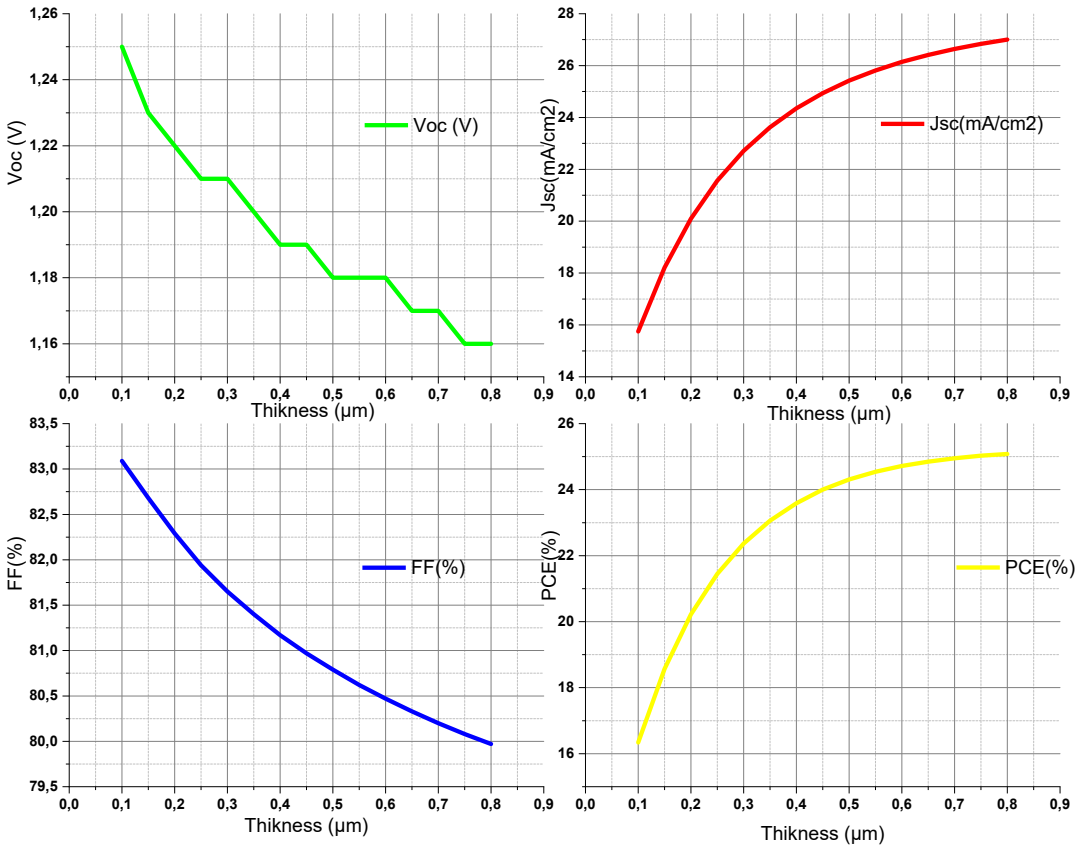


Figure III 3. J-V characteristics of the 3D PVK based solar cell using the photovoltaic parameters obtained from simulation for optimized device:

AZO/WS2/3D PVK/D-PBTTT-14

With thickness: Green) Variation of Voc, Red) Variation of Jsc, Bleu) Variation of FF and Yellow) Variation of PCE as function of Thickness (µm) .

In this work, we changed the thickness of the perovskite layer to achieve good results, and we obtained the following results in the table above. From a thickness of 0.1 to 0.45 micrometers, we observed an increase in PCE (%), but at a thickness of 0.75 micrometers, we achieved the highest PCE (%) rate, with a result of 25.03%.

Perovskite thickness increased the photoconversion efficiency, but the interesting point is that the increase did not continue in the same shape after the maximum thickness (0.75 micrometers). Interestingly, this shows that there is a limit to the benefit of perovskite increase, and this may be due to factors such as light absorption or the distribution of charges within the cell.

III.3.2 The temperature effect on solar cell efficiency:

In this part we will analyze the effect of temperature on the efficiency of the perovskite solar cell of an active layer $((FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09})$ 900nm thick. **Table III4** shows the results of this simulation.

Table 4: Temperature-dependent degradation of cell performance:

Temperature (K)	Vco (V)	*Jsc*(mA/cm^2)	FF (%)	Rendement (%)
300	**1.18**	**25.81**	**80.62**	**24.54**
350	**1.11**	**25.81**	**80.69**	**23.08**
400	**1.03**	**25.81**	**78.92**	**21.09**
450	**0.96**	**25.82**	**76.32**	**18.92**

These results clearly indicate that the increase in temperature has a negative impact on the performance of the perovskite-based solar cell. Higher temperature results in a decrease in $\mathbf{V_{OC}}$ open circuit voltage, **FF** fill factor and overall **PCE** efficiency. As well as short-circuit current density even though it appeared relatively stable, but can also show a slight decrease at higher temperatures. **Figure III4** shows significantly the decrease of the remdement of the cell as a function of the temperature increase.

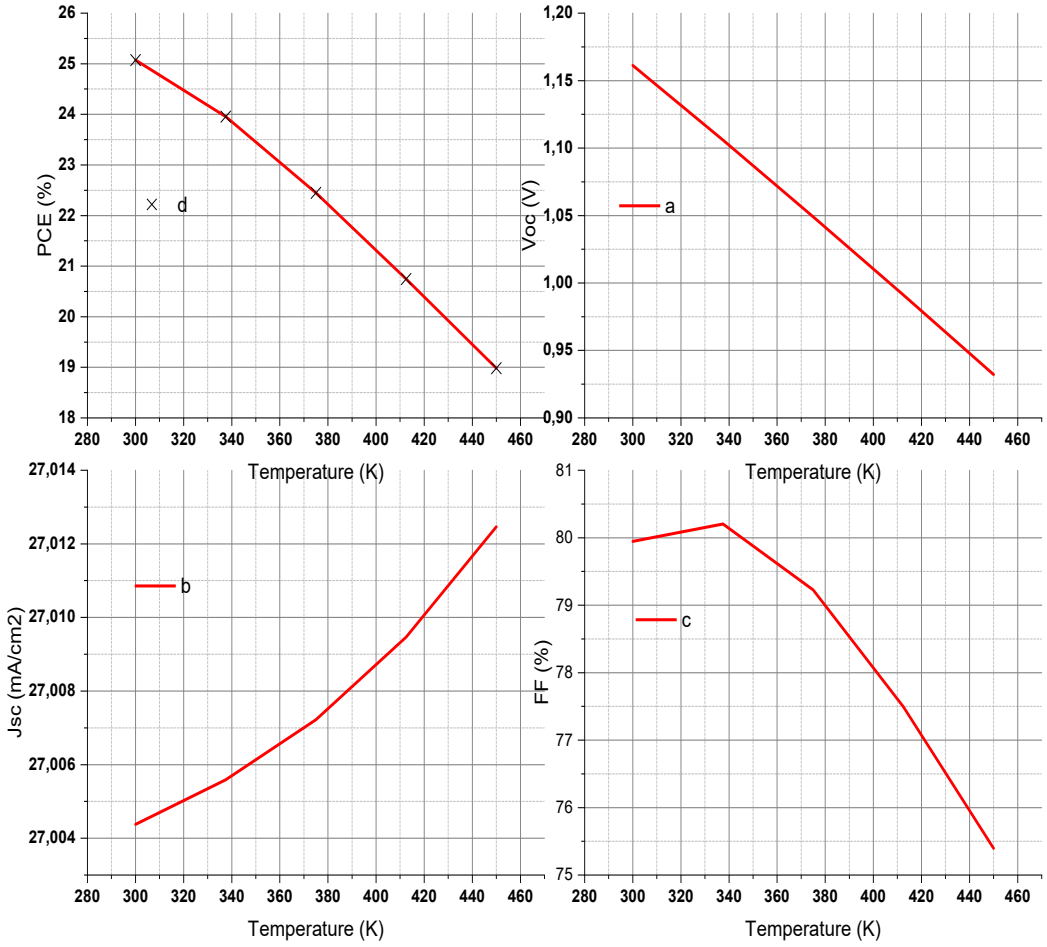


Figure III 4. the influence of the temperature increase on the photovoltaic parameters: a) VOC , b) JSC, c) FF and d) PCE

General conclusion:

General conclusion:

Perovskite is the subject of research over the past two decades, solar cells based on structured materials based on perovskite have attracted great attention in recent years, and sutout hybrid organic-inorganic trible cations such as $((FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09})$.

Therefore, we first conducted a brief state of the art of solar cells, their electrical characteristics, and then the performance of a photovoltaic cell.

Our project was a numerical modification based on the effect of active layer thickness and temperature on solar cell perfomances. A modification of the solar cell based on perovskite 3D PVK, using the SCAPS software was made. The model of the cell with the structure N-I-P 'AZO/WS_2/3D PVK/D-PBTTT-14' was created and simulated first, and then we optimized the thickness of the active layer.

The simulation results show that the cell performance was significantly improved by increasing the thickness of the active layer. On the other hand the temperature increase of the perovskite based solar cell $((FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09})$ a negative inference on cell performances.

We have clued that the cell yield reaches its maximum value of 25.08% with an 800nm thickness of the active layer $((FAPbI3)_{0.77}(MAPbBr3)_{0.14}(CsPbI3)_{0.09})$, this yield is considered a good record in perovskite-based solar cells $((FAPbI_3)_{0.77}(MAPbBr_3)_{0.14}(CsPbI_3)_{0.09})$.

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