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Highest Efficiency of Perovskite Structure Solar Cells

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Abstract: Perovskite solar cells are the most promising photovoltaic technology in the current generation due to their rapid rise in efficiency (high absorption and large diffusion length), availability Initial the materials, low cost, easy to manufacture under very normal conditions, and high yield. This work concerned about modeled Titanium dioxide-based perovskite simulation model with FTO / TiO_2 / $CH_3NH_3PbI_3$ / NiO/Pt and used the solar cell capacitance simulator (SCAPS-1D) for analyzed. In this study NiO we used as Hole Transport Layer (HTM), TiO_2as electron Transport Material (ETL) and CH3NH3PbI3 is the perovskite absorber. We study effects for change of the thicknesses for $CH_3NH_3PbI_3$ absorber material and NiO as the (HTM) layer, TiO_2 as the (ETL) layer, addition to environment temperature and work function on the major parameters of our device solar cells. The effected thickness of CH3NH3PbI3 various from (0.05 to 0.8) µm and the best efficiency are observed at 0.05 µm. When using the best thickness for layer $CH_3NH_3PbI_3$ efficiency is constant at variant temperatures.

Keywords: ETL, HTM, Perovskites Structure, Solar Cells

1 Introduction

Recent years have seen a significant increase in interest in perovskite solar cells based on $CH_3NH_3PbX_3$ due to their simple manufacturing process and rapidly rising photoelectric conversion efficiency (PCE), which increased from 3.81% in 2009 to 22.1% in 2016 [1-7]. Due to limitations electron length and hole diffusion in perovskite absorption layers, the PCE of a corresponding perovskite solar cell is not increasing, although an increase in perovskite density would boost their luminous output. There are also accessible other perovskite parameters, such as a high absorption coefficient and a solid conveyor [8–11]. The corresponding simulation work provided the basic literature data for the construction of this model [12-14]. The software is arranged in a Set of panels where the consumer can set parameters or calculate outcomes [15]. The recombination profiles, the distribution of electric fields, the carrier transport mechanism, and the individual current densities are all explained and analyzes model physics by SCAPS.ETL and HTL are typically utilized in PSCs broad bandgap hole blocking and electron blocking materials respectively [16].

2 Numerical modeling and Device simulation

Simulation is a crucial technique for realizing a deep insight into the physical activity, the viability of the suggested physical interpretation, and the effect of physical changes on the solar cell devices' performance. For the simulation of solar cells, there are numerous simulation models available (SCAPS, AMPS, SCAP, etc). SCAPS (Solar Cell Power Simulator) is a one-dimensional simulation program with seven semiconductor input layers developed by a group of solar cell researchers from the Electronics and Information System Department, University of Ghent, Belgium Building a solar cell without stimulation works is unpractical, as is waste of time and money. It not only minimizes the risk, time, and money but also analyzes the properties of the layers and their function to maximize the efficiency of the solar cell [1]. For the work currently underway, SCAPS used to model the TiO_2/$CH_3NH_3PbI_3$/NiO perovskite solar cells in perovskite. The nanostructure of TiO_2/$CH_3NH_3PbI_3$/NiO solar heterojunction cells was simulated at different working point Thickness and was subjected to different ambient temperatures for heat investigation using SCAPS [17].

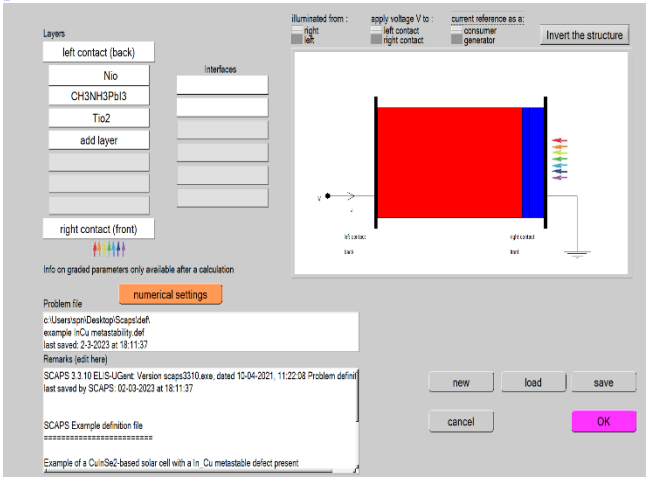

Fig. 1: SCAPS panel showing the TiO_2/$CH_3NH_3PbI_3$/NiO heterojunction solar cells definition.

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3 Solar cells capacitance simulation (SCAPS)

The simulation package of solar cells structures adapted firstly at Gent University using the structure of CdTe and $CuInSe_2$ family [16]. The SCAPS describes the performance of a solar cells mathematically using finite difference methods to solve the differential equations with number of laws and relation in physics of solar cells [18]. The express of equations as shown below:

$$J_p = -q\mu_p\, p\, \nabla U_p - K\, T\, \mu_P\, \nabla_P \quad (1)$$

$$J_n = -q\mu_n\, n\, \nabla V_n + K\, T\, \mu_n n \quad (2)$$

$$V_p = V - (1-\gamma)\Delta G/g \quad (3)$$

$$V_n = V + \gamma\Delta G/g \quad (4)$$

Equations 2 and 3 reflect the current density of the hole and the electron. Where V_b and V_n are the potential effectives expressed in Eqs 3 and 4. ΔG represents the band structure variance, μ_n, μ_p, respectively, indicate electron and hole mobility .A typical $CH_3NH_3PbI_3$ based solar cell structure consists of an absorber layer and at the top p-type (NiO) and n-type (TiO_2) is arranged at the bottom side. The cell is illuminated schematically as shown in Figure 2.

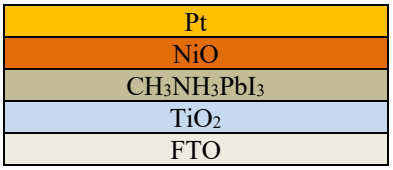


Fig. 2: Schematic representation device architecture (FTO/TiO_2/$CH_3NH_3PbI_3$ /NiO/Pt).

Under steady-state conditions, SCAPS can solve the fundamental 1-Dimensional semiconductor equations.

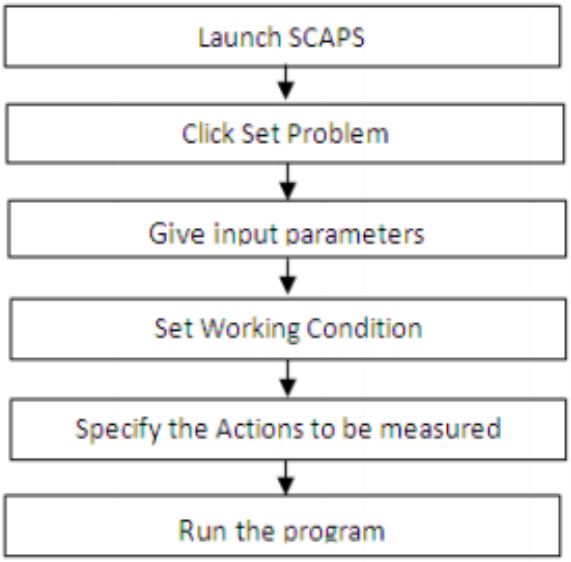


Fig. 3: Explains the simulation process using SCAPS.

4 Simulation results

1. SCAPS simulation of TiO_2/Perovskite/ NiO

Note that all simulation parameters for each layer in the device are carefully selected from those reported experimental data and other literature [19-20]. Table 1 summarizes all of the primary parameters for simulation use.

Table 1: Material properties of HTM, absorber, and ETL.

parameters	NiO	$CH_3NH_3PbI_3$	TiO_2
Band gap (ev)	3.6	1.5	3.200
Electron effinity (ev)	1.8	3.9	4.100
Dielectric permittivity	11.7	10	9.000
CB effective density of states ($1/cm^2$)	2.5E+20	2.75E+18	2.200E+18
VB effective density of states ($1/cm^2$)	2.5E+20	3.9E+18	1.000E+19
Electron mobility ($cm^2/v.s$)	2.000E+1	1.00E+1	2.000E+1
Hole mobility ($cm^2/v.s$)	1.000E+1	1.0E+1	1.000E+1

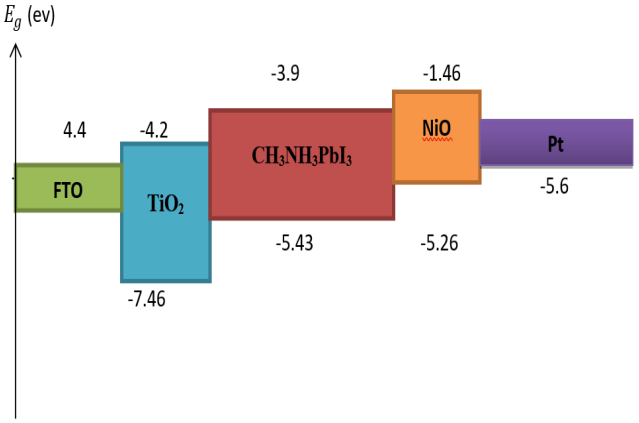


Fig. 4: Device structure and energy level diagram of the TiO_2/$CH_3NH_3PbI_3$/NiO/Pt.

Table 2: Devise Parameters use in the numerical analysis.

Left contact electrical properties (Pt)	
Thermionic emission /surface recombination Velocity of electron (cm/s)	10^7
Thermionic emission /surface recombination	10^7

Velocity of hole (cm/s)	
Metal (Pt) work function (ev)	5.6
Right contact electrical properties	
Thermionic emission /surface recombination Velocity of electron (cm/s)	10^7
Thermionic emission /surface recombination Velocity of hole (cm/s)	10^7
work function of FTO (ev)	4.4

1	1.2445	17.696089	81.57	17.96
1.05	1.2445	17.694566	81.53	17.95
1.1	1.2445	17.693040	81.49	17.94
1.15	1.2445	17.691508	81.45	17.93
1.2	1.2459	17.689968	81.31	17.92
1.25	1.2459	17.688418	81.27	19.91
1.3	1.2458	17.686858	81.23	17.90
1.35	1.257	17.685285	81.19	17.89
1.4	1.2457	17.685285	81.09	17.86
1.45	1.2456	17.682065	80.99	17.84
1.5	1.2456	17.680438	80.93	17.82

5 Result and Discussion

1. Effect of the TiO_2 layer thickness change on solar cells

Must be specified the best thickness in the absorber layer for absorb the largest number of photons thus create electron-hole pairs. We study change the thickness of TiO_2 as the ETL layer from (0.1 to 1.5) µm. We notice from the drawing that increase the thickness of the TiO_2 material leads to a decrease in efficiency, and upper value for efficiency at 1.25 µm is 19.91% as in table (3), then the efficiency decreases with increasing thickness (amount of radiation received is few). Because of partial absorption of received light by the ETL layer, bulk and surface recombination at the interface. Figure 5 shows the variation of photovoltaic parameters with the thickness of the TiO_2 (HTM). The graph shows that the FF, J_{sc} decreased as we go from thickness (0.1-1.5) µm. But there is an increased V_{oc} generally from (1.2443 -1.2456) volt.

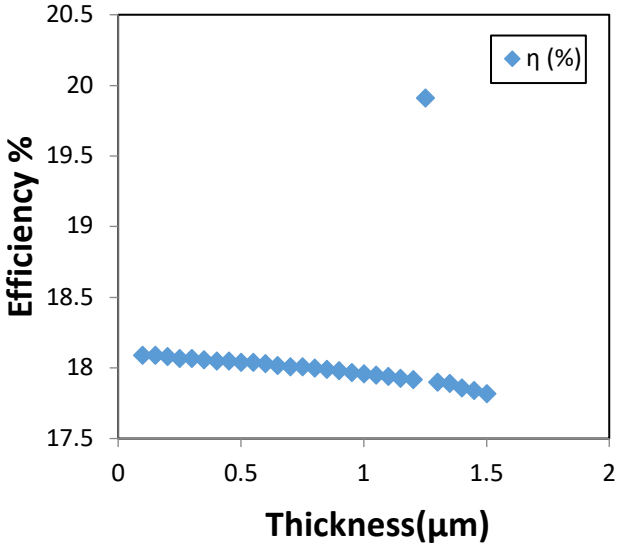
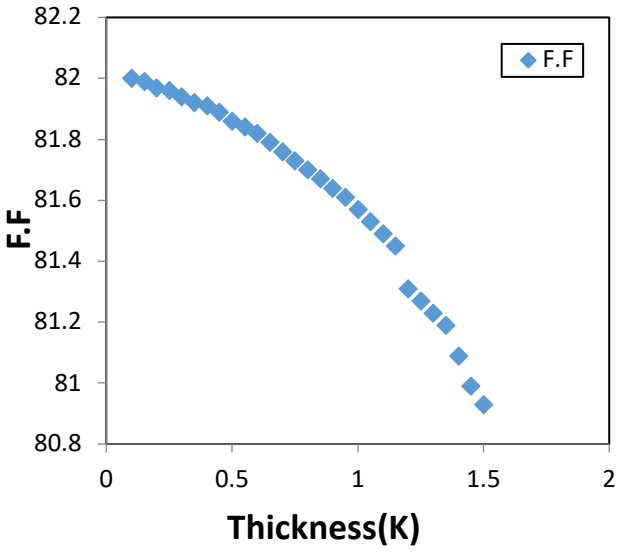


Table 3: Variation of Thickness for TiO_2 with device parameters.

Thickness(µm)	V_{oc}(V)	J_{sc}(mA /cm^2)	F.F (%)	η (%)
0.1	1.2443	17.734637	82.00	18.09
0.15	1.2443	17.728581	81.99	18.09
0.2	1.2443	17.724656	81.97	18.08
0.25	1.2443	17.721753	81.96	18.07
0.3	1.2443	17.719371	81.94	18.07
0.35	1.2443	17.717284	81.92	18.06
0.4	1.2443	17.715363	81.91	18.05
0.45	1.2443	17.713552	81.89	18.05
0.5	1.2443	17.711817	81.86	18.04
0.55	1.2444	17.710137	81.84	18.04
0.6	1.2444	17.708494	81.82	18.03
0.65	1.2444	17.706887	81.79	18.02
0.7	1.2444	17.705305	81.76	18.01
0.75	1.2444	17.703743	81.73	18.01
0.8	1.2444	17.702196	81.70	18.00
0.85	1.2445	17.700660	81.67	17.99
0.9	1.2445	17.699135	81.64	17.98
0.95	1.2445	17.697611	81.61	17.97



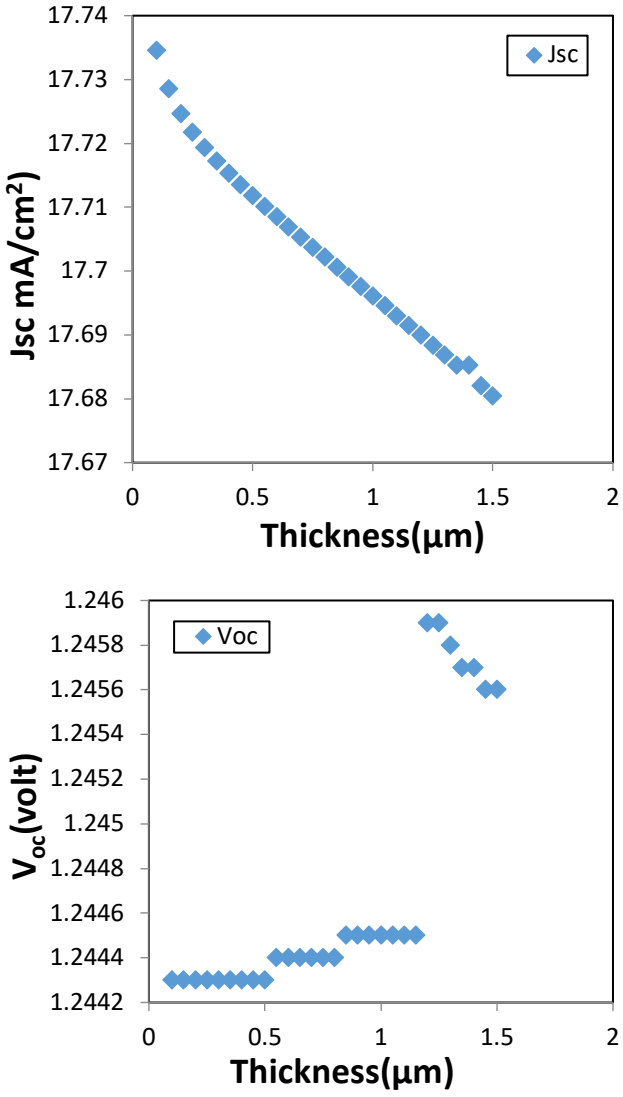


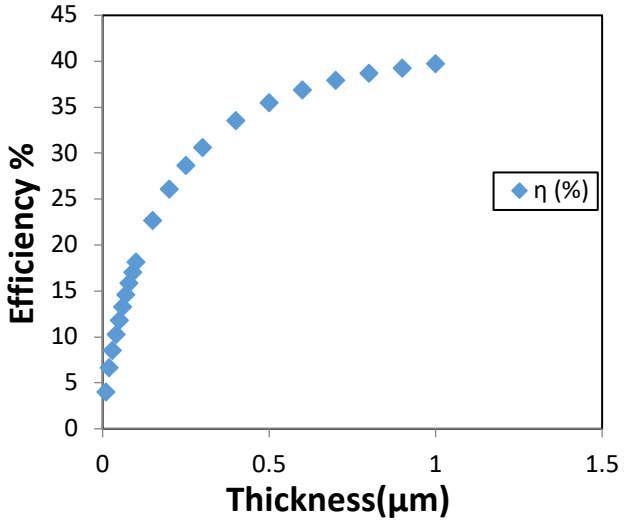
Fig. 5: Variation of PV parameters by varying the thickness of TiO_2.

2. Effect of the NiO layer thickness change on solar cells

The thickness of NiO layer range (0.01 to 1) µm, The efficiency 4 % to 39.71 %. in this study, the thickness of the optimum absorber layer is 1 µm, where absorb a lot of photons and generation electron-hole pairs. When increasing the thicknesses of NiO as the HTM the parameter of device increase, V_{oc}, J_{sc}, and η (1.2054 to 1.2645) volt, (3.965777 to 35.394582) (mA/cm^2) and (4 to 39.71) % while the FF decrease at thinner thickness (0.02,0.03) µm, then it increases with the transition to thicker layers of NiO (83.78 to 88.73) %. enhanced exciton production led to the efficiency increase.

Table 4: Variation of Thickness for NiO with device parameters.

Thickness(µm)	V_{oc}(V)	J_{sc}(mA /cm^2)	F.F (%)	η (%)
0.01	1.2054	3.965777	83.78	4.00
0.02	1.2180	7.232356	75.07	6.61
0.03	1.2245	9.544587	72.99	8.53
0.04	1.2291	11.101524	74.91	10.22
0.05	1.2329	12.444247	76.76	11.78
0.06	1.2361	13.668157	78.34	13.24
0.07	1.2388	14.798239	79.53	14.58
0.08	1.2410	15.847292	80.50	15.83
0.09	1.2427	16.823699	81.31	17.00
0.1	1.2443	17.734637	82.00	18.09
0.15	1.2499	21.489390	84.26	22.63
0.2	1.2535	24.259299	85.62	26.04
0.25	1.2561	26.363546	86.39	28.61
0.3	1.2580	28.002036	86.92	30.62
0.4	1.2605	30.359848	87.58	33.52
0.5	1.2618	31.950626	87.99	35.47
0.6	1.2627	33.078721	88.26	36.86
0.7	1.2634	33.907485	88.44	37.89
0.8	1.2639	34.534333	88.57	38.66
0.9	1.2642	35.016530	88.66	39.25
1	1.2645	35.394582	88.73	39.71



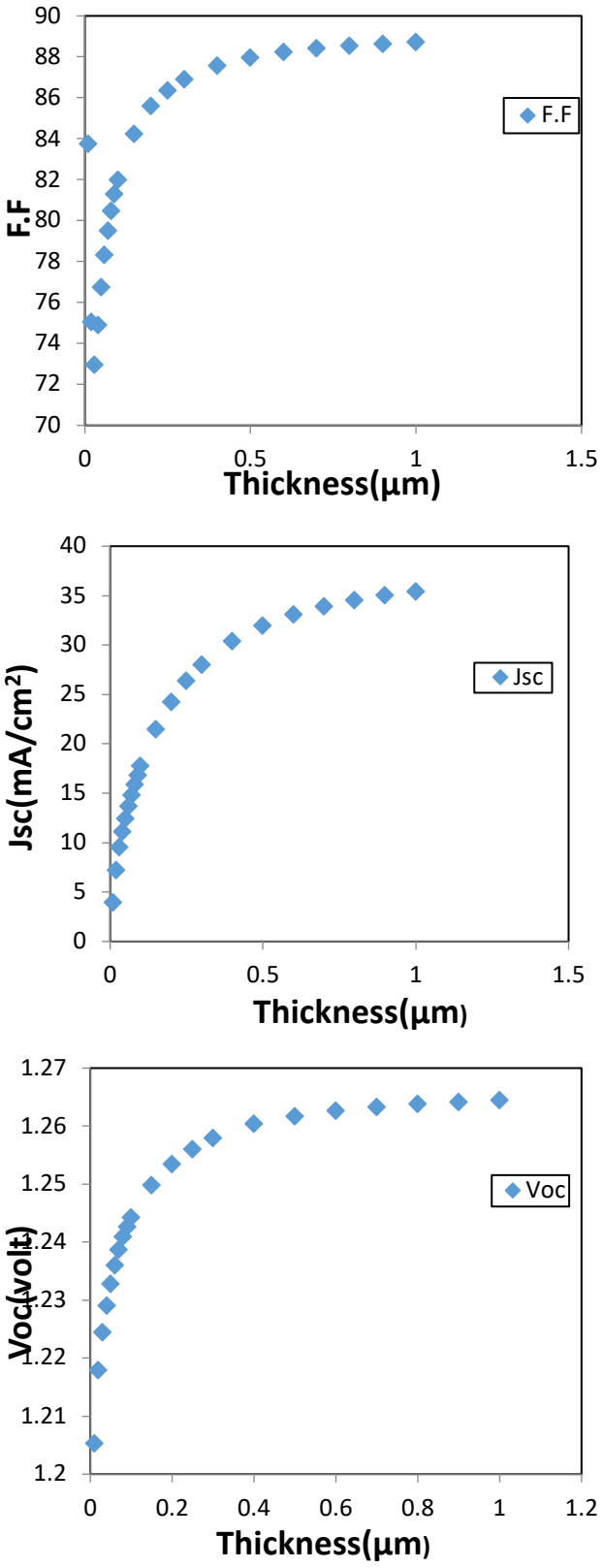


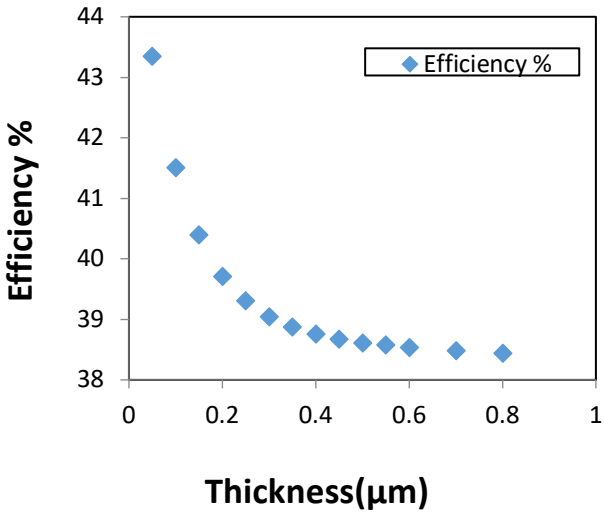
Fig. 6: Variation of PV parameters by varying the thickness of NiO.

3. Effect of the $CH_3NH_3PbI_3$ layer thickness change on solar cells

The overall performance of the solar cells greatly affected the thickness of the absorber layer, with NiO as the HTM layer and TiO_2 as the ETL layer. We took the thicknesses of TiO_2 and NiO with the best efficiency and we change the thickness of the absorbent layer $CH_3NH_3PbI_3$ from(0.05 to 0.8) µm, and high efficiency at thickness 0.05 µm is 43.34 % as illustrated in table (5) .The absorber layer $CH_3NH_3PbI_3$at the thickness from(1.2667 to 1.2637) the V_{oc} decreases while the J_{sc}, FF and η decrease (38.551467 to 34.289712) (mA/cm2), (88.76 to 88.72) % and (43.34 to 38.44) %.The reason for this is that the absorbent layer, when it reaches a certain thickness, begins to scatter the light that reaches it, which leads to a decrease in the number of excitons generated and this leads to a decrease in efficiency.

Table 5: Variation of Thickness for $CH_3NH_3PbI_3$ with device parameters.

Thickness(µm)	V_{oc}(V)	J_{sc}(mA /cm^2)	F.F (%)	η (%)
0.05	1.2667	38.551467	88.76	43.34
0.1	1.2656	36.950613	88.75	41.50
0.15	1.2649	35.979841	88.74	40.39
0.2	1.2645	35.394582	88.73	39.71
0.25	1.2643	35.034159	88.73	39.30
0.3	1.2641	34.806326	88.72	39.04
0.35	1.2640	34.657949	88.72	38.87
0.4	1.2639	34.558019	88.72	38.75
0.45	1.2639	34.488186	88.72	38.67
0.5	1.2638	34.437433	88.72	38.61
0.55	1.2638	34.399042	88.72	38.57
0.6	1.2638	34.368853	88.72	38.53
0.7	1.2637	34.323524	88.72	38.48
0.8	1.2637	34.289712	88.72	38.44



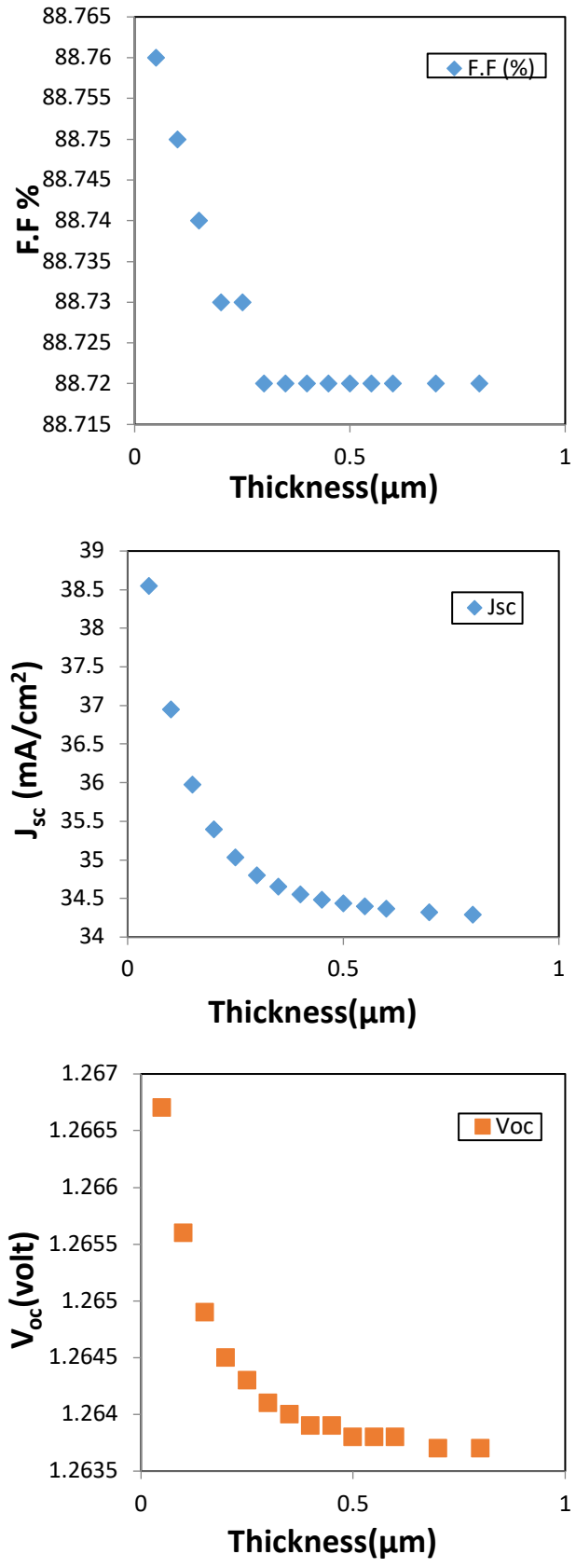


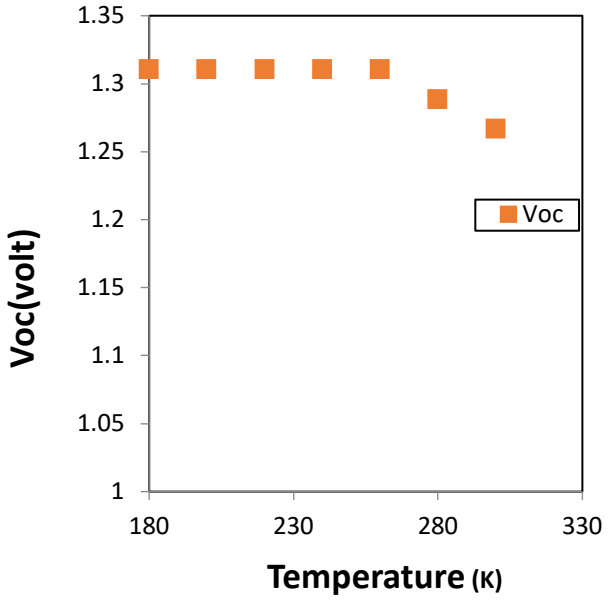
Fig. 7: Variation of PV parameters by varying the thickness of $CH_3NH_3PbI_3$.

4. Effect of annealing temperatures for $CH_3NH_3PbI_3$

The results of simulation I-V property such as PCE, J_{sc}, FF, and V_{oc} of the perovskite solar cells with different temperature as in table (6) we notice the highest efficiency is (45.08) % with J_{sc} = 38.346759 mA/cm^2, FF =89.71 % and V_{oc}=1.3105 volt is achieved when the temperature at (180) k, also remain PCE, J_{sc}, FF, V_{oc} constant on same values at temperatures (200,220,240,260) K, then decrease at temperatures (280,300) thus the best result at very low temperatures. after the temperature is increasing from 180 k to 300 k the PCE, and J_{sc} decrease because reducing in the create of the electron-hole pairs in the perovskite layers when increasing temperature as in Figure 8. Due to control of the recombination, create, and a set of the charge carriers it can tuning the efficiency with temperature so the better temperature of perovskite solar cells with $CH_3NH_3PbI_3$ as PVSC is 180 k. In the time same, we notice that the device of perovskite solar cells of $CH_3NH_3PbI_3$ with temperature has very high stability as in the Figure 8 the changing in parameter is small, thus that the stability base temperature is stable and resistant to temperature.

Table 6: The parameter of the NiO/ $CH_3NH_3PbI_3$/TiO2 heterojunction solar cell.

T(K)	V_{oc}(V)	J_{sc}(mA /cm^2)	FF	Efficiency%
180	1.3105	38.346759	89.71	45.08
200	1.3105	38.346759	89.71	45.08
220	1.3105	38.346759	89.71	45.08
240	1.3105	38.346759	89.71	45.08
260	1.3105	38.346759	89.71	45.08
280	1.2887	38.453874	89.37	44.29
300	1.2667	38.551467	88.76	43.34



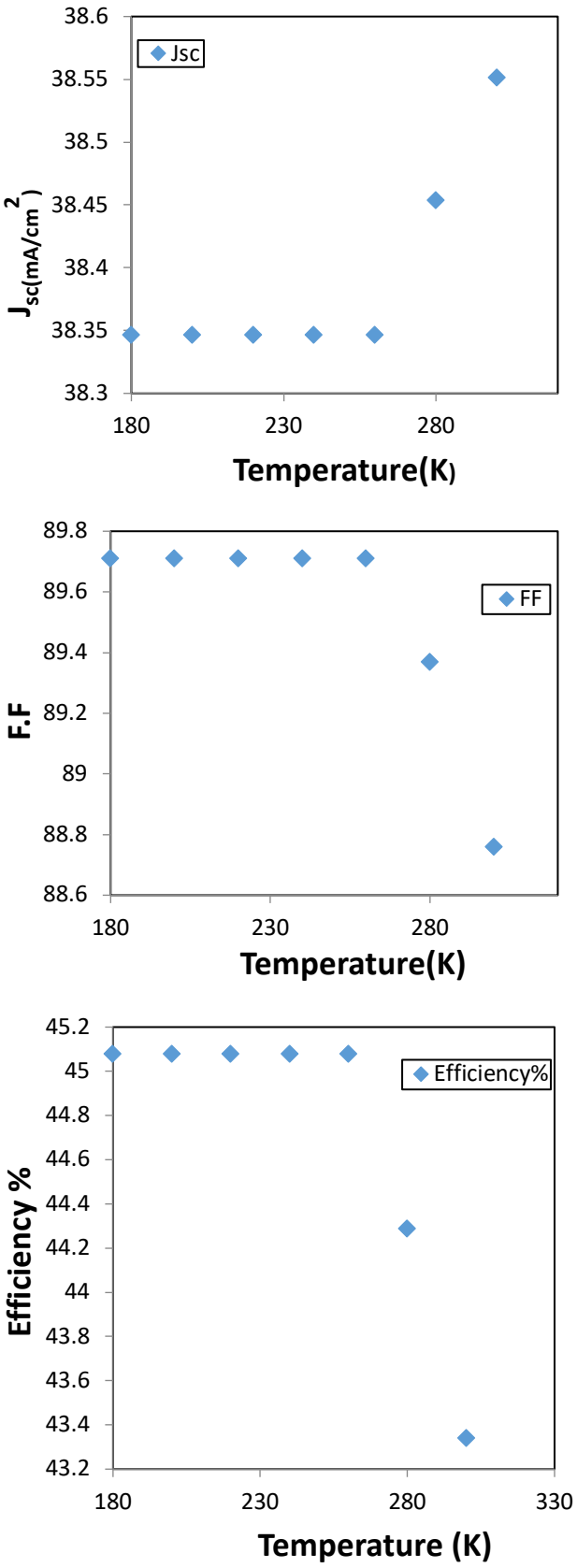


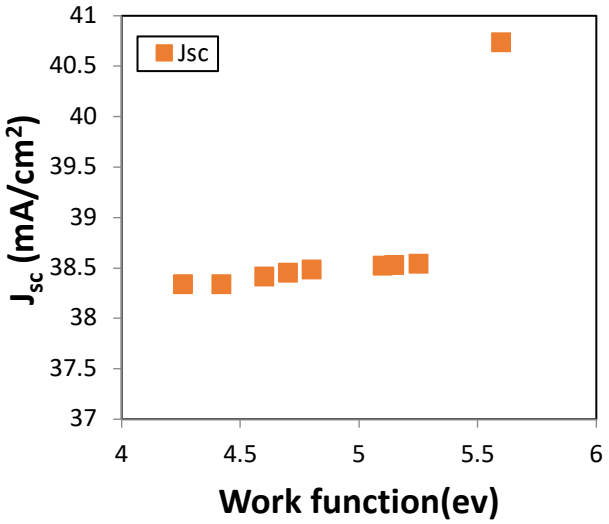
Fig. 8: The variation of solar cell parameters with the temperature.

5. Effect of different back contact material

Low thermal stability of the back contact and high cost are the prime barriers to perovskite solar cells commercialization. When choosing appropriate work function material for manufactured the back contact, result a reasonable built-in voltage. As we note from the table, a different value of the work function (Back) was chosen from (4.26_5.6) ev for in order to obtain a back connection with better specifications to simulate the device. The increase in the work function material lead to increase value of V_{oc} (0.8911 to 1.2682) volt, J_{sc} (38.339785 to 40.737906) (mA/cm^2), F.F (79.73 to 89.16) % and η (27.24 to 46.06) % observed in figure (9).Work function (back contact) increases lead to the Schottky barrier (produced at the NiO/back contact interface) lowers, causing to simple mobility of the hole from NiO for back contact, thus increasing in the parameters.

Table 7: Shows effect of various metal contact on efficiency of the cell.

Metals	Work Function (ev)	V_{oc}(V)	J_{sc}(mA/cm^2)	FF	Efficiency %
Al	4.26	0.8911	38.33978	79.73	27.24
Sn	4.42	0.8911	38.33978	79.73	27.24
Cu	4.6	1.0711	38.41401	82.33	33.88
Ag	4.7	1.1705	38.45166	83.49	37.58
Fe	4.8	1.2511	38.48663	85.42	41.13
Au	5.1	1.2667	38.52350	88.76	43.31
Ni	5.15	1.2667	38.52827	88.76	43.32
Ir	5.25	1.2667	38.542530	88.76	43.33
Pt	5.6	1.2682	40.737906	89.16	46.06



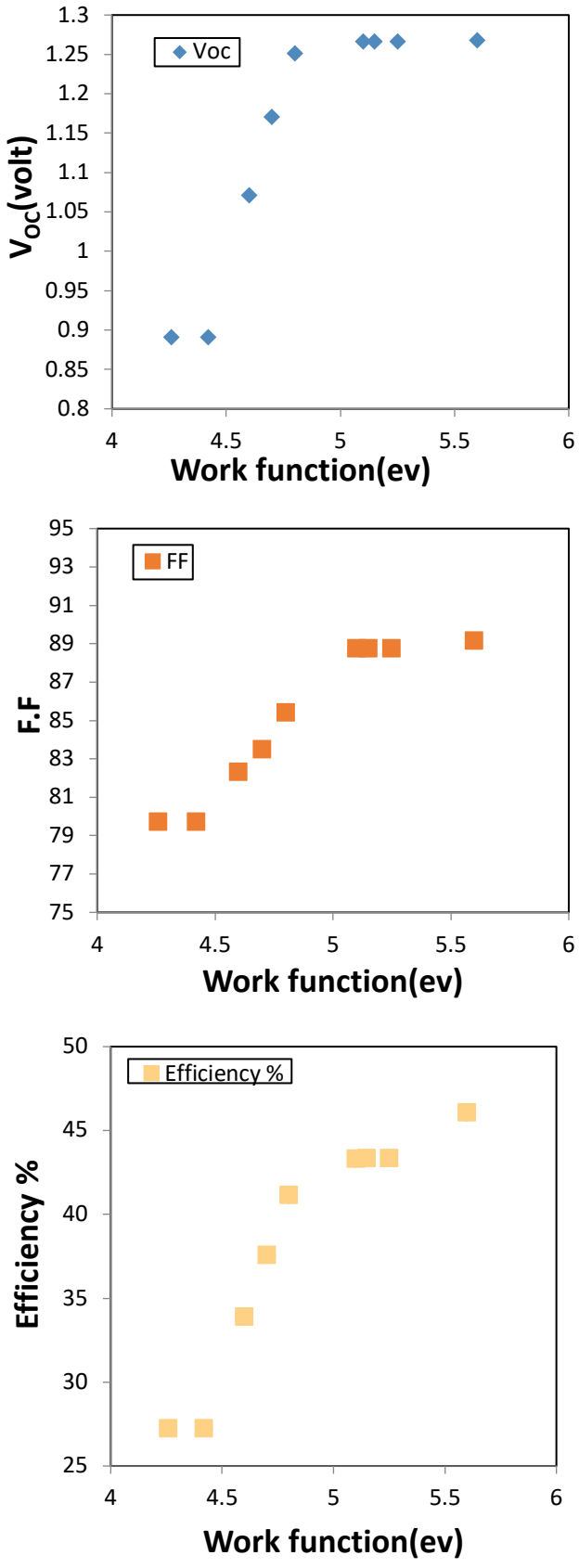


Fig. 9: J-V characteristics, FF and η of PSC as a function of work function.

6 Conclusions

In this study, we discussed simulation results the perovskite solar cells using two three layers NiO as the HTM layer and TiO_2 as the ETL layer and Perovskite $CH_3NH_3PbI_3$ by using SCAPS as simulation tool. Increase efficiency with increase thickness NiO material, because of photons number that reaches this layer great lead to generate sufficient number of excitons, as for TiO_2, $CH_3NH_3PbI_3$ materials decrease efficiency at increase thickness, where begins the absorber layers in distribution the light that reaches it, the moment it reaches a specific thickness which thus a decrease in the number of excitons create. Then we studied the change in temperature where it was noticed that best efficiency 45.08 % at 180 k, to be device work wonderfully in low temperature. After that we dealt in this research, study change work function where the efficiency more improves to reach of 46.06% at 5.6 ev.

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