

## Hole Transporting Material Effect on Sandwiched Perovskite Based Solar Cells Using SCAPS-1D

Ismaila Taiwo Bello<sup>1</sup>, Kamaldeen Olasunkanmi Suleman<sup>3</sup>, Yetunde Ajoke Ajayeoba<sup>4</sup>, Sulaiman Ayomide Ayinla<sup>2</sup>, Ayomide Eunice Awosika<sup>2</sup> and Hassan Adebayo Shittu<sup>2\*</sup>

<sup>1</sup>Department of Physics, CSET, University of South Africa, Johannesburg 1710, South Africa.

<sup>2</sup>Department of Pure and Applied Physics, Ladoke Akintola University of Technology, Ogbomosho, Nigeria

<sup>3</sup>Department of Physics, Nigerian Maritime University, Okerenkoko, Delta State, Nigeria.

<sup>4</sup>Department of Physics, Osun State University, Osogbo, Nigeria.

Author Correspondence: [hashittu23@student.lautech.edu.ng](mailto:hashittu23@student.lautech.edu.ng), [talk2dprof@gmail.com](mailto:talk2dprof@gmail.com).

### Abstract

In this research, the simulation of Sandwiched Perovskite Based Solar Cells (PSCs) was investigated using computer based software known as solar cell capacitance simulator (SCAPS-1D). The effect of Hole Transporting Material (HTM) on the sandwiched perovskite was determined by the electrical. The solar cell structures used are n-FTO/ZnO/p-CZTS/p-PSC/p-CZTS/HTM and n-FTO/ZnO/p-CZTS/p-PSC/p-CZTS. The simulations were performed under ambient temperature (300K) and AM 1.5 Sun of the Solar spectrum parameters ( $V_{oc}$ ,  $J_{sc}$ , FF) and efficiency generated by the SCAPS-1D. From the results obtained, the model band gap for the two devices and graphs were plotted and the efficiencies recorded. It was observed that with the increase of perovskite thickness from 50 to 500 nm, the efficiencies of the sandwiched perovskite increases. It was also observed that the device with HTM had a greater efficiency than the device without the HTM. The efficiencies of 20.56 % and 15.53 % were recorded for the sandwiched perovskite with HTM and the sandwiched Perovskite without HTM. The continuous increase in the efficiencies of the device with HTM shows that it has a positive effect on the perovskite.

**Key words:** Perovskite, sandwiched, Hole Transporting Material (HTM), efficiency.

## 1.0 Introduction

Methylammonium lead halide ( $\text{CH}_3\text{NH}_3\text{PbX}_3$ ,  $X = \text{Cl, Br or I}$ ) kind of perovskite solar cells (PSCs) have reveal notable enhancement in power conversion efficiencies (PCE) over the past years. The universal chemical formula for perovskite compounds is  $\text{ABX}_3$ , where X is an anion that bonds the two cations of extremely distinct sizes A and B. The A have larger atoms than 'B' atoms. The perfect cubic-symmetry configuration has the B cation in six-fold organization, encircled by an octahedron of anions, also 12-fold cuboctahedral organization of the A cation in [1].

The natural characteristics of the perovskite materials ranging from; high dielectric constant, binding energy, low exciton, ambipolar transfer characteristics larger than a long range to intrinsic ferroelectric polarization have made this possible in solar cell application [2]. PSCs have gained enhancement in PCE from 3.8% to 22.1% within the little span of time has been achieved through easy device manufacturing and classic material synthesis with solution processability, low-cost, and high-power conversion efficiency. Likewise, the electrontransport and hole transport layers also play a notable function in determining the resultant device output performance, which is reliant on the charge removal characteristics [3-4]. To enhance PCE, most of the research is now paying cognitive attention on optimization of monolithic tandem silicon-based PSCs which have achieved output efficiency above 25% [5]

Researchers' efforts have also been called to improving and modifying HTMs to attain improved stability from its' hygroscopic character and to enhance the general device performance [2].

HTMs play a significant task in influencing the device performance and researchers have to consider the subsequent aspects for the introducing new HTMs; energy levels of the preferred HTMs must be slightly advanced to that of the perovskite, it should have fitting energy levels, providing the driving force for charge transfer (i.e. the highest occupied molecular orbital, HOMO,

materials). It must act as a barrier between perovskite layer and anode to block electrons without entering the anode. HTM should possess a sufficient hole transfer efficiency (preferably  $> 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) to assist hole conduction and avert charge recombination. Splitting of the quasi-fermi-energy levels of the perovskite by the influence of HTM favoring the open circuit voltage [6]. Meanwhile it must also evade the diffusion between the perovskite layer and backside electrode metal. Cost-effectiveness of the material should be considered and should possess high thermal stability and overcome the peripheral degradation factors for an efficient device performance and must be environmental friendly.

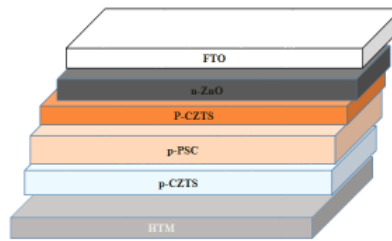
Optical absorption coefficient of  $\text{MAPbI}_3$  is advanced than other photovoltaic materials such as amorphous Si:H, Si and CdTe, so the absorber thickness can be reduced to approximately 300 nm, thereby reducing the cost of the material [7-8]. When compared to organic photovoltaic materials, the exciton binding energy of 30-50 meV allows autonomous exciton separation to free charges after optical absorption [9-10]. However, an approximate 1 nm extended diffusion lengths, the high electron and hole mobility in the range of  $10 - 60 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and the long carrier lifetime ( $\sim 100 \text{ ns}$ ) results in long diffusion lengths ( $\sim 1 \mu\text{m}$ ) so that charge carriers can be freely transported across the 300 nm thick perovskite absorber before recombination [11-12].

Thin film solar cells have developed interest in a quaternary semiconducting compound Copper zinc tin sulfide (CZTS). The group of associated materials includes group I-II, group IV-VI such as copper zinc tin selenide and the sulfur-selenium alloy CZTSSe. CZTS is one of the potential materials to be employed as an absorber layer in solar cell, owing to its efficient optical properties (the band gap varies from 1.4 to 1.5 eV) [13-14]. In this research work, a one-dimensional simulation program with seven semiconductor input layers called SCAPS (Solar Cell Capacitance Simulator) was used, which was developed by a group of solar cell researcher at the Department of

electronics and information System, University of Gent, Belgium[15].

## 2.1 Device Structure

The solar cell structures used are FTO/n-ZnO/p-CZTS/p-PSC/p-CZTS/HTM and n-FTO/ZnO/p-CZTS/p-PSC/p-CZTS. This is shown below in figure 1.



**Figure 1:** Simulation Structure

## 2.2 Device Simulation

The resolution of the simulation is based three prevailing semiconductor equations and are follows: electron and hole continuity equations, Poisson's equation. Numerical solutions of these 3 joined partial differential equations can be done by SCAPS for the electron and hole concentration as well as electrostatic potentials as function of positions x.

### 2.2.1 Poisson equation

Both the charge and electric potential  $\Phi$  are connected together by Poisson equation:

$$\frac{d}{dx} \left( -\varepsilon(x) \frac{d\Phi}{dx} \right) = q [p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)]$$

Where p and n denote the free hole density and the free electron density respectively, ionized donor density is represented by  $N_D^+(x)$  while ionized acceptor density is represented by  $N_A^-(x)$ , the trapped electron density is denoted by  $n_t(x)$  while the trapped hole density is

denoted by  $p_t(x)$  and  $\epsilon$  is the dielectric constant of the medium.

SCAPS the following unknown variables However, in a photovoltaic cell simulation, the electrical potential the carrier concentrations of free hole density and free electron density determined using SCAPS to solve the joined partial differential equations. The simulations were performed under ambient temperature (300K) and AM 1.5 Sun of the Solar spectrum parameters (Voc, Jsc, FF) and efficiency generated by the SCAPS-1D.

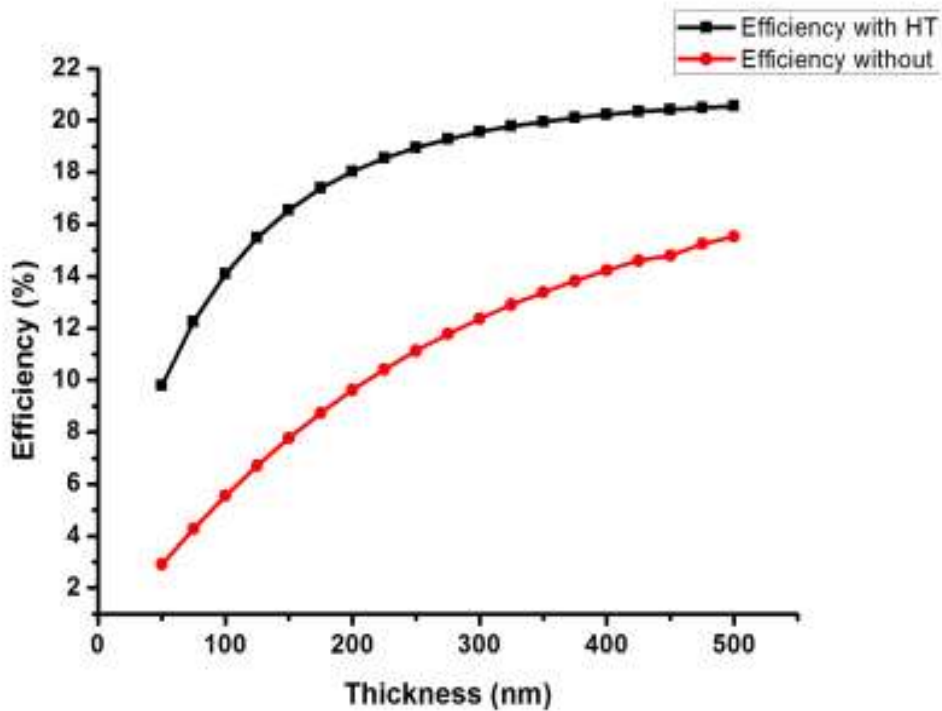
**Table 1:** Material parameters used in simulation [16-17].

Parameter	FTO	ZNO	CZTS	CH <sub>3</sub> NH <sub>3</sub> PbCl <sub>3</sub>	HTM
Thickness, $x$ (nm)	500	50	250	500	350
Bandgap, $E_g$ (eV)	3.500	3.350	1.550	1.550	2.450
Electron affinity, $\chi$ (eV)	4.00	4.210	4.500	3.900	3.00
Dielectric ratio, $\epsilon/\epsilon_0$	9.000	9.000	10.000	6.500	3.00
Density of states, $N_c$ ( $cm^{-3}$ )	2.200E+18	2.200E+18	2.200E+18	2.200E+18	1.000E+15
Density of states, $N_v$ ( $cm^{-3}$ )	1.800E+19	1.800E+19	1.800E+19	1.800E+19	1.000E+19
Elect.Mobility, $\mu_p$ ( $cm^2/Vs$ )	2.000E+1	2.500E+1	1.000E+2	1.600E+0	2.000E-4
Hole mobility, $\mu_p$ ( $cm^2/Vs$ )	1.000E+0	1.000E+2	2.000E+1	2.000E-1	2.000E-4
Defect density, $N_t$ ( $cm^{-3}$ )	-	-	-	-	10E+15
Thermal velocity of electron (cm/s)	1.000E+7	1.000E+7	1.000E+2	3.000E+7	1.000E+7
Thermal velocity of hole (cm/s)	1.000E+7	1.000E+7	1.000E+7	3.000E+7	1.000E+7
$N_A$ ( $cm^{-3}$ )	0.000E+0	0.000E+0	8.220E+18	6.000E+18	2.000E+18
$N_D$ ( $cm^{-3}$ )	2.000E+19	1.000E+18	0.000E+0	0.000E+0	0.000E+0

### 3. Results and discussion

In the model simulated, different thickness of the component of the Perovskite (PSC) (50 nm-500 nm), ZnO (50 nm), CZTS (25 nm-250nm) are varied with step-height of 25 nm. The generated data such as Voc, Jsc, FF and efficiency are used for further analyses. The condition of simulation was changed from dark to light which had a great effect on the result obtained. The graph is drawn and the J-V curves were obtained. The band alignment and band offset were also determined.

#### 3.1 Effect of HTM on the Efficiency



**Figure 2:** Performance evolution of the thickness of Sandwiched PSC as a function of Efficiency with and without HTM

It was observed from figure 2 that, when the Perovskite material thickness was 50 nm, the efficiency of the PSC with Hole Transporting Material (HTM) and without HTM was 9.80 % and 2.91% respectively with the efficiency increment of 70.31 %. At 75 nm, the efficiencies of 12.25 % and 4.28 % with the efficiency increment of 65.02 % were observed for PSC with HTM and without HTM respectively. At 100 nm, the efficiencies of 14.09 % and 5.55 % were observed for PSC with HTM and without HTM respectively with the efficiency increment of 60.61 %. When the PSC material was 125 nm, the efficiency of the PSC with HTM and without HTM were 15.48 % and 6.71 % respectively with the efficiency increment of 56.65 %. At 150 nm, the efficiencies observed for PSC with HTM and without HTM were 16.55 % and 7.77 % respectively with the efficiency increment of 53.05 %. The efficiencies of 17.38% and 8.74% was observed when the thickness of 175 nm Of PSC was simulated with HTM and without HTM respectively with the efficiency increment of 49.71 %. At 200 nm, the efficiencies obtained for PSC with HTM was 18.02 % and 9.26 % was observed for PSC without HTM with the efficiency increment of 48.61 %. At 225 nm, the efficiencies of 18.54 % and 10.41 % was observed for PSC with HTM and without HTM respectively with the efficiency increment of 43.85 %. At 250 nm, the efficiencies of 18.95 % and 11.13 % was observed for PSC with HTM and without HTM respectively with the efficiency increment of 41.26 %. However, at 275 nm, the efficiency of 19.28 % was observed for PSC with HTM, while 11.78% was observed for PSC without HTM with the efficiency increment of 38.90 %. At 300 nm, the efficiencies of 19.55 % and 12.37 % was observed for PSC with and without HTM with the efficiency increment of 36.72 %. At 325 nm, the efficiencies of 19.77% and 12.90 % was observed for PSC with and without HTM with the efficiency increment of 34.74 %. However, at 350 nm, the efficiency of 19.95 % was observed for PSC with HTM and 13.38% for PSC without HTM with the efficiency

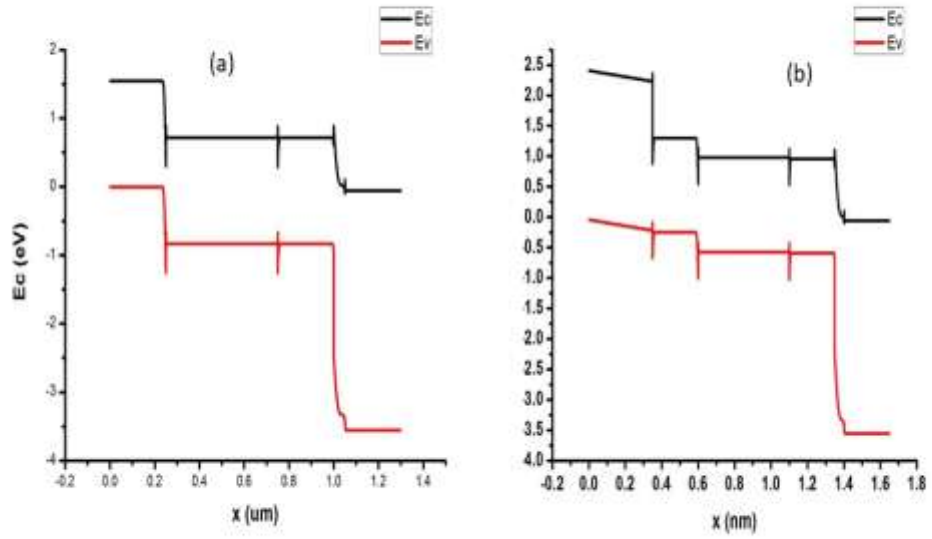


increment of 32.93 %. At 375 nm, the efficiencies of 20.10 % and 13.82 % were obtained for PSC with and without HTM respectively with the efficiency increment of 31.24 %. The efficiencies of 20.22 % and 14.23% were observed when simulating the PSC of 400 nm thickness with and without HTM respectively with the efficiency increment of 29.62 %. At 425 nm, the efficiencies of 20.33 % and 14.60 % were observed when simulating the PSC with and without the HTM with the efficiency increment of 28.18 %. When the PSC of 450 nm was simulated, the efficiencies of 20.42 % and 14.80 % were observed for PSC with HTM and without HTM respectively with the efficiency increment of 27.52 %. At 475 nm, the efficiencies obtained for PSC with HTM was 20.49 % and 15.24 % without HTM with the efficiency increment of 25.62 %. Lastly, at 500 nm, the efficiencies obtained for PSC with HTM was 20.56%, while 15.53 % was obtained for PSC without HTM with the efficiency increment of 24.46 %. Therefore, there is no great increment in the efficiency of the PSC after the thickness of 500 nm.

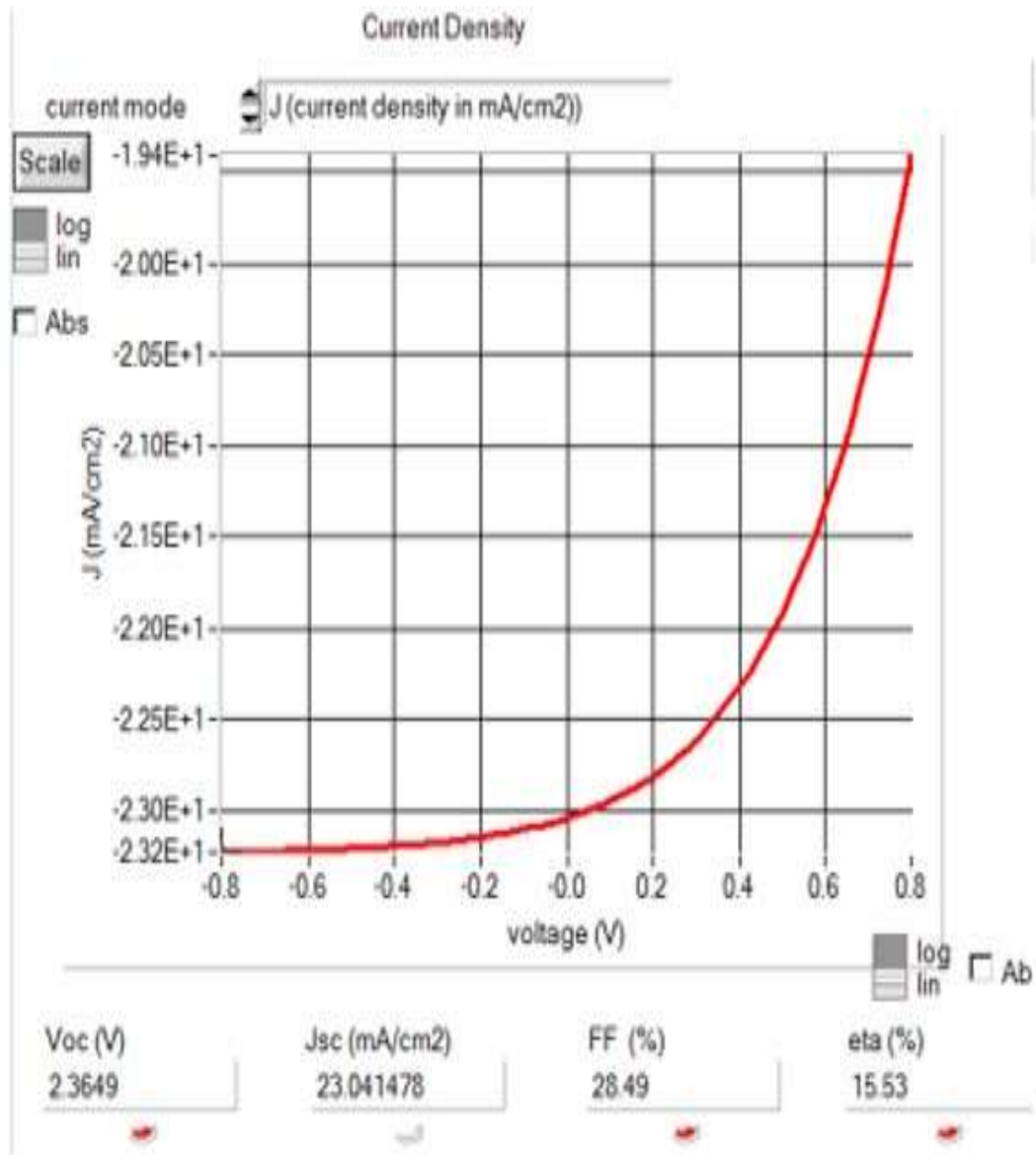
It was observed from the simulation done, that the efficiency of the device which has the Hole Transporting Material (HTM) had a greater efficiency than the device without the HTM.

### **3.2 The Bandgap diagram**

Figures 3a and 3b, show the band diagram of the Sandwiched Perovskite with Hole Transporting Material (HTM) and Sandwiched Perovskite without HTM respectively. The band gap line up model of the simulated device (FTO/Zno/CZTS/PSC/CZTS) and (FTO/ZnO/CZTS/PSC/CZTS/HTM) were derived from the data obtained from the SCAPS under the ambient temperature (300K).



**Figure 3:** (a) Simulated Band Gap without HTM (b) Band Gap with HTM



**Figure 4:** J-V characteristics plot of the cell without HTM at 500nm thickness of the absorber layer

## **Conclusion**

Sandwiched Perovskite without Hole Transporting Material (HTM) and Sandwiched Perovskite Based solar cell with Hole Transporting Material (HTM) has been successfully simulated using One-Dimensional Solar Cell Capacitance Simulator (SCAPS-1D). The output results of the simulation were recorded plotted across the thickness variation of the absorber layers which varies from 50nm to 500nm. It was discovered that the higher the absorber thickness the higher the efficiencies and others electrical parameters output in the solar cell. The efficiencies of 15.53% and 20.56% were achieved for the Sandwiched Perovskite-Based solar cell with HTM and Sandwiched Perovskite-Based solar cell without HTM respectively.

## **ACKNOWLEDGEMENT**

An immense support of this work was gotten from SCAPD-1D, a numerical tool developed by Prof. Marc Burgelman and his research group, Department of Electronics and Information Systems, University of Gent, Belgium.

## REFERENCES

- [1]. Bello I T Awodele M K Adedokun O Akinrinola O Awodugba A O 2018 Modelling and simulation of CZTS-perovskite sandwiched tandem solar cell.
- [2]. Hsiao Y C Wu T Li M Liu Q Qin W Hu B 2015 Fundamental physics behind high-efficiency organo-metal halide perovskite solar cells *J. Mater. Chem. A* **3** pp 15372–15385.
- [3]. Abdulrazzaq O A Saini V Bourdo S Dervishi E Biris A S 2013 Organic solar cells: A review of materials, limitations, and possibilities for improvement. Part. Sci. Technol. **31** pp 427–442.
- [4]. Noh J H Im S H Heo J H Mandal T N Seok S I 2013 Hybrid nanostructured solar cells *Nano Lett. Chemical management for colorful, efficient, and stable inorganicorganic* **13** pp 1764–1769.
- [5]. Correa B J P Abate A Saliba M Tress W Jesper J T Gratzel M Hagfeldt A 2017 The rapid evolution of highly efficient perovskite solar cells. *Energy Environ Sci.* **10** pp 710–727.
- [6]. Bakr Z H Wali Q Fakharuddin A Schmidt-Mende L Brown T M Jose R 2017 Advances in hole transport materials engineering for stable and efficient perovskite solar cells. *Nano Energy* **34** pp 271–305.
- [7]. Yin W J Shi T T and Yan Y F 2014 Unique properties of halide perovskites as possible origins of the superior solar cell performance *Advance Mater.* **26** (27) pp 4653–4658.
- [8]. Stefaan D W Jakub H Soo-Jin M Philipp L Bjoern N Martin L Franz J H Jun-Ho Y and Christophe B 2014 Organometallic halide perovskites: sharp optical absorption edge and its relation to photovoltaic performance *J. Phys. Chem. Lett.* **5** (6) pp 1035–1039.
- [9]. Ponceca C S Savevenije J Tom J Mohammed A Kaibo Z Arkady Y Tobjom P Tobias H Pavel C Tonu P Andrey S 2014 Organometal halide perovskite solar cell materials rationalized: ultrafast charge generation, high and microsecond-long balanced mobilities, and slow recombination *Journal of America Chemical Society.* **136** (14) pp 5189–5192.
- [10]. Stranks S D Burlakov V M Leijtens T, Ball J M Goriely A and Snaith H J 2014 Recombination kinetics in organic-inorganic perovskites: excitons free charge and subgap states *Physical Review Applied* **2** (3) pp 034007.
- [11]. Stranks S D Eperon G E Grancini G Menelaou C Alcocer M J P Leijtens T Herz L M Petrozza A and Snaith H J 2013 Electron-hole diffusion lengths exceeding 1 micrometer in an organometal trihalide perovskite absorber *Science* **342** pp 341–344.

- [12]. Leijtens T Stranks S D Eperon G E Lindblad R Johansson E M McPherson I J Rensmo H Ball J M Lee M M Snaith H J 2014 Electronic properties of meso-superstructured and planar organometal halide perovskite films: charge trapping, photodoping, and carrier mobility *ACS Nano* **8**(7) pp 7147–7155.
- [13]. Wangperawong A King J S Herron S M Tran B P and Pangan O K 2011 Aqueous bath process for deposition of Cu<sub>2</sub>ZnSnS<sub>4</sub> photovoltaic absorbers *Thin Solid Films* **519** (8) pp 2488-2492.
- [14]. Zhao W Zhou W and Miao X 2012 Numerical Simulations of Thin Film Solar Cells *Proc. the 7th IEEE International Conference on Nano/Micro Engineered and Molecular Systems (NEMS '12)*, Kyoto.
- [15]. Alex N Marc B Decock K Verschraegen J Degrave S 2013 SCAPS Manual. University of Gent.
- [16]. Takashi M Masashi M 2014 *J. Appl. Phys.* **116** pp 054-505
- [17]. Gloeckler M Fahrenbruch A L Sites J R 2003 *In 3rd World Conference Proceedings: Photovoltaic Energy Conversion. Grand Cube, Osaka, Japan, 11-18 May.*