

# Optical and Electrical Modeling of a hybrid Solar Cell based on a Mesostructured Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ : Influence of the Depth and Thickness of the Photoactive Layer

Abdoulaye Ndiaye Dione\*, Sossé Ndiaye, El Hadji Oumar Gueye, Allé Dioum, Alioune Aidara Diouf, Mahamat Bichara Abderaman, Balla Diop Ngom, Aboubaker Chedikh Beye

Department of Physics (Laboratory of Solid State Physics and Materials Sciences),  
Cheikh Anta Diop University of Dakar, Dakar, Senegal  
\*Corresponding author: bayfalldione@yahoo.fr

**Abstract** In this paper we propose an analytical model to investigate the influence of the depth and thickness of the composite photoactive layer, on the optical and electrical properties of the hybrid solar cell based on the mesostructured perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$ . Using Bruggeman theory, energy conservation equation and charge density continuity equation, allowed us to determine the optical generation rate and the short-circuit current density. The results obtained show that the optical generation rate decreases according to the depth. We also see that this optical generation rate increases with the thickness of the photoactive layer. For the short-circuit current density, we note that it increases with the thickness and there is an optimum thickness at 850 nm. Our results agree with those found in literature.

**Keywords:** mesostructured perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  solar cell, optical and electrical parameters, bruggeman theory, conservation equation, continuity equation

**Cite This Article:** Abdoulaye Ndiaye Dione, Sossé Ndiaye, El Hadji Oumar Gueye, Allé Dioum, Alioune Aidara Diouf, Mahamat Bichara Abderaman, Balla Diop Ngom, and Aboubaker Chedikh Beye, "Optical and Electrical Modeling of a hybrid Solar Cell based on a Mesostructured Perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$ : Influence of the Depth and Thickness of the Photoactive Layer." *American Journal of Nanomaterials*, vol. 5, no. 2 (2017): 68-71. doi: 10.12691/ajn-5-2-4.

## 1. Introduction

Recently, the investigation of perovskite based hybrid solar cell has attracted the attention of researchers and scientists in the whole world because of their important and remarkable luminous characteristics [1]. These perovskite materials are known for their abundance in the nature, their manufacturing process at very low temperatures, their less expensive processing technical and for the spontaneous organization of their crystalline structure. Furthermore, they freely generate charges in the material after light absorption, which allows generation and collection of these created charges. They also have good intrinsic optical and electrical properties [2,3]. The mesostructured perovskite hybrid cells have the same architectural design as the Dye-sensitized solar cells (DSCs). Only the dye is replaced by perovskite. It is a mesostructure of metal oxide (e.g.,  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{Al}_2\text{O}_3$ ) and methylammonium of metal halide ( $\text{CH}_3\text{NH}_3\text{MX}_3$ ) with M a metal ( $\text{M} = \text{Pb}$ ,  $\text{Sn}$ ) and X a halogen ( $\text{X} = \text{I}$ ,  $\text{Br}$ ,  $\text{Cl}$ ) sandwiched between

two electrodes: a transparent anode which allows light to pass and a metal cathode which reflects the light towards the photoactive layer (Figure 1). The rapid evolution of conversion rates [4] places these types of materials very competitively in front of third generation (organic) and conventional (silicon) materials that have been studied for decades. To improve the efficiency and performance of these new cells, several experimental studies have been developed in recent years [5-10]. However, the developed models that we have encountered in the literature did not consider a composite photoactive layer composed of titanium dioxide ( $\text{TiO}_2$ ) and methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) [11,12]. It is in this perspective that we propose an analytical model taking into account this heterogeneity. This model allows to study the influence of depth and thickness on the optical and electrical parameters of the cell. To determine these parameters, Bruggeman theory, energy conservation equation and density continuity equation are used. After presenting our model, we establish the analytical expressions of the optical and electrical parameters of the photoactive layer. We present and discuss our results before concluding.

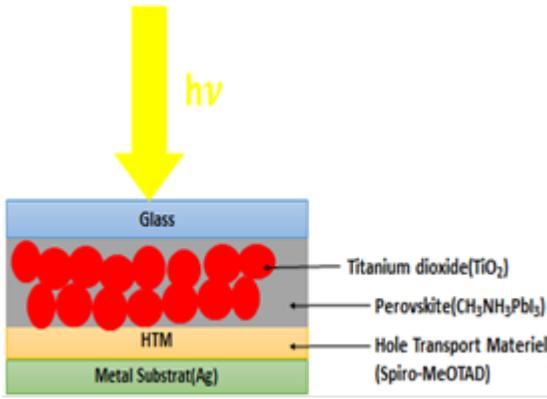


Figure 1. Structure of the mesostructured perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  solar cell

## 2. Computational Model

The model considered is depicted in Figure 2. Where  $z$  and  $d$  represent respectively the depth and the thickness of the composite photoactive layer. So we are only interested of this photoactive layer composed of a mixture titanium dioxide ( $\text{TiO}_2$ ) and perovskite ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) sandwiched between two electrodes.

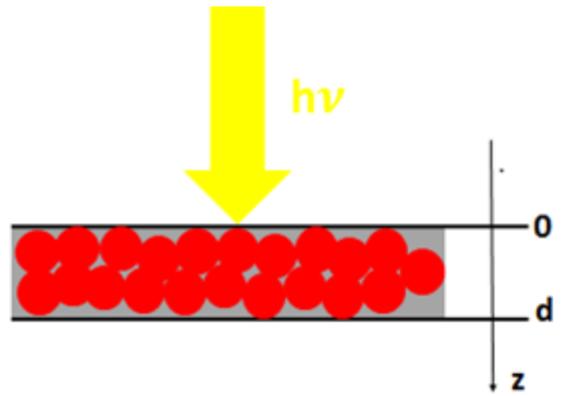


Figure 2. Schematic of the composite photoactive layer

### 2.1. Optical Parameters

In this part, we determine the expression of the optical generation rate which is linked to the various complex refractive indices. The complex refractive indices of titanium dioxide ( $\text{TiO}_2$ ) and perovskite ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) for visible wavelengths range (350 nm-800 nm) have been obtained in the literature [13]. On the other hand, the refractive index of the photoactive layer was obtained by considering the Bruggeman theory [14,15,16,17,18] for supposedly spherical particles. It leads to an equation of the second degree given by relation (1):

$$2\varepsilon_m^2 + [(3p - 2)\varepsilon_a + (1 - 3p)\varepsilon_b] \varepsilon_m - \varepsilon_a \varepsilon_b = 0 \quad (1)$$

Where  $\varepsilon_m$  is the average dielectric constant (effective permittivity) of the composite medium,  $\varepsilon_a$  and  $\varepsilon_b$  are respectively the dielectric permittivity of titanium dioxide and perovskite and  $p$  the porosity of titanium dioxide [19]. By solving this equation, we obtain the average dielectric constant of the composite medium and we deduce its complex refractive index ( $N$ ) by the relation (2):

$$\varepsilon_m = N^2. \quad (2)$$

Using theories based on electromagnetism and considering the energy conservation equation in static regime [20] defined by the relation (3),

$$Q + \text{div} \bar{P} = 0 \quad (3)$$

we easily obtain the optical generation rate for a depth  $z$  of the Photoactive layer according to the relation (4):

$$G_e(z) = \eta_{inj} G_a(z) \quad (4)$$

Where we have respectively  $Q$  the total energy density per unit time,  $\bar{P}$  the Poynting vector and  $\eta_{inj}$  the injection rate of photons. The absorption rate of photons  $G_a(z)$  is given by the relation (5):

$$G_a(z) = \int_{\lambda} \frac{Q(z, \lambda)}{\frac{hc}{\lambda}} d\lambda. \quad (5)$$

Where  $h$  and  $c$  are respectively the Planck constant and the velocity of light in vacuum.

The relation (6) gives the total energy density per unit time.

$$Q(z, \lambda) = \frac{1}{2} \alpha(\lambda) . N.Y. |E|^2 \quad (6)$$

Where  $\lambda$ ,  $Y$ ,  $E$ , and are respectively the Wavelength of light in the visible range, the impedance of the wave and the electric field. The absorption coefficient  $\alpha(\lambda)$  of the composite photoactive layer is given as in [21].

### 2.2. Electrical Parameters

For this part we determine the analytical expressions of the charges density and short-circuit current which depend on the previous generation rate. For the photoactive layer considered, only the perovskite material is responsible for the absorption of light. In addition, the transport and recombination properties of mesostructured perovskite solar cells are similar to those of dye-sensitized solar cells. Charge transport in perovskite cells is dominated by conduction electron within the mesoporous  $\text{TiO}_2$  [22]. It has also been suggested that the high dielectric constant of perovskites allows the photogenerated excitons to dissociate immediately into free carriers (electrons and holes) [23,24]. The photogenerated electrons diffuse through the photoactive layer before being collected by the anode. Consequently, it is important to develop an analytical electrical model to solve the electrons density continuity equation in static mode along the photoactive layer [12]. It is given by the following relation (7):

$$\frac{\partial^2 \rho(z)}{\partial z^2} - \frac{\rho(z)}{L^2} + \frac{G_e(z)}{D} = 0 \quad (7)$$

Where  $\rho$ ,  $D$  and  $L$  represent respectively the electrons density photogenerated, the diffusion coefficient and the diffusion length. This equation has been simplified by ignoring the recombination of the carriers in the absorber layer because their diffusion length in the perovskite

material is very high [25,26]. The final solution of equation (7) is obtained from the boundary conditions at the anode/photoactive layer ( $z = 0$ ) and cathode/photoactive layer ( $z = d$ ) interfaces:

$$\frac{\partial \rho(z)}{\partial z} \Big|_{z=0} = \frac{S_1}{D} \rho(0) \quad (8)$$

$$\frac{\partial \rho(z)}{\partial z} \Big|_{z=d} = -\frac{S_2}{D} \rho(d) \quad (9)$$

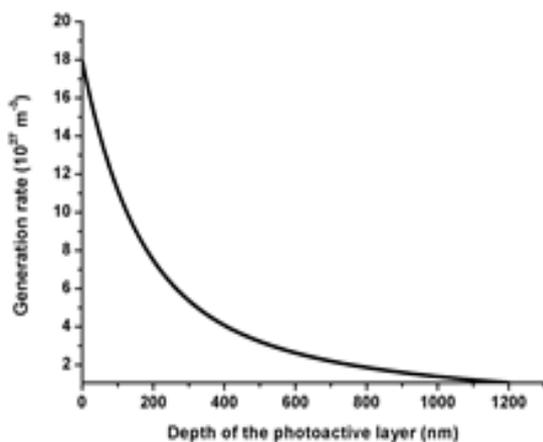
Where  $S_1$  and  $S_2$  denote respectively the recombination rates of the electrons at the interfaces ( $z = 0$ ) and ( $z = d$ ). After having determined the analytical expression of the photogenerated electrons density, we have deduced that of the short-circuit current density given by the relation (10):

$$J_{cc} = qD \frac{\partial \rho(z)}{\partial z} \Big|_{z=0} \quad (10)$$

Where  $q$  is the electron charge.

### 3. Résultats et Discussions

After determining the analytical expressions of the macroscopic parameters cited above, a numerical code is established. The obtained results are presented in this section. The evolution of the optical generation rate and the electron density according to the depth of the photoactive layer was investigated. Similarly, an investigation was made on the evolution of the optical generation rate and the short-circuit current density as a function of the thickness. The analytical model was validated by data found in the literature.

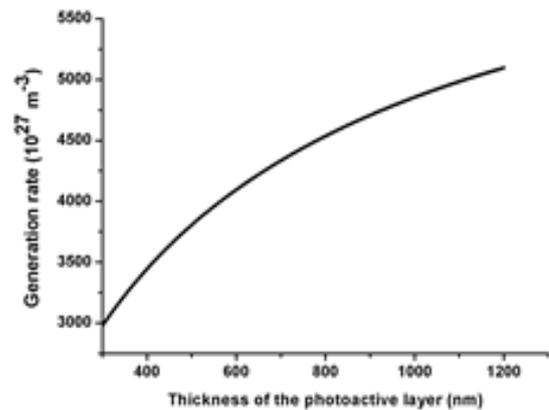


**Figure 3.** Optical generation rate depending on the depth of the photoactive layer

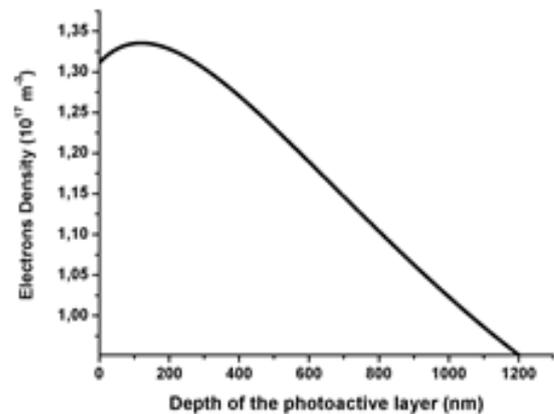
The Figure 3 shows the evolution of the optical generation rate depending on the depth of the photoactive layer. We note, this optical generation rate decreases in accordance with the progress in depth. The same pace has been found in the literature [12]. This behavior is due to the attenuation of the wave amplitude according to the depth.

The Figure 4 shows the evolution of the optical generation rate as a function of the thickness of the photoactive layer. The analysis of the graph shows that the optical generation rate increases with the thickness of the

photoactive layer. This same phenomenon has been observed in dye-sensitized solar cells [19] including the transport and recombination properties are similar to those of our cell.

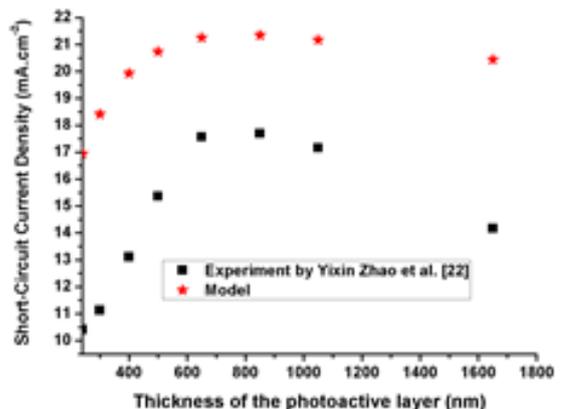


**Figure 4.** Optical generation rate as a function of the thickness of the photoactive layer



**Figure 5.** Electrons Density depending on the depth of the photoactive layer

The profile of the electrons density generated in the photoactive layer along the depth has been shown in Figure 5. The analysis of this graph shows a high electrons concentration in the environment of the anode/photoactive layer interface which decreases in depth. This density being related to the optical generation rate; its behavior is also related to the attenuation of the amplitude of the wave along the depth.



**Figure 6.** Short-circuit current density as a function of the thickness of the photoactive layer

In Figure 6, we presented the evolution of the short-circuit current density as a function of the thickness of the photoactive layer. The analysis of the graph shows that the short-circuit current density increases with the thickness. We note an optimum thickness of 850 nm. The same behavior was observed by Yixin Zhao et al [22] for a thickness varying from 240 nm to 1650 nm.

## 4. Conclusion

Our model allowed us to investigate the influence of the depth and thickness of the photoactive layer on the optical and electrical properties of a hybrid solar cell based on mesostructured perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$ . We observed that the optical generation rate decreases along the depth of the photoactive layer. We also noticed that the optical generation rate increases with thickness. For the electrons density, we observed a high concentration at the anode/photoactive layer interface. About the short-circuit current density, we found that there is an optimum thickness of 850 nm which agree with the result found in the literature. The model makes it possible to know the optimal thickness of the composite photoactive layer. It allowed us as well to analytically determine the optical generation rate and the electrons density which cannot be measured directly. However, it would be interesting to study the influence of the recombination rates at the interfaces on the optical and electrical properties of such a solar cell for better optimization. See also the influence of the wavelength of incident light would be important.

## References

- [1] Wolf, S.D., Holovsky, J., Moon, S.J., Löper, P., Niesen, B., Ledinsky, M., Haug, F.J., Yum, J.H and Ballif, C, "Organometallic Halide Perovskites: Sharp Optical Absorption Edge and its Relation to Photovoltaic Performance", *Physical Chemistry Letters.*, 5(6).1035-1039. March. 2014.
- [2] Fan, J., Jia, B and Gu, M, "Perovskite-based low-cost and high-efficiency hybrid halide solar cells", *Photonics Research*, 2(5). 111-120. October.2014.
- [3] Sun, S., Salim, T., Mathews, N., Duchamp, M., Boothroyd, C., Xing, G., Sumbce, T.C and Lam, Y.M, "The origin of high efficiency in low-temperature solution-processable bilayer organometal halide hybrid solar cells", *Energy Environ. Sci.*, (7). 399-407. October.2014.
- [4] Park, N.G, "Perovskite solar cells: an emerging photovoltaic technology", *Materials Today*, 00(00).August.2014.
- [5] Kojima, A., Teshima, K., Shirai, Y and Miyasaka, T, "Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells", *American Chemical Society*, 131. 6050-6051. April.2009.
- [6] Liu, D., and Kelly, T.L., "Perovskite solar cells with a planar heterojunction structure prepared using room-temperature solution processing techniques", *Nature Photonics*, 8. 133-138. December. 2013.
- [7] Bi, D., Yang, L., Boschloo, G., Hagfeldt, A and Johansson, E.M.J, "Effect of Different Hole Transport Materials on Recombination in  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Perovskite Sensitized Mesoscopic Solar Cells", *Physical Chemistry Letters*, 4 (9). 1532-1536. April. 2013.
- [8] Boix, P.P., Nonomura, K., Mathews, N and Mhaisalkar, S.G, "Current progress and future perspectives for organic/inorganic perovskite solar cells", *Materials Today*, 17(1). 16-23. January-February. 2014.
- [9] Zhu, L., Shi, J., Lv, S., Yang, Y., Xu, X., Xu, Y., Xiao, J., Wu, H., Luo, Y., Li, D and Meng, Q, "Temperature-assisted controlling morphology and charge transport property for highly efficient perovskite solar cells", *Nano Energy*, 15.540-548. July.2015.
- [10] Brenner, T.M., Egger, D.A., Kronik, L., Hodes, G and Cahen, D, "Hybrid organic-inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties", *Nature Reviews Materials*, (15007). January. 2016.
- [11] Foster, J.M., Snaith, H.J., Leijtens, T and Richardson, G, "A model for the operation of perovskite based hybrid solar cells: formulation, analysis and comparison to experiment", *SIAM Journal on Applied Mathematics*, 74(6). 1935-1966. November. 2014.
- [12] Sun, X., Asadpour, R., Nie, W., Mohite, A.D and Alam, M.A, "A Physics-Based Analytical Model for Perovskite Solar Cells," *IEEE Journal of Photovoltaics*, 5(5).1389-1394. July.2015.
- [13] Palik, E.D and Ghosh, .G, *Handbook of Optical Constants of Solids*, Academic Press, Orlando, 1985, 577-580.
- [14] S.Berthier and J. Lafait. "Modelisation des proprietes optiques des milieux inhomogenes a structure complexe", *Journal de Physique Colloques*, 42 (1), Jan 1981.
- [15] A.M.Jayannavar and N.Kumar, "Generalization of Bruggeman's unsymmetrical effective medium theory to a three-component composite", *Physical Review*, 44(21), December 1991.
- [16] M.Louge and M.Opie, "Measurements of the effective dielectric permittivity of suspensions", *Powder Technology*, 62(1), July 1990.
- [17] P. Mallet, "Diffusion électromagnétique par des matériaux hétérogènes rugueux: homogénéisation et étude du couplage", Thèse de doctorat. Aix-Marseille 3, France, 2006.
- [18] S. Orlowska, "Conception et prédiction des caractéristiques diélectriques des matériaux composites à deux et trois phases par la modélisation et la validation expérimentale", Thèse de doctorat, Ecole Centrale De Lyon, France, 2003.
- [19] Gueye, E.H.O., Tall, P.D., Ndao, C.B., Dioum, A., Dione, A.N and Beye, A.C, "An Optical and Electrical Modeling of Dye Sensitized Solar Cell: Influence of the Thickness of the Photoactive Layer", *American Journal of Modeling and Optimization*, 4(1). 13-18. 2016.
- [20] D. Allé, "Etude en 3D de cellules photoactives organiques bicouches composées de phthalocyanine de cuivre (CuPc) et de fullerene ( $\text{C}_{60}$ ): Influence de la dissociation des excitons aux interfaces actives", thèse de doctorat de troisième cycle, Université Cheikh Anta Diop de Dakar, Sénégal, 2010.
- [21] L. Jylhä and A. Sihvola, "Equation for the effective permittivity of particle-filled composites for material design applications", *Journal of Physics D: Applied Physics*, 40 (16).4966-4973. August. 2007.
- [22] Zhao, Y., Nardes, A.M and Zhu, K, "Solid-State Mesostructured Perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Solar Cells: Charge Transport, Recombination, and Diffusion Length", *Physical Chemistry Letters*, 5(3) 490-494. January.2014.
- [23] D'Innocenzo, V., Grancini, G., Alcocer, M. J., Kandada, A. R. S., Stranks, S. D., Lee, M. M and Petrozza, A, "Excitons versus free charges in organo-lead tri-halide perovskites", *Nature Communications*, 5. 3586. April.2014.
- [24] Lee, M. M., Teuscher, J., Miyasaka, T., Murakami, T. N and Snaith, H. J, "Efficient hybrid solar cells based on meso-superstructured organometal halide perovskites", *Science*, 338(6107). 643-647. Novembre. 2012.
- [25] Dong, Q., Fang, Y., Shao, Y., Mulligan, P., Qiu, J., Cao, L and Huang, J, "Electron-hole diffusion lengths >175 nm in solution grown  $\text{CH}_3\text{NH}_3\text{PbI}_3$  single crystals", *Science*, 347(6225). 967-970. February .2015.
- [26] Gonzalez-Pedro, V., Juarez-Perez, E. J., Arsyad, W.-S., Barea, E. M., Fabregat-Santiago, F., Mora-Sero, I and Bisquert, J, "General Working Principles of  $\text{CH}_3\text{NH}_3\text{PbX}_3$  Perovskite Solar Cells", *Nano Letters*, 14(2). 888-893. January. 2014.