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Improved Optical and Electrical Characteristics of PTB7:PCBM Organic Solar Cells via ZnO Spacer Integration

Fathi Brioua 1, Chouaib Daoudi 2
Electrical Engineering Department, University of Ahmed Draia - Adrar, Algeria 1
Département Génie Électrique, Université 20 Août 1955, Skikda, Algeria 2

INTRODUCTION & AIM

Organic solar cells (OSCs) have emerged as strong contenders for next-generation photovoltaic technologies, offering advantages such as mechanical flexibility, lightweight design, and low-cost fabrication. Nevertheless, their power conversion efficiency (PCE) remains constrained by insufficient light absorption and suboptimal charge extraction in the PTB7:PCBM-based active layer [1].

To address these limitations, this study aims to enhance the overall device performance by incorporating a zinc oxide (ZnO) optical spacer layer. Using finite element method (FEM) simulations, the research investigates how inserting a ZnO layer between the PEDOT:PSS and the active blend can :

- Improve the optical field distribution, exciton generation rate, and light-harvesting capability of the OSC.

METHOD

Two-dimensional optical simulations were performed using the Finite Element Method (FEM) to analyze an OSC stack consisting of a glass substrate, a SiO_2 buffer layer, an indium tin oxide (ITO) anode, a PEDOT:PSS hole transport layer, a ZnO buffer layer, a PTB7:PCBM active region, and an aluminum (Al) cathode. The optical field distribution and exciton generation rate (G) were evaluated under monochromatic illumination at different incident wavelengths, as well as under the AM1.5G solar spectrum at 100 mW/cm². The active layer comprised a PTB7 donor blended with a PCBM acceptor to examine the influence of the ZnO optical spacer on the overall device performance.

Two device configurations were : a reference structure (Glass / SiO_2 / ITO / PEDOT:PSS / PTB7:PCBM/Al) and a modified design **incorporating a ZnO spacer layer** inserted between the PEDOT:PSS and the active blend (Glass/SiO_2/ITO/PEDOT:PSS/**ZnO**/PTB7:PCBM/Al).

Dissipated energy (W.m-2 nm-1) $\varphi(z,\lambda) = \alpha(\lambda)\frac{n_i}{n_0} I_{solar}\left|\frac{E(z)}{E_0}\right|^2$

Optical model [2]

$$G(z) = \sum_{\lambda=300}^{900} G(z,\lambda) \quad G(z,\lambda) = \frac{\varphi(z,\lambda)}{\hbar\upsilon}$$

Electrical model [3]

Poisson equation

$$\frac{d^2\emptyset}{dx^2} = -\frac{q}{\varepsilon_0\varepsilon_r}(p-n)$$

Current densities

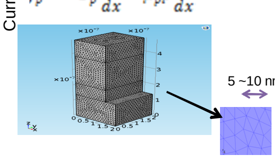
$$J_n = -D_n\frac{dn}{dx} + \mu_n n\frac{d\emptyset}{dx}$$

$$J_p = -D_p\frac{dp}{dx} - \mu_p p\frac{d\emptyset}{dx}$$

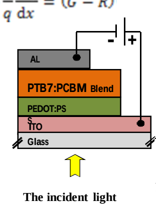
Charge continuity equations

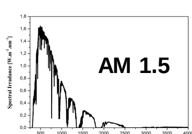
$$\frac{1}{q}\frac{dJ_n}{dx} = (G-R)$$

$$-\frac{1}{q}\frac{dJ_p}{dx} = (G-R)$$

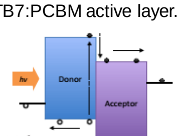


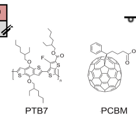
Mesh of the studied structure (FEM)





The Energy potential diagram PTB7:PCBM active layer.





Chemical structure of P3HT:PCBM

RESULTS & DISCUSSION

Figure 1: Electric field intensity profile **without the ZnO** space layer inside the PTB7: PCBM active layer.

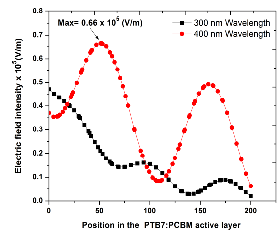


Figure 2: Energy distribution of electrical field intensity of structure (PTB7:PCBM active layer).

a) Structure with ZnO at 450 nm

b) Structure without ZnO at 450 nm

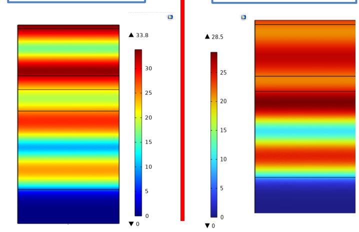


Figure 3 : Electric field intensity profile **with the ZnO** space layer inside the PTB7: PCBM active layer

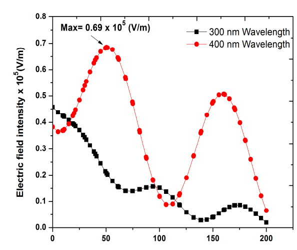


Figure 4: Generation rate inside the PTB7: PCBM active layer for 40, 100, 150 and 220 nm thick.

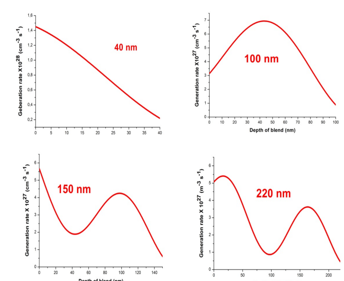


Figure 5 *:* Calculated current (I-V) for structure with ZnO material based on our numerical model results under AM 1.5 G illumination.

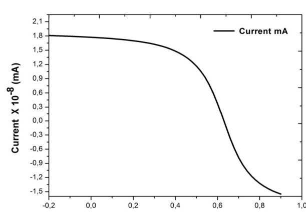
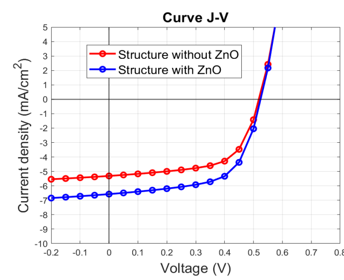


Figure 6: Short circuit current density (mA/cm2) with and without ZnO material.



CONCLUSION

- The insertion of a ZnO spacer layer enhances the internal electric field distribution within the active region.
- Reflection losses at the PEDOT:PSS/active interface are reduced, leading to improved light confinement and exciton generation.
- The ZnO layer simultaneously acts as an optical spacer and an electron-transporting interfacial layer, resulting in higher light absorption and overall device efficiency.
- Finite element simulations using COMSOL Multiphysics strongly correlated with experimental data, validating the design's effectiveness in optimizing performance.

FUTURE WORK / REFERENCES

Future work will focus on integrating optimized ZnO spacer thickness and morphology with experimental fabrication to validate simulation results and further enhance the optical–electrical synergy in organic solar cells.

[1] Brioua, F., Remram, M., Nechache, R., et al. **Appl. Phys. A**, 123, 704 (2017).
[2] Fathi, B., Chouaib, D. **Iran. J. Mater. Sci.**, 21(2), 1 (2024).
[3] Brioua, F., Daoudi, C., Mekimah, B., Lekouaghet, B. **Phys. Scr.**, 99, 085951 (2024)