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P3HT:PCBM as an active layer to enhance the efficiency of organic solar cells

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INTRODUCTION & AIM

Organic solar cells have gained significant attention in recent years due to their properties of low material cost, light weight, and high-throughput roll-to-roll production. However, their low efficiency and stability remain major challenges. Despite significant advancements in organic solar cells, challenges remain in optimizing photon harvesting, minimizing optical losses, and enhancing the electric field distribution, all of which are crucial for improving device efficiency [1].
The objective of this work is to address these challenges by optimizing the optical and structural properties of the active layers to enhance the performance and stability of organic solar cells (P3HT:PCBM). Using a coupled optical-electrical model, Finite Element Method (FEM) simulations performed in COMSOL Multiphysics software are employed to calculate:

- The spatial distribution of the electric field and the photon absorption generation rate.
- The short-circuit current densities as a function of the active layer thickness, based on the exciton generation rate (G).

METHOD

To properly study the effect of optimizing the optical and structural properties on enhancing the short-circuit current from semiconductor active layer materials, we modeled the structure: Indium Tin Oxide (ITO) / PEDOT:PSS/ P3HT:PCBM (Blend active layer)/ (AL). The illumination conditions were calibrated based on a standard solar cell with an intensity of 100 mW/cm² and AM 1.5 G.

COMSOL MULTIPHYSICS

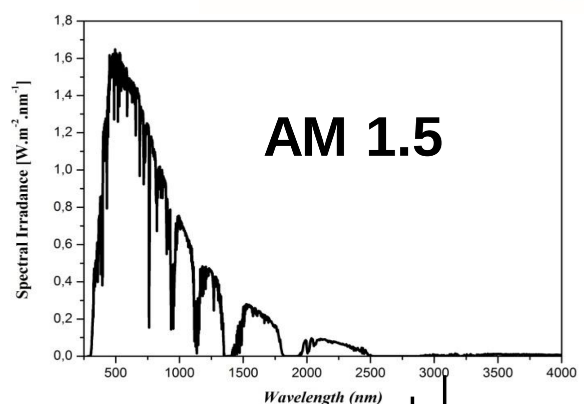
Optical model [2]

Dissipated energy (W.m-2 nm-1)

$$\varphi(z,\lambda) = \alpha(\lambda)\frac{n_i}{n_0}\, I_{solar} \left|\frac{E(z)}{E_0}\right|^2$$

$$G(z,\lambda) = \frac{\varphi(z,\lambda)}{\hbar\upsilon}$$

$$G(z) = \sum_{\lambda=300}^{900} G(z,\lambda)$$



Electrical model [3]

Poisson equation

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

Charge continuity equations

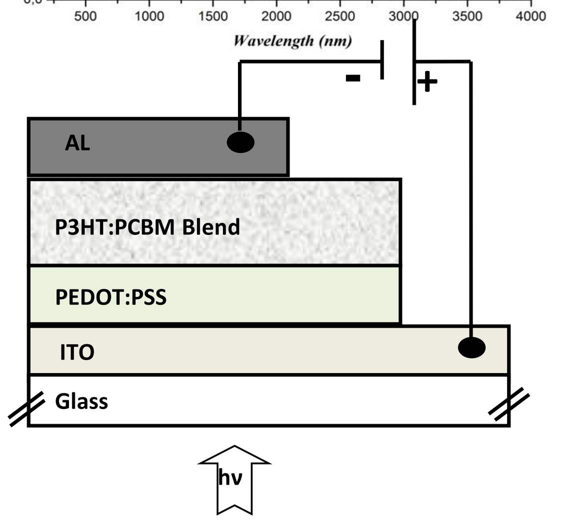
$$\frac{1}{q}\frac{dJ_n}{dx} = (G-R)$$

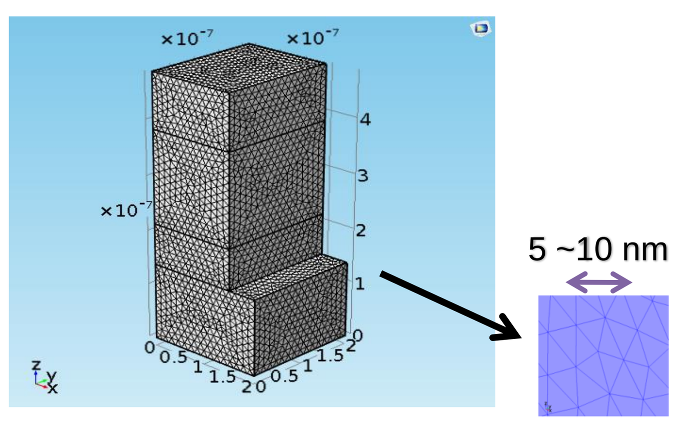
$$-\frac{1}{q}\frac{dJ_p}{dx} = (G-R)$$

Current densities

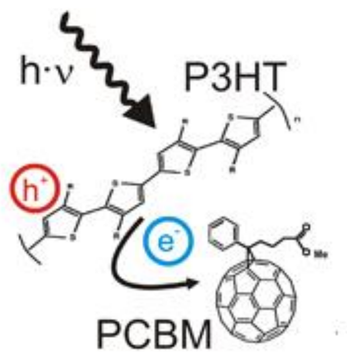
$$J_n = -D_n\frac{dn}{dx} + \mu_n n\frac{d\emptyset}{dx}$$

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

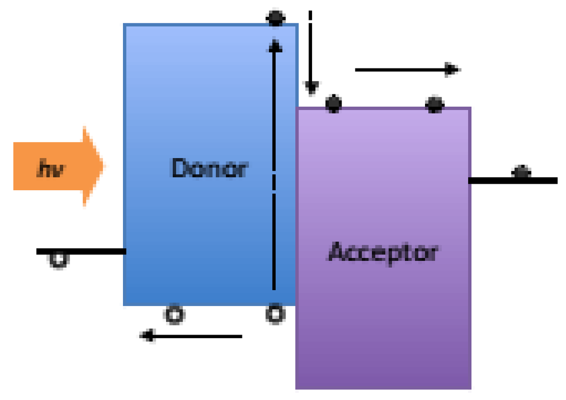




Mesh of the studied structure (FEM)



Chemical structure of P3HT:PCBM



The Energy potential diagram P3Ht:PCBM active layer.

RESULTS & DISCUSSION

Figure 1: Normalized electric field intensity of P3HT:PCBM.

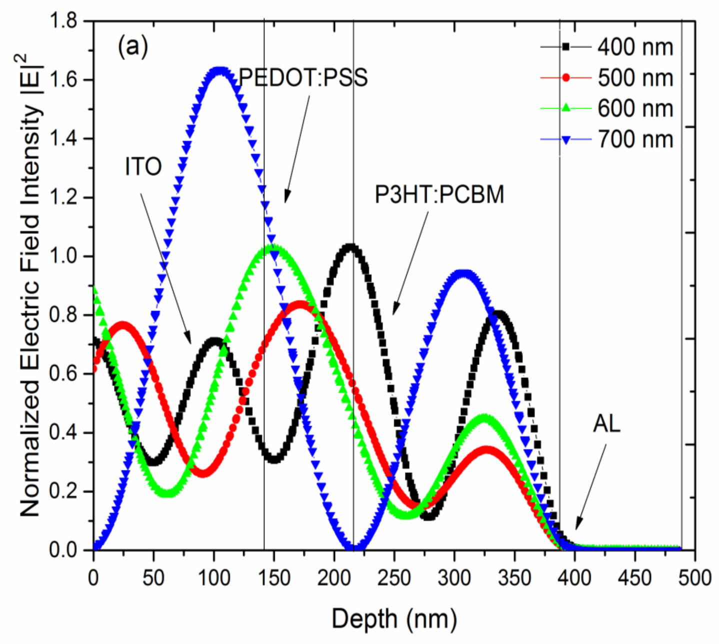


Figure 2: Energy distribution of hole concentration for P3HT:PCBM.

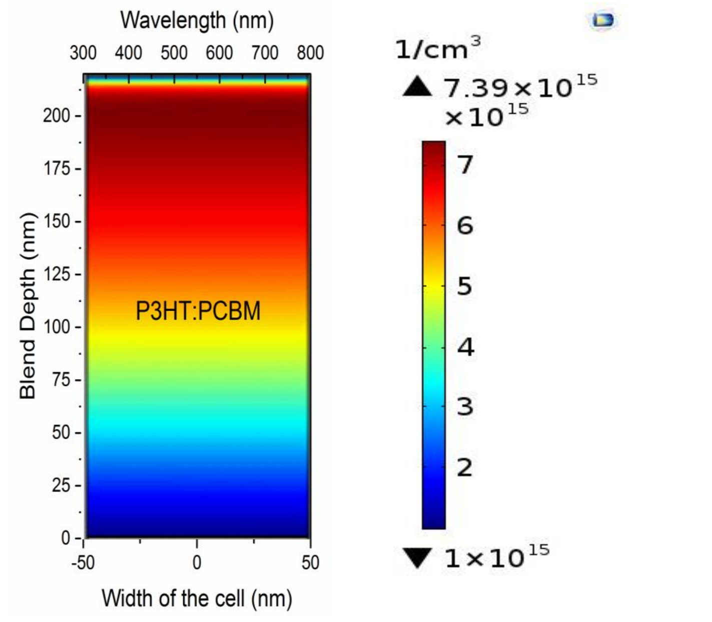


Figure 3 : Generation rate with different active layer thicknesses based of P3HT:PCBM.

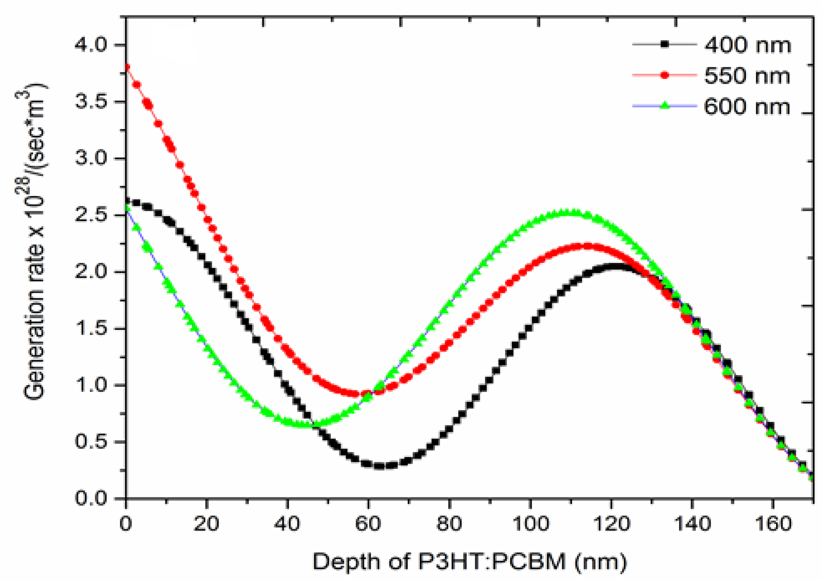


Figure 4 : Variations in light intensity versus wavelength for P3HT:PCBM Material.

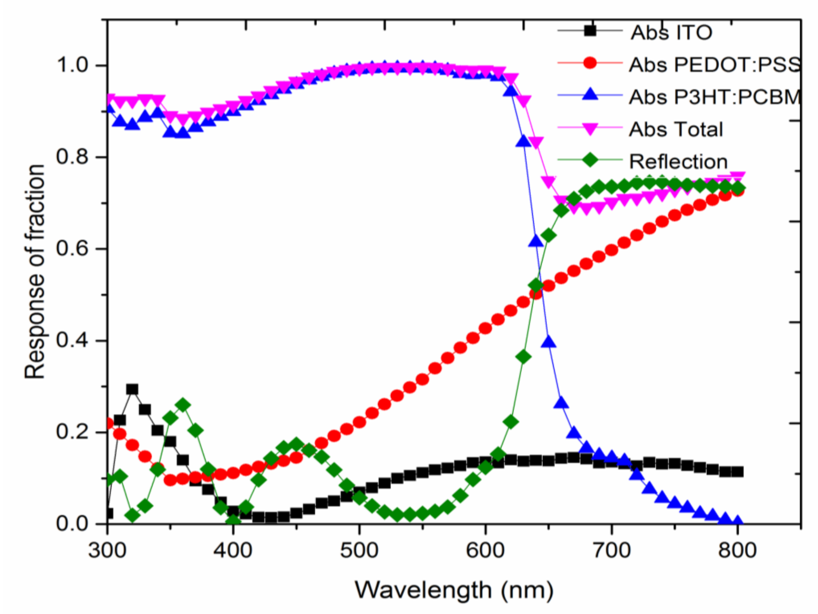


Figure 5 : Short-circuit current density (Jsc) of P3HT:PCBM with varying active layer thicknesses.

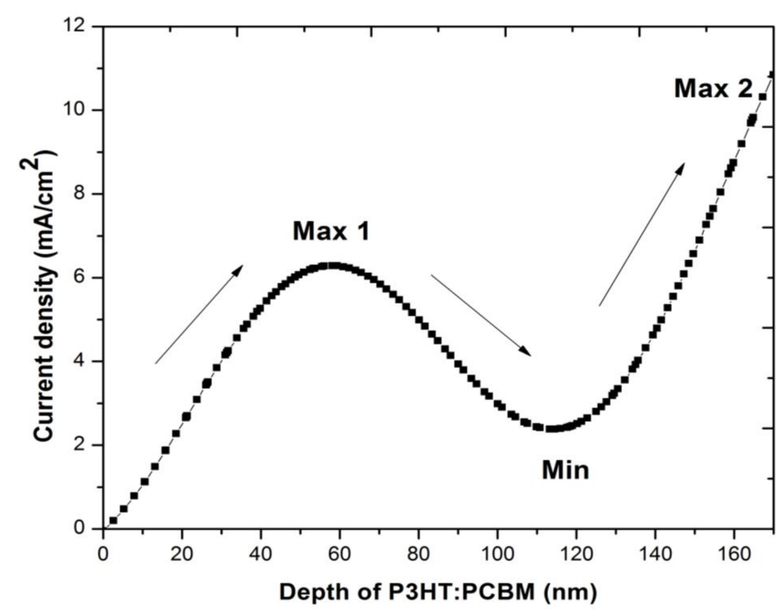
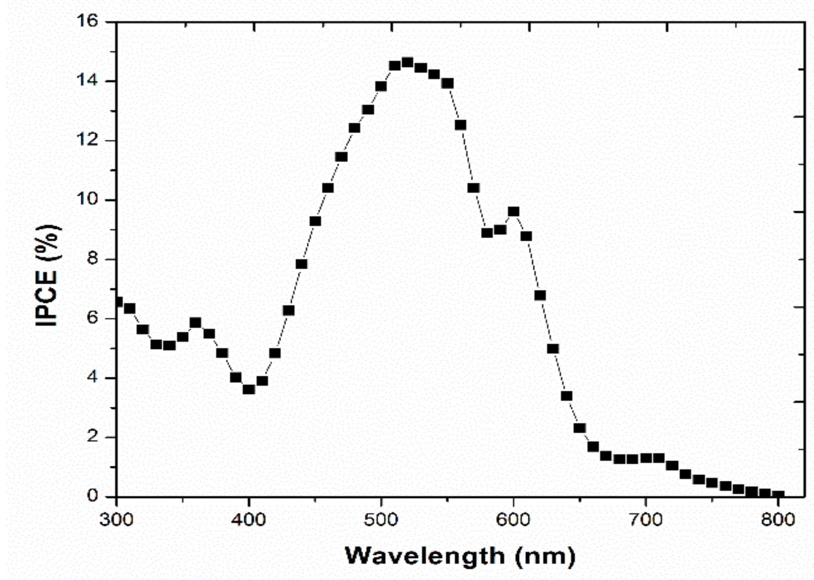


Figure 6: Incident Photon-to-Current Efficiency (IPCE) as a function of wavelength.



CONCLUSION

•This study investigates the impact of optical interferences on organic solar cell performance, analyzing electric field intensity, generation rate, absorption profiles, and transmission.
• A short-circuit current density of 11.35 mA/cm² is achieved, demonstrating high absorption within the active layer.
• Finite element simulations using COMSOL Multiphysics strongly correlated with experimental data, validating the design's effectiveness in optimizing performance.

FUTURE WORK / REFERENCES

As a perspective, we propose using ZnO nanoparticles to enhance the initial part of the optical response, which in turn improves the electrical response and overall efficiency.

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