Evaluation the Efficiency of Organic Solar Cell with other vital Parameters via Simulation models

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الملخص

تمتلك الخلايا العضوية الكهروضوئية مستقبلاً واعداً كبديلٍ لخلايا الطاقة الشمسية التقليدية المُصنعة من السيلكون، لعدة أسباب اقتصادية وبيئية، إضافةً إلى الاستهلاك العالمي للطاقة المتزايد سنوياً، مع نمو الأنشطة البشرية المختلفة، لهذه الأسباب يعمل الباحثون على تصنيع خلايا طاقة شمسية جديدة ذات كفاءة مناسبة، باستخدام مواد جديدة، لا تسبب تلوثاً بيئياً، وبتكلفة إنتاج أقل من خلايا السيلكون، من بين هذه المواد التي أُستخدمت لهذا الغرض، البوليمرات العضوية التي تمتلك خواص شبه موصلة، التي لفتت أنظار الباحثين والعلماء لخواصها الفريدة، وانخفاض تكلفة تصنيعها، إضافةً لعدم إضرارها بالبيئة، لهذا، قمنا بهذه الدراسة عبر استخدام نماذج المحاكاة للخلايا العضوية الكهروضوئية، لتقييم كفاءة تحويل الطاقة للخلية، ومجموعة من العوامل التي تؤثر على الإنتاجية الإجمالية للخلية كمعامل سعة الخلية، فرق جهد الدائرة المفتوحة، الطاقة القصوى المتولدة من الخلية، أظهرت النتائج قيماً مختلفةً لهذه العوامل مع أي تغيير في سمك الطبقة النشطة للخلية حيث تتناقص كفاءة تحويل الطاقة للخلية مع كل زيادة في سمك الطبقة النشطة، والعكس صحيح، بقية العوامل لم تتأثر بشكل كبير. هذا النوع من الدراسات يوفر الجهد والوقت خلال عملية التصنيع الفعلية في المختبر، وتعطي مؤشرات جيدة على الظروف المثلى لإنتاج الخلايا العضوية الكهروضوئية عمليا.

الكلمات المفتاحية: الخلايا العضوية الكهروضوئية، الطبقة النشطة، المحاكاة، كفاءة أداء الخلية، معامل السعة، الطاقة المتولدة القصوى

ABSTRACT

The Organic Solar Cells, (OSCs) have a promising future as an alternative for traditional Silicon Solar Cells, (SSCs) for many economic and environmental reasons, in addition to global consumption of energy, that increases annually, with growth of human activities, due to these factors , researchers are working to make new solar cells, with appropriate efficiency, by using new materials, that not polluting the environment, and less cost than silicon solar panels, between the materials used for this purpose, organic polymers which is have semi-conductive properties attracted intention of researchers and scientists for unique properties and low cost fabrication, as well they haven't negative impacts on environment. Hence, we presented this Simulation Study, for organic solar cell, to evaluate the Performance Cell Efficiency, (PCE) and other important parameters, that effected on the whole cell productivity, such as Fill Factor, Open-Circuit Voltage and Maximum Power Produced by the cell, the results shows different values for these parameters, with any changing in active layer thickness, where is the performance cell efficiency decreased with increase in thickness of active layer, and vice versa, other parameters didn't effects widely, this type of study reduces consuming time and efforts during real production in the laboratory and gives good indications about the optimum conditions to product organic solar cell in the real production.

Keywords: Organic Solar Cells, Active layer, Simulation, Performance Cell Efficiency, Fill Factor, Maximum Produced Power

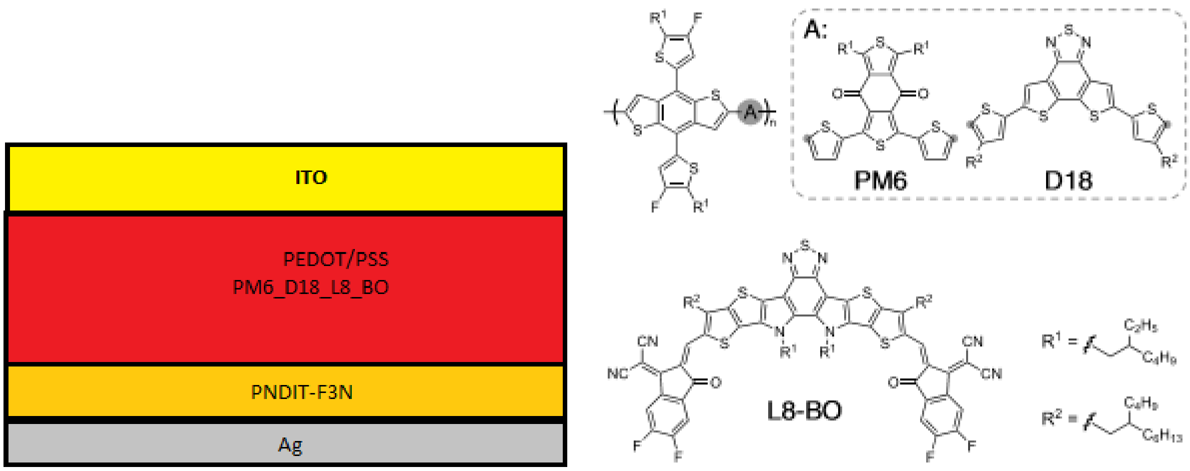
1. Introduction

Organic solar cells have more attraction to researcher rather than Silicon based solar cells, due to low cost, easy production process, as economic values [1]. In addition to environmental factors relating to materials included in organic solar cells fabrication, which is more environment friendly [2], there are many techniques used in fabrication of organic solar cells, Bulk Hetero-Junction based organic solar cells have increasing intention of researchers because they have unique optical and physical properties [3], this technique improved the performance of the OSC [4], the most challenge in the organic solar cells, is how we can raising the cell performance more than other types of solar cells [3], the BHJ approach including blending the Donor (D) and acceptor (A) materials to increasing the D:A interfacial area this leads to enhance charges separation and efficiency [5], compared to bilayer architecture [6], the active layer materials is the main factor that determines the efficiency of the cell [7], so we focused in our research to study it particularly, with clearing its effects on other parameters that controlling on device performance.

Our aims in this paper to demonstrating the effects of active layer thickness on the most important parameters such as Fill Factor, open circuit voltage, the maximum current produced by the cell, and finally the Performance cell efficiency based on changing of active layer thickness by simulation models.

2. Models and Methods:

We assume a cube lattice for the active layer that interact with incident light photons, The cell structure is Glass/ITO/PEDOT/PSS/PM6-D18-L8-BO, and the chemicals and their structure used in this research are shown in Fig 1A, and Supplementary Fig. 1. L8-BO (2,2′-((2Z,2′Z)-((3,9-bis(2-butyloctyl)-12,13-bis(2-ethylhexyl)12,13-dihydro-[1,2,5]thiadiazolo[3,4-]thieno[2″,3″:4′,5′] thieno[2′,3′:4,5]pyrrolo[3,2-g]thieno[2′,3′:4,5]thieno[3,2-b]indole-2,10-diyl)bis(methaneylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile) primarily absorbs light between 550 and 900 nm [8], PM6 (poly((4,8-bis(5(2-ethylhexyl)-4-fluoro-2-thienyl)benzo[1,2-b:4,5-b′]dithiophene-2,6-diyl)-2,5-thiophenediyl(5,7-bis(2-ethylhexyl) -4,8-dioxo-4H,8H-benzo[1,2-c:4,5-c′]dithiophene-1,3-diyl)2,5-thiophenediyl)) and D18 (poly(dithieno[3,2-e:2′,3′-g]-2,1,3-benzothiadiazole-5,8-diyl(4-(2-butyloctyl)-2,5-thiophenediyl) (4,8-bis(5-(2-ethylhexyl)-4-fluoro-2-thienyl) benzo[1,2-b:4,5-b′] dithiophene-2, 6-diyl) (3-(2-butyloctyl)-2,5-thiophenediyl))), PM6 and D18 used together as donors to absorb short wavelength photons in the range 400-700 nm, and to make high quality phase of the donors,



(a) **(b)**

Fig 1: (a) The structure of the cell, (b) chemical structure of active layer materials.

Poly[(9,9bis(30-(N,N-dimethylamino)pro-pyl)2,7-fluorene)-alt-5,50-bis(2,20-thiophene)-2,6-naphthalene1, 4,5,8-tetracabox-ylic-N,N0-di(2-ethylhexyl)imide] (PNDIT-F3N) used as material transporter for electrons [9], the Ag as other electrode for the cell as sown in Fig 1a.

For the model Study, we used the OghmaNano software, which is 1D,2D drift diffusion model simulation software, the most benefits for this model it goes to the trouble of explicitly solving the ShockleyRead-Hall equations as a function of energy and position space, This enables one to model effects such as mobility/recombination rates changing as a function of carrier population and enables one to correctly model transients as one does not have to assume all the carriers in the trap states have reached equilibrium. Things such as ToF transients, CELIV transients etc. Can be modelled with ease. Of course can be used for more ordered materials as well, you then just need to turn the traps of [10]. Table 2.1 shows the simulation process parameters.

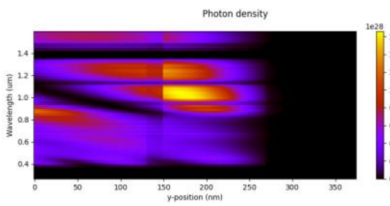
Table 2.1: Simulation Parameters:

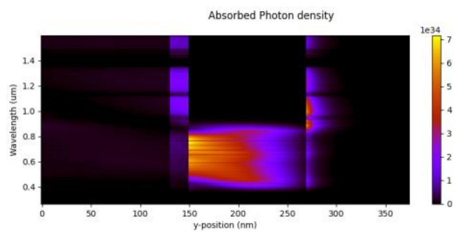
Parameter	Value
ITO Thickness	60 nm
Substrate Material	Glass

Substrate Thickness	200 nm
Active Layer Thickness	120-320 nm
Light Density	1.5AM

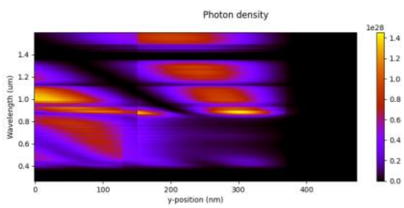
3. **Results & Discussion:**

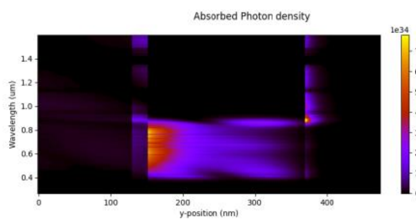
3.1 Optical Absorbance:



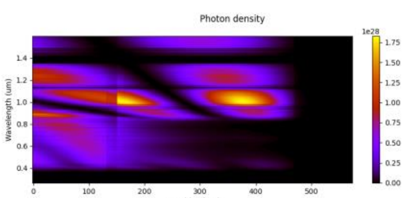


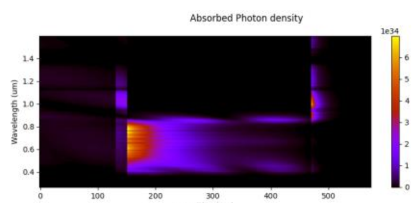
(a) **(b)**





(c) **(d)**





(e) **(f)**

Fig 2: (a) spectrum represents the photo density, (b) spectrum represents the absorbed photon for the active layer no 1, while (c) & (d) for the active layer 2, (e) & (f) for the active layer no 3 respectively.

Fig 2, it's clarifying the increasing in range of the absorbed photon density with increasing in the active layer thickness, so, the Layer 3 has absorbed photon density higher than layer 1 &2, but it doesn’t mean has more efficiency as we will see next section.

3.2 The Cell Efficiency Parameters:

The following Table shows the vital parameters, those effects directly on the whole electrical power conversion of the modelled cells:

Table 3.2: The Vital parameters of the modelled cells:

The active Layer Thickness (m)	Fill Factor (a.u)	Open Circuit Voltage (V)	Short circuit current (Am-2)	Power conversion efficiency (%)
1.2×10^{-7}	0.8039	0.8742	-2.4366	17.12
2.2×10^{-7}	0.6941	0.8608	-2.5289	15.11
3.2×10^{-7}	0.5338	0.8503	-2.4866	11.28

From the results shown in Table 3.2, we can see the high efficiency of the cells belongs to the Layer 1, which has higher value in Fill Factor, Open circuit voltage, and power conversion efficiency, and then the layer 2 has the medium values, finally the layer 3, has the less value for these vital parameters.

4. Conclusions

In this research paper, we found that optimum power conversion of the modelled cells in 400 nm by computational tool OghmaNano software simulation. The other important parameters has been explained by the changing the thickness of active layer, we can enhance the efficiency of the organic solar cell by changing active layer thickness and testing other conductor polymers that may lead to get high cell efficiency.

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