



شبكة المعلومات الجامعية
التوثيق الإلكتروني والميكرو فيلم

بسم الله الرحمن الرحيم



MONA MAGHRABY



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التوثيق الإلكتروني والميكروفيلم



شبكة المعلومات الجامعية التوثيق الإلكتروني والميكروفيلم



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التوثيق الإلكتروني والميكروفيلم

جامعة عين شمس

التوثيق الإلكتروني والميكروفيلم

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AIN SHAMS UNIVERSITY

FACULTY OF ENGINEERING

Electronics Engineering and Electrical Communications

Modeling and simulation of bulk heterojunction organic solar cell

A Thesis submitted in partial fulfillment of the requirements of the degree of

Doctor of Philosophy in Electrical Engineering

(Electronics Engineering and Electrical Communications)

by

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Master of Science in Electrical Engineering

(Electronics Engineering and Electrical Communications)

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Statement

This thesis is submitted as a partial fulfillment of Doctor of Philosophy in Electrical Engineering Engineering, Faculty of Engineering, Ain Shams University.

The author carried out the work included in this thesis, and no part of it has been submitted for a degree or a qualification at any other scientific entity.

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Abstract

The non-fullerene acceptor organic solar cells (NFA-OSCs) have attracted lots of interest due to their higher stability and greater efficiency compared with traditional fullerene acceptor solar cells. Throughout this thesis, we improved the performance parameters of a bulk heterojunction (BHJ) structure of NFA-OSC by adjusting the transport layers characteristics which can be achieved experimentally. The validation of the optimization is done using simulation. SCAPS program has been utilized to simulate the structure and the validity of its simulation has been verified by comparing the I-V characteristics with measurements from a reported literature. In addition, we studied the impact of several parameters such as the thickness of the active layer and its trap density on the cell performance using simulation. According to our presented optimization, some encouraging results were obtained: a short circuit current (J_{sc}) of 16.2 mA/cm², open circuit voltage (V_{oc}) of 1.06 V, fill factor (FF) of 82.95% and power conversion efficiency (PCE) of 14.25%. The obtained results pave the way for high efficiency NFA solar cells.

In addition, the design guidelines for the graded bulk heterojunction (GBHJ) structure, with an active layer of donor-blend-acceptor are provided. Also, a comparative study is performed between the presented GBHJ with conventional bulk heterojunction (BHJ) and bi-layer solar cells using simulation to compare the main performance parameters, collection efficiency, recombination and generation of all structures. The results indicate that GBHJ has the highest power conversion efficiency (PCE) of 10.15%, while BHJ

has the highest collection efficiency (η_{coll}) of 96.71%. The GBHJ performance is optimized by inspecting each layer individually and interfacial and bulk trap states. Further, an improvement of the performance of GBHJ is achieved by using other candidates of non-fullerene acceptors (NFAs) with higher reported blend mobilities. A short circuit current density (J_{sc}) of 19.88 mA/cm², open circuit voltage (V_{oc}) of 0.798 V, fill factor (FF) of 78.68 %, PCE of 12.49 % and η_{coll} of 95.12 % is obtained.

Key words:

non-fullerene acceptor (NFA), bulk heterojunction (BHJ), organic solar cells (OSCs), SCAPS , graded bulk heterojunction (GBHJ), collection efficiency.

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