Ain Shams University
Faculty of Engineering
Electronics and Communications Department

Modeling and Simulation of Perovskite Solar Cells

A Thesis
Submitted in partial fulfillment of the requirements of
a Master of Science Degree in Electrical Engineering
(Electronics and Communications Engineering)

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Faculty of Engineering – Ain Shams University

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Statement

This dissertation is submitted to Ain Shams University for the degree of Master of Science in Electrical Engineering (Electronics and Communications Engineering).

The work included in this thesis was carried out by the author at the Electronics and Communications Engineering Department, Faculty of Engineering, Ain Shams University, Cairo, Egypt.

No part of this thesis was submitted for a degree or a qualification at any other university or institution.

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Abstract

Perovskite solar cells (PSCs) have attracted considerable attention as a competitor technology in solar cells due to the rapid enhancement in their power conversion efficiency (PCE) in recent years. PSCs have several advantages such as their bandgap tunability, lower cost, tolerance of high impurities, long diffusion length and wide optical absorption. In this thesis, different electron transport materials (ETMs) have been analyzed with a new Copper Iodide (CuI) Hole Transport Material (HTM) to replace the conventional electron and hole transport materials for PSCs, such as the titanium dioxide (TiO_2) and the expensive Spiro-OMeTAD which has been known to be suffer from performance degradation. Moreover, the influence of the electron transport layer (ETL), hole transport layer (HTL) and the perovskite layer thicknesses on the overall cell performance, is studied. The design of the proposed PSC is performed utilizing SCAPS-1D simulator (Solar Cell Capacitance Simulator-one dimension). Because of its high electron affinity and tunable bandgap, zinc oxysulfide (ZnOS) is found to be the best replacement for TiO_2 as ETM. The results show that lead-based PSC with CuI as HTM is an efficient arrangement and better than the easily degradable and expensive Spiro-OMeTAD. According

to the presented simulation and tuning of various layers thicknesses, the highest designed efficiency is 26.11%. In addition, different ETMs have been simulated with copper oxide (CuO) as HTM in Iodide/chloride mixed halide perovskite $MAPbI_{3-x}Cl_x$ by incorporation of Chlorine (Cl) in perovskite lead halides ($MAPbI_3$) is used because $MAPbI_{3-x}Cl_x$ films have a long term of thermal stability than $MAPbI_3$ and better carrier diffusion length. In addition, a proposal for tuning the features and parameters of the PSCs, such as the thickness and defect density of the perovskite layer, the electron, and hole transport layers, the doping concentrations, and the bandgap energy, has been introduced. The results showed that the tuned mixed halide PSCs with ZnOS as an electron transport material and CuO as a hole transport material have the highest performance with a power conversion efficiency of 30.82%. This achievement represents a 4.71% increase in conversion efficiency.

Keywords — Copper iodide; Copper oxide; Electron transport materials; Hole transport materials; Perovskite Solar Cell; SCAPS-1D.

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