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Improved Organometal Halide Perovskite Solar Cell Performance via Morphological Control and Substrate Parameter Optimization

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KEYWORDS

Abstract:
This research presents a comparative analysis of solar cells utilizing organometal halide perovskite, with titanium dioxide (TiO_2) and zinc oxide (ZnO) employed as electron transport materials (ETMs). Utilizing SCAPS-1D simulations, the study investigates the influence of absorber and ETM thickness, interface trap density of states, and dopant concentration on photovoltaic solar cell performance. The findings reveal that increasing the thickness of the $MAPbI_3$ perovskite layer up to 700 nm enhances power conversion efficiency (PCE), while thickness increments beyond 90 nm for TiO_2 and ZnO layers diminish efficiency. The research underscores the importance of controlling the morphology of $CH_3NH_3PbI_3$ perovskite solar cells (PSC) for achieving high efficiency and explores experimental and theoretical approaches to attain efficiencies of up to 29%. Additionally, the study examines the significance of optimizing thickness, reducing defect density, and incorporating a back contact with a higher work function, suggesting that replacing the TiO_2 layer with a ZnO layer could enhance solar cell performance.

Introduction:
Perovskite solar cells (PSC) have emerged as a promising technology for solar energy conversion, boasting a certified power conversion efficiency (PCE) of 29% within a short timeframe [1-6]. Compared to silicon alternatives, PSC offers advantages such as lower cost, lighter weight, increased flexibility, and compatibility with roll-to-roll production, making it a competitive option for future commercialization. Achieving precise control over perovskite morphology is crucial for optimal device performance, especially in planar junction PSCs, where the crystalline layer must maintain self-supporting structure [7-10]. However, manipulating perovskite crystal growth remains challenging. This study investigates the impact of 3-aminopropanoic acid self-assembled monolayers (SAM) on ZnO layers, resulting in enhanced $CH_3NH_3PbI_3$ perovskite film structure and improved energy level alignment at the interface. The study also compares the use of TiO_2 and ZnO as ETMs in perovskite solar cells, exploring their significance in enhancing module performance [11-13].

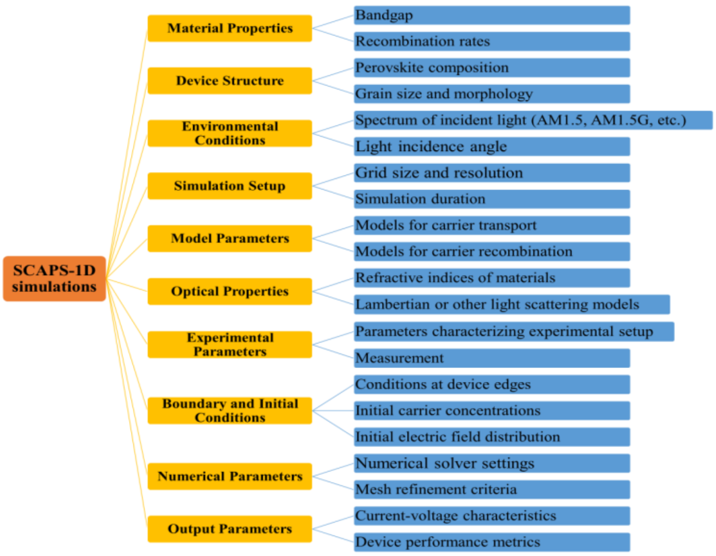

Figure 1. SCAPS-1D simulation steps and process use in this work [14-17].

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Experimental Methodology:

The study employed materials from Sigma Aldrich Corp. and Spiro-OMeTAD from Lumi. Tech. Corp. in Taiwan, conducting experiments using various instruments including AFM, XRD, UV-Vis absorption spectroscopy, SEM, PL spectroscopy, and UPS [18]. SCAPS software was utilized for modeling heterojunction solar cells with input layers consisting of spiro-MeOTAD, HTM, $MAPbI_3$, TiO_2, ZnO, FTO, and Au [19-22]. Experiments were conducted under 1 Sun light conditions, with the FTO substrate subjected to washing, rinsing, drying, and cleaning processes. The perovskite layer was synthesized using a two-step technique in a nitrogen gas-filled glove box, with spiro-OMeTAD film exposed to ambient conditions for conductivity enhancement. Back contact application was performed via thermal evaporation [23-26].

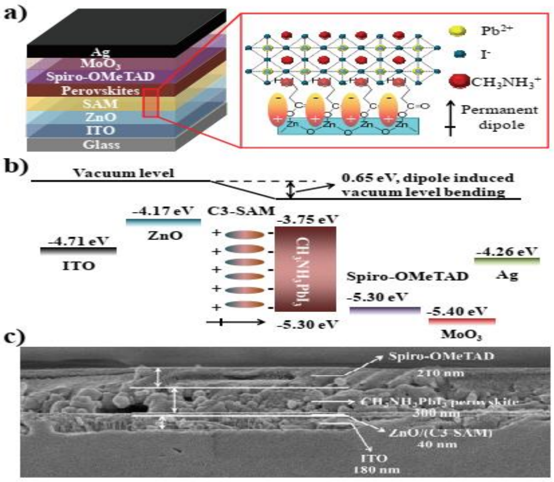

Figure 2. The diagram depicts the structure of a perovskite solar cell, highlighting the formation of a permanent dipole and the role of the self-assembled monolayer in perovskite crystals.

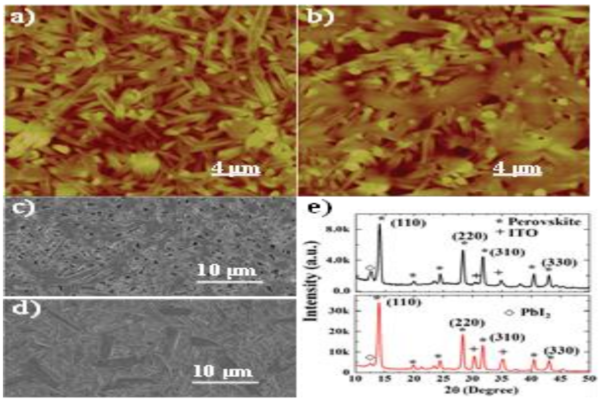

Figure 3. AFM images of $CH_3NH_3PbI_3$ perovskite.

Results and Discussion:

The study observed morphological improvements in $CH_3NH_3PbI_3$ perovskite films following PEDOT:PSS deposition on ZnO, attributed to enhanced compatibility between substrate and perovskite [27-33]. XRD analysis revealed enhanced crystalline quality of perovskite films with PEDOT:PSS, while AFM and SEM images depicted larger crystalline domains [34]. Device performance evaluation showed a significant increase in PCE with PEDOT:PSS modification, emphasizing its importance in PSC optimization. Simulation results demonstrated a positive correlation between absorber thickness and PCE, highlighting the critical role of substrate parameters in solar cell performance.

Conclusion:

In conclusion, this research emphasizes the efficacy of incorporating SAM on ZnO layers to enhance perovskite film structure and device performance. Comparative analysis of TiO_2 and ZnO as ETMs underscores their significance in optimizing solar cell

efficiency. The study's findings provide valuable insights into morphological control techniques and substrate parameter optimization for enhancing PSC performance, paving the way for further advancements in perovskite solar cell technology.

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Conflict of Interest Statement

The authors conducted ethical and transparent research, demonstrating the importance of ethical practices in scientific research.

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