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Design and Analysis of Quantum Dot Solar Cell Using SCAPS-1D Software

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Abstract

Compared to conventional solar cells, quantum dot solar cells (QDSCs) have drawn a lot of attention due to their hybrid structure, low production cost, and greater power conversion efficiency. Nevertheless, carrier recombination in the quasi-neutral region (QNR) continues to limit their performance. The electron transport layer (ETL) and hole transport layer (HTL) are two of the layers that are most important in determining the overall efficiency of the device. The SCAPS-1D simulator was used in this work to conduct a numerical investigation with indium gallium zinc oxide (IGZO) as the ETL, CdS as the buffer layer, Sb_2Se_3 as the absorber layer, and PbS as the HTL. After optimizing the device construction, doping concentrations were thoroughly examined. In this work, the SCAPS-1D simulation program was used to conduct a thorough numerical analysis of a QDSC structure. Lead sulfide (PbS) is the HTL, cadmium sulfide (CdS) is the buffer layer, antimony selenide (Sb_2Se_3) is the absorber layer, and IGZO is the ETL in the suggested device architecture. Key photovoltaic characteristics, such as fill factor, open-circuit voltage, short-circuit current density, and total power conversion efficiency, were thoroughly examined in relation to material selection and layer arrangement. In order to lower recombination losses and enhance charge carrier extraction, the effects of doping concentration modifications in the transport and absorber layers were carefully investigated after initial device optimization. The modified device reached a maximum power conversion efficiency of 35.67% thanks to the improved performance of IGZO.

Keywords: IGZO, quantum dot solar cell, features of SCAPS-1D, fill factor (FF), Voc, JSC, power conversion efficiency (PCE), quantum efficiency (QE), and JV characteristics

INTRODUCTION

Given the rapid advancement of technology and population expansion, modern science and technology have a crucial role to play in meeting the increasing need for sustainable and clean energy [1]. Making the switch to renewable energy sources is crucial to reducing pollution brought on by excessive fossil fuel use and maintaining the natural equilibrium of Earth's ecosystems [2]. Solar energy is particularly plentiful among renewable sources; of the more than four million exajoules (10^{11} J) of solar energy that reach Earth each year, around 5×10^1 EJ can be practically harvested, which is enough to meet the world's energy and electricity needs. Solar energy is unique among renewable energy sources because of its long-term sustainability, accessibility, and abundance. It is anticipated that more than four million exajoules (10^{11} J) of solar energy reach the Earth annually, of which around 5×10^1 exajoules can be feasibly harnessed utilizing present and emerging technology. This vast potential greatly exceeds the

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present global energy and electricity consumption, showcasing solar power as a vital alternative for future energy systems. As a result, solar cells and photovoltaic technologies are widely used to effectively transform sunlight into electrical energy, making clean power generation possible for utility-scale, industrial, and household applications. As a result, solar cells are frequently used to transform sunlight into electrical power.

Owing to their superior light absorption and extended carrier diffusion lengths, organic–inorganic hybrid perovskite solar cells (PSCs) are attractive options for next-generation photovoltaic technology. The power conversion efficiency (PCE) of PSCs has significantly improved since their first report in 2009, increasing from 3.8% to 25.7% in just ten years [3–5]. Despite this rapid development, the poor durability of perovskite materials in the presence of moisture, heat, and extended light exposure makes their large-scale commercialization difficult [3].

Because they can effectively convert solar photons into electrical energy, quantum dot solar cells (QDSCs) have attracted interest as possible substitutes for upcoming photovoltaic systems [6]. Nanoscale semiconductor crystals, which offer special optoelectronic characteristics, size-dependent tunable bandgaps, and dimensions smaller than the exciton Bohr radius, are used as absorber materials in QDSCs [7].

In a conventional solar cell arrangement, the absorber layer is positioned between the electron transport layer (ETL) and the hole transport layer (HTL). However, QDSCs frequently have poor PCE because of their low carrier concentration and mobility [8–15]. Extensive research has focused on investigating appropriate materials for each device layer to improve efficiency and practical applications to overcome these restrictions.

The ETL and HTL have the greatest impact on the overall performance of all layers in a solar device [8, 16–18]. Thus, it is crucial to choose materials that are both affordable and capable of producing high PCE. With a PCE of 13.94% when combined with a PbS–TBAI quantum dot absorber and PbS–EDT HTL, TiO_2 is currently one of the most widely utilized ETL materials [19].

In this study, a device with a suitable electron transport material was modeled to construct and analyze an effective QDSC. The suggested structure uses WS_2 as the ETL placed on indium-doped tin oxide (ITO), PbS–EDT as the HTL, CdS as the buffer layer, and Sb_2Se_3 as the absorber layer [20–23].

Following a thorough examination of this arrangement, indium gallium zinc oxide (IGZO) was used in place of the WS_2 ETL, and the modified apparatus was thoroughly examined.

The photovoltaic performance metrics of both device designs, including the fill factor (FF), PCE, short-circuit current density (Jsc), and open-circuit voltage (Voc), were assessed and compared. Furthermore, the impact of the HTL doping density was examined.

Here, FF is defined as the ratio of the maximum output power to the product of Voc and Jsc, PCE is computed as the ratio of the maximum output power to the incident solar power, Jsc is the maximum current density generated under short-circuit conditions, and Voc is the maximum voltage produced when no external current flows.

Additionally, the impacts of the shunt and series resistances were investigated. For both devices, contour charts showing the link between ETL thickness and bandgap were created, and the effect of the operating temperature on device performance was investigated. An ideal device configuration was determined after a thorough comparison of the outcomes.

DEVICE STRUCTURE AND OPERATION

With approximately half of its energy falling into the infrared portion of the spectrum, the Sun alone can supply the world's ever-expanding energy needs [24]. The capacity of QDSCs to efficiently capture energy from the infrared spectrum is one of their main advantages over traditional solar cells. An ETL, absorber layer, buffer layer, and HTL constitute the four-layer device structure used in this study. Figure 1 shows the entire device architecture [16, 17, 25, 26].

ITO, as depicted in Figure 1, is connected to a WS_2 layer that functions as the ETL and as the front contact through which incident solar energy enters the device [26, 27].

Because they lead to increased stability, improved adhesion, and decreased sheet resistance, electrical characteristics are more important than optical transparency. ITO films are better suited for this application than fluorine-doped tin oxide (FTO) films because they are smoother, can be deposited over larger regions, and require lower processing temperatures. Cadmium sulfide (CdS) serves as the buffer layer and antimony triselenide (Sb_2Se_3) as the absorber layer.

The Sb_2Se_3 absorber was interfaced with CdS at the device junction, allowing for effective incident radiation absorption. The PbS–EDT HTL was covered with a layer of gold (Au) for the back contact.

In the changed device arrangement, ITO was maintained as the front contact, but IGZO replaced WS_2 as the ETL. The buffer layer in this structure is CdS, the absorber is Sb_2Se_3, and the HTL is PbS–EDT. After analysis, the device structure that was first calibrated, ITO/WS_2/CdS/Sb_2Se_3/PbS-EDT/Au, was redesigned as ITO/IGZO/CdS/Sb_2Se_3/PbS/Au. Higher electron mobility, a wider bandgap, increased efficiency, environmental friendliness, and more affordable fabrication are just a few of the advantages of IGZO over WS_2.

SCAPS

By simulating the quantum dot layer as an efficient semiconductor absorber, SCAPS can be utilized to model and study the electrical performance of QDSCs. Quantum dots in QDSCs offer significant light absorption and size-dependent band gaps; these characteristics can be integrated into SCAPS by varying the bandgap energy, electron affinity, density of states, and defect levels. By establishing bulk and interface defect distributions, SCAPS can be used to study the localized states and increased recombination, which are frequently introduced by quantum dots.

To learn how dot size, defect density, and interface quality impact device performance, researchers can use SCAPS to mimic the J-V characteristics, quantum efficiency (QE), and recombination mechanisms of QDSCs.

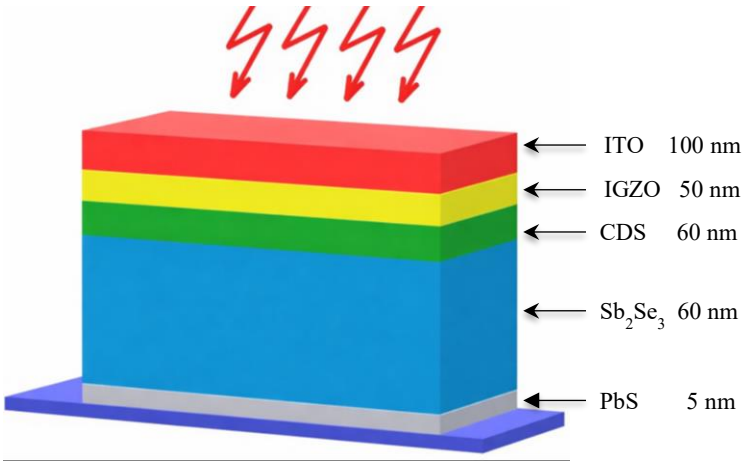

Figure 1. Diagram of a solar cell.

Additionally, it aids in assessing the band alignment and charge transport constraints between the transport and quantum dot layers. Overall, SCAPS offers a useful and efficient paradigm for maximizing the design of QDSCs by connecting the material characteristics of quantum dots to macroscopic device behavior.

RESULTS AND DISCUSSION

The QDSC simulated using SCAPS-1D software exhibited steady and effective device performance in terms of current density–voltage (J–V) characteristics. The current density remained nearly constant at approximately 40 mA/cm² as the applied voltage increased from 0.2 V to approximately 0.85 V, suggesting efficient charge carrier production and transport, as well as effective photon absorption by the quantum dot absorber layer.

This flat current region indicates that the device structure has a low series resistance and low recombination losses. The open-circuit voltage (V_oc) of the QDSCs is represented by a significant fall in the J–V curve about 0.9–0.95 V. After this, the current density quickly decreased and turned negative, indicating the cut-off region when the device stopped providing power. The prominent knee of the curve indicates good junction quality and a high fill factor.

The wavelength-dependent photo-response of the device is demonstrated by the quantum efficiency (QE) characteristics of the QDSCs derived from the SCAPS-1D simulation, as shown in Figure 2. Higher surface recombination losses and absorption in the front window or buffer layers are responsible for the comparatively low QE in the 300–400 nm range. The QE continuously improves as the wavelength increases from 400 nm to approximately 700 nm, indicating better photon absorption within the quantum dot absorber layer and more effective charge carrier generation and collection, as shown in Figure 3.

The QE curve steadily approaches saturation in the longer wavelength range beyond 700 nm, indicating that most of the input photons are efficiently absorbed and transformed into charge carriers. This behavior validates the potent light-harvesting capacity of QDs throughout a wide spectral range.

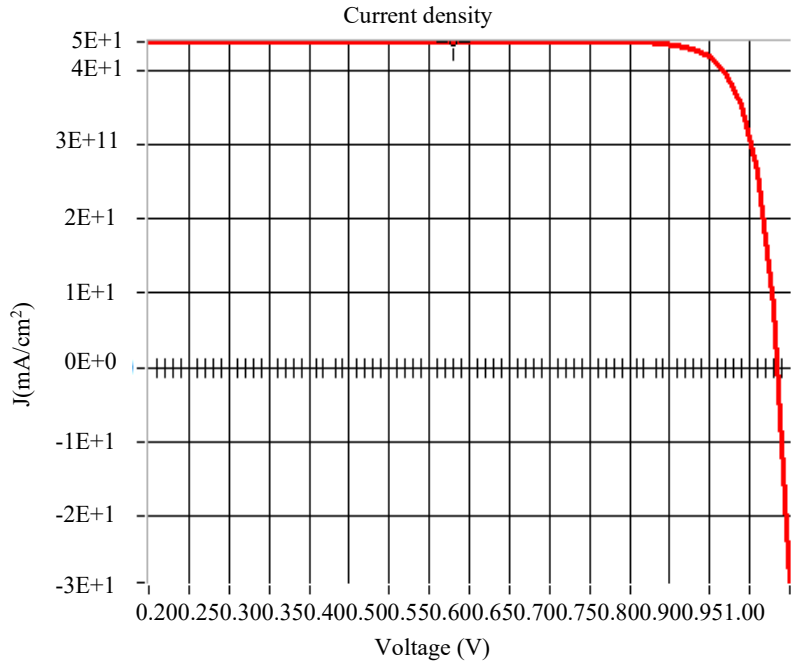

Figure 2. J–V Characteristics of solar cells.

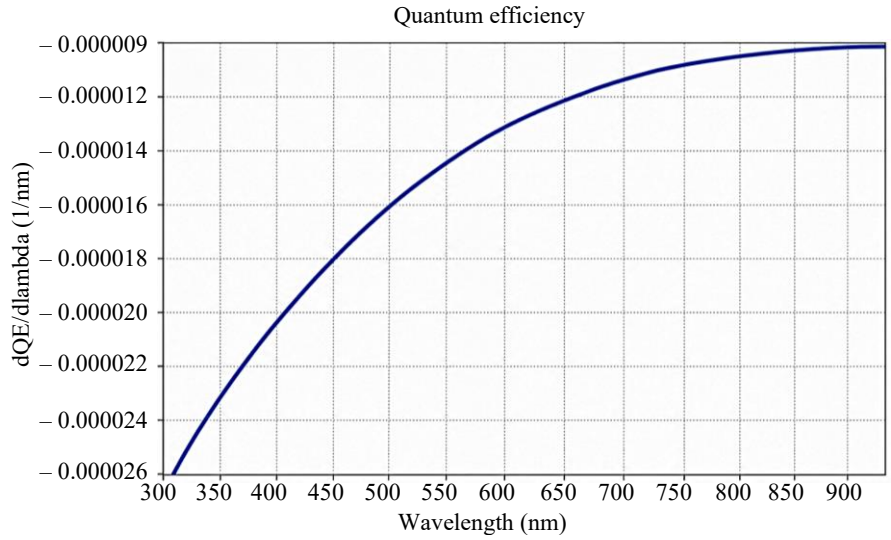

Figure 3. Quantum efficiency derivative versus wavelength graph.

CONCLUSION

In this study, we used the SCAPS-1D modeling program to systematically build and analyze a high-performance QDSC. We examined how important device layers, especially the HTL and ETL, affect the overall device performance. An optimal device design was successfully created using IGZO as the ETL, CdS as the buffer layer, Sb_2Se_3 as the absorber layer, and PbS as the HTL. Charge transport and collection were improved, and carrier recombination in the quasi-neutral area was greatly decreased by careful material parameter and doping concentration adjustment. Consequently, the suggested QDSC demonstrated a significant improvement over traditional designs, with a maximum PCE of 35.67%. These results demonstrate the great potential of IGZO-based quantum dot solar cells for next-generation photovoltaic applications and validate that careful selection and optimization of transport layers are critical for boosting QDSC performance.

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