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# Theoretical modeling and optimization: Cd-free CTS/Zn(O,S)/ZnO thin film solar cell

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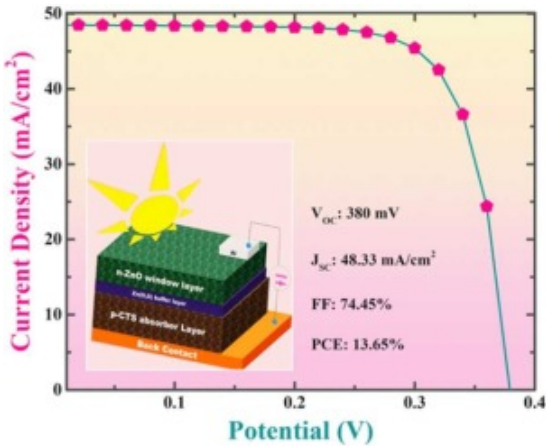
## Abstract

Latterly Zn(O, S) has gained utmost attention as an eco-friendly buffer layer with controllable energy levels for high-performance thin-film solar cell (TFSCs) devices. The article discusses that the conventional detrimental Cd-containing buffer is replaced by the non-toxic Zn(O,S) buffer and yielded a comparable high efficiency. Using SCAPS software, the modeling and numerical simulations of the CTS based solar cell are systematically analyzed. Detail investigations of the band alignment between the CTS absorber and Zn(O, S) buffer layer has been studied as a function of the S/(S+O) ratio along with the effects of thickness, carrier concentration, defect density of buffer layer and absorber layer with interface defect density. The final optimized results of p-CTS/Zn(O,S)/n-ZnO/Al heterojunction revealed that the obtained figure of merit value is comparably high ($\eta$=13.65%, $V_{OC}$ = 0.3802 V, $J_{SC}$ = 48.33 mA/cm$^2$, and FF = 74.45%) than the previously reported values. All in all, the present study suggests that Zn(O, S) can be a suitable alternative candidate for the CdS-buffer layer in a CTS-based solar cell.

## Graphical Abstract

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## Introduction

Since the last few years, scientists around the world are interested in the developments of second-generation solar cells; currently, CdTe and CIGS absorber based thin-film solar cells (TFSCs) are sharing the solar cell market. Despite having high power conversion efficiency up to ~22% [1], both the materials are facing the critics of containing Cd-like toxic material and costly rare metal Indium respectively [2], [3]. Scientists are looking towards the earth-abundant photovoltaic materials which can fulfill the energy necessities of the world in terms of cost-effectiveness and high power conversion efficiency (PCE) TFSCs devices. $Cu_2SnS_3$ is one of the potential solar cell materials and $Cu_2SnS_3$ based TFSCs devices could be an alternative for other commercial TFSCs. $Cu_2SnS_3$ compound is one of the several compounds of Cu-Sn-S system made by adding an earth-abundant tin (Sn) material in Cu-S system to form a stable compound. Cu-Sn-S system consists of several ternary compounds ($Cu_2SnS_3$, $Cu_3SnS_4$, and $Cu_4SnS_4$) that have already been scrutinized for solar cell applications as absorber material [4]. Like CZTS material $Cu_2SnS_3$ (CTS) also consists of earth-abundant and less-toxic materials but it is superior than CZTS due to its unique properties like; a wider range of phase stability, lesser elements, and low structural complexity [5]. CTS has p-type conductivity, structural dependent tunable direct bandgap (0.91 eV to 1.35 eV), and higher absorption coefficient (~$10^4$ to $10^5$ $cm^{-1}$) and these properties are similar to those of CIS, CIGS, CIGSe, and CZTS [6], [7], [8], [9]. CTS absorber materials are gaining considerable interest to develop cheaper, highly efficient TFSC devices. In this regard, there are several reports on the development of CTS absorber material [5] and of CTS based solar cells [10], [11], [12], [13], [14], [15], [16]. Furthermore, dopant materials like Ba, Co, Ge, Ag, etc. used to enhance the performance of CTS TFSCs [17], [18], [19], [20], [21]. Till now, in the development of CTS based TFSCs several cell structures have been developed and studied experimentally as well as theoretically. From the previous reported literature, we found that most of the experimentally developed CTS based solar cells consist of toxic CdS-buffer layer and similar structures further investigated theoretically. CdS

buffer layer performs well with CTS but due to its toxic nature and disadvantage of photocurrent loss due to its small bandgap, which is not sufficiently large for transmitting the entire portion of the visible spectrum and this result in limiting the PCE of devices.

We need to find out the replacement of the Cd-buffer layer which should be eco-friendly, has a large bandgap, high transparency, suitable band lineup with absorber material, high resistivity, cost-effective, low interface recombination, and gives a high performance with better stability to device. $ZnO_{1-x}S_x$ is the one, which provides all the mentioned aspects with a unique advantage of tunable and controllable bandgap by ratio (x) factor [22], [23]. Zn(O,S) as buffer layer has been used with different absorber layers such as CIGS, CIGSe, CZTS, Si and SnS to fabricate high PCE devices and these studies include both the experimental and theoretical analysis [24], [25], [26], [27], [28], [29], [30], [31]. There are several reported methods including Chemical bath deposition (CBD), evaporation, sputtering, an ion layer gas reaction (ILGAR), and atomic layer deposition (ALD) for the synthesis of Zn(O,S) semiconductor which possess wide-bandgap [32], [33], [34], [35]. All these reported methods have ease in controlling the ratio of oxygen and sulfur. However, CBD-Zn(O,S) often necessitates post-air annealing and light soaking to improve PCE. Khemiri et al. also report that Zn(O,S) as buffer layer can substitute CdS material in CZTS or sulfosalt TFSCs and Zn(O, S) thin films were synthesized via vacuum thermal evaporation method [36]. Physical vapour deposition can also be used to grow buffer layers, but we need to think about how to optimize the coverage of the layers on the CIGS films [35], [37]. Kobayashi et al. (2016) [37] has investigated for the Zn(O,S) layer via sputtering method which is a feasible and also a well-developed method at the manufacturing scale. Furthermore, the oxygen-to-sulfur ratio is a major determinant of Zn(O,S) properties, which may be easily controlled using the sputtering technique [35], [37].

In this article, we have explored the possibility of Zn(O, S) could be a suitable buffer layer for CTS-based thin film solar cells to grow as a high efficiency solar cell device. SCAPS-1D program has been utilized for numerical investigation; which is the proclaimed software for device modeling of thin-film solar cells and its results are relevant with the experimental results [38], 39, [40]. This simulation program was developed by Marc Burgleman et al. (2000) at ELIS of the National University of Gent [41]. There are several solar cell device physical parameters (AC & DC) measured under illumination condition; steady-state band diagrams, open-circuit voltage ($V_{OC}$), quantum efficiency (QE), short-circuit current density ($J_{SC}$), Fill-Factor (FF), efficiency ($\eta$), carrier recombinations for proposed CTS/Zn(O, S)/ZnO cell structure [42]. In present work, we have investigated the performance assessment of CTS TFSCs under the influence of the Zn(O, S) buffer layer by considering its physical properties such as S/(S+O) ratio, layer thickness, donor density concentration and with the variable properties of the absorber layer.

## Section snippets

## Device modeling and materials parameters

To illustrate the performance of proposed cell structure back contact/p-CTS/n-Zn(O, S)/n-ZnO/Al in details, a simulation was performed. Fig. 1 depicts the heterojunction solar cell structure comprising layer by layer of three different semiconductors with front and back contacts. In brief, back contact, p-CTS as an absorber layer with 2.5μm, n-Zn(O, S) as buffer layer with 50nm, n-ZnO as window layer with 200nm, and then Aluminium as front contact. This cell structure was further…

## Results and discussion

Following the numerical investigation based on significant parameters of three layers (absorber, buffer and window layer) of this proposed CTS/Zn(O, S)/ZnO solar cell structure. Initially, we had investigated this CTS/Zn(O, S)/ZnO solar cell structure with the flat band contacts (Front and Back contacts) to optimize the final optimal parameters of the absorber, buffer, and window layer. Finally, the performance of CTS based solar cell structure illustrated using final optimized parameters with…

## Influence of S/(S+O) ratio in Zn(O, S) buffer layer

In this section, we have first investigated the influence of S/(S+O) ratio (x) in the proper band alignment of buffer layer with absorber layer and secondly the influence of ratio on solar cell performance. To perform the simulation first the bandgap and electron affinity for each ratio (x) in Zn(O, S) should be calculated. The bandgap (2.6 eV to 3.6 eV) and electron affinity (3.6 eV to 4.6 eV) values of Zn(O,S) can be adjusted by altering the S/(S+O) ratio (x)[27]. Buffere et al. reported that…

## Influence of thickness and acceptor concentration ($N_A$) of CTS layer

CTS material with the direct narrow bandgap ($E_g$ = 0.91 eV) can absorb maximum incident AM 1.5 G radiations. There are other parameters like thickness which play an important role in the performance of TFSCs as well as in the device fabrication. Furthermore, factors like deposition techniques and sulfurization of the CTS layer may change their grain size and thickness. According to some literature surveys, the Cu/Sn ratio might be responsible for the acceptor type defects or carrier…

## Impact of Interface defect density CTS/Zn(O, S)

From the experimental point of view, in a heterojunction structure, the electron-hole pair movement is effective with a smooth and friendly contact of interfaces. Unless the device is irregular and less dense, there is a strong likelihood of charge trapping which will deteriorate the solar cell overall performance [5]. The interface defects are generally responsible for the recombination of electron-hole pairs at the interface between absorber/buffer layers. Here, the

effect of the density…

## Final CTS TFSC performance with back contacts

To analyze the final simulation of CTS cell structure with the optimized parameters, Aluminium (Al) as front contact and variable back contacts, details are arranged in Table 2. In this simulation, to optimize the back contact work function, we have varied work function values in a range of 5.0 eV to 5.6 eV. The performance of CTS solar cell vs back contact work function has illustrated in Fig. 12. The simulation results show that Al with a work function of 4.08 eV is suitable as front contact…

## Conclusion

In conclusion, it is evident that this study has shown that Zn(O, S) was best alternative as a buffer layer in the CTS/ZnO solar cell structure provides earth-abundant and environmentally friendly solar cell model. Summing up the results for the optimum physical properties with the help of simulations are kept nearly similar as in reported experimental CTS/CdS cell structures to compare easily their solar cell performances. Initially, the band-alignment of the buffer layer with the CTS absorber …

## Author Statement

*Vishnu V. Kutwade:* designed the model and the computational framework and analyzed the data. *Ramphal Sharma:* Supervise and helped in discussion. *Ketan P. Gattu:* assisted with the material selection and simulations. *Makrand E. Sonawane, Dipak A. Tonpe, Ibrahim M. S. Mohammed:* contributed in calculations and writing the manuscript with *Vishnu V. Kutwade*. All authors delivered constructive feedback and helped shape the research, analysis, and manuscript.…

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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