Physica B 740 (2026) 419128

Contents lists available at ScienceDirect

Physica B: Condensed Matter

journal homepage: www.elsevier.com/locate/physb

ZnO/SnS_2 nanoplate composite cathode buffer layer for performance enhancement of organic solar cells

Adarsh Raj K P [a], Divya Vandananikal Sivarajan [a], Anoop C. Sathyadevan Nair [a], Abhijith Thazhathenair [b,c], Raghu Chatanathodi [a,**], Vari Sivaji Reddy [a,*]

[a] Department of Physics, National Institute of Technology Calicut (NITC), Kozhikode, Kerala, 673601, India
[b] Department of Physics, PSG Institute of Technology and Applied Research, Neelambur, Coimbatore, Tamil Nadu, 641062, India
[c] Department of Nanoscience and Technology, PSG Institute of Advanced Studies, Peelamedu, Coimbatore, Tamil Nadu, 641004, India

ARTICLE INFO

Keywords:
ZnO cathode buffer layer
Interface engineering
SnS_2 nanoplates
Organic solar cells
Power conversion efficiency

ABSTRACT

The performance of organic solar cells (OSCs) based on the widely used zinc oxide (ZnO) cathode buffer layer (CBL) is severely affected by the surface defects, energy level mismatch with the common acceptor materials and its intrinsic hydrophilic nature. Developing novel materials to passivate surface defects and improve the properties of ZnO CBL is one of the prime areas of research in OSCs. In this work, hydrothermally synthesized SnS_2 nanoplates of average size 26 nm were successfully used to modify the surface of ZnO CBL in PTB7:PC_{70}BM based OSCs. The average power conversion efficiency of the OSCs increased from 6.13% to 6.84% after the surface modification. The XPS and DFT studies revealed passivation of oxygen deficiency defects and reduction in work function of CBL leading to decrease in energy barrier for flow of electrons from the active layer to cathode. Due to the efficient passivation of surface defects by the SnS_2 nanoplates, the conductivity of ZnO increased from 0.92×10^{-4} S/m to 1.63×10^{-4} S/m. Moreover, the SnS_2 modification significantly enhanced the hydrophobicity of ZnO, benefitting the formation of a good interfacial contact with the organic active layer. Significantly low leakage current observed in the case of OSCs based on ZnO/SnS_2 composite CBL reveals substantial decrease in charge recombination as a result of defect passivation. The present study demonstrates that interface engineering using metal dichalcogenide nanostructures is a promising approach to improve the properties of ZnO CBL/active layer interface in OSCs.

1. Introduction

Organic solar cells (OSCs) have garnered significant attention in the field of solar energy conversion owing to their numerous advantages such as flexibility, solution processability, roll-to-roll printing, low cost and lightweight [1,2]. The power conversion efficiency (PCE) of OSCs has recently surpassed 20% due to advancements in device architecture, design and the synthesis of novel active layer materials and interfacial engineering [3,4]. Fine tuning of active layer/electrode interfaces using suitable buffer layers is crucial for improving the performance of OSCs [5]. Materials with appropriate energy level alignment with the active layer, high optical transparency, chemical stability and charge selectivity are employed as buffer layers [6,7]. OSCs are categorized into conventional and inverted types based on the position and type of the buffer layers, which determine the direction of charge transport [6]. ZnO is widely used as the cathode buffer layer (CBL) in inverted OSCs owing to its high electron mobility, good hole-blocking ability and transparency in the visible region [8]. However, the defects on ZnO surface act as charge trapping centers and promote charge carrier recombination, adversely affecting the performance of OSCs [8]. The energy level mismatch between ZnO and commonly used acceptor materials hampers charge transport [9]. The hydrophilic nature of ZnO leads to poor interfacial contact with the hydrophobic active layer and also affects the long-term stability of OSCs due to the adsorption of oxygen and moisture [10]. Passivation of surface defects on ZnO, especially oxygen deficiency defects, is crucial for improving the performance of inverted OSCs. Several strategies including the use of a thin interlayer, UV-ozone or plasma treatment, and low-temperature annealing under an oxygen rich environment were successfully utilized to mitigate the drawbacks associated with ZnO surface defects

* Corresponding author.
** Corresponding author.
E-mail addresses: raghuc@nitc.ac.in (R. Chatanathodi), sivaji@nitc.ac.in (V.S. Reddy).

https://doi.org/10.1016/j.physb.2026.419128
Received 15 May 2026; Received in revised form 10 July 2026; Accepted 23 July 2026
Available online 26 July 2026
0921-4526/© 2026 Elsevier B.V. All rights are reserved, including those for text and data mining, AI training, and similar technologies.

[11–13]. Among these methods, depositing a thin interlayer is considered more advantageous due to its versatility, reproducibility, and better interfacial control with different active layer systems. Various classes of materials, such as organic small molecules, conjugated and non-conjugated polyelectrolytes, ionic liquids, fullerene derivatives and self-assembled monolayers have commonly been employed as interlayers on top of the ZnO surface [10,14–17]. However, despite their strong defect passivation abilities, the majority of these organic materials exhibit lower electrical conductivity, making the thickness of interlayers a crucial factor controlling the device performance. Hence, novel 2D materials that exhibit higher conductivity and promising optoelectronic properties need to be explored as interlayers to improve the surface properties of ZnO CBL.

Recently, metal dichalcogenides (MDCs), a new class of 2D layered materials, have attracted significant research attention due to their favorable properties, such as a tunable bandgap, solution processability, high mobility, large surface area and chemical stability arising from their low dimensionality [18,19]. MDCs such as MoS_2, WS_2, and $NbSe_2$ were explored as the hole transport layers in conventional OSCs to replace the acidic and hygroscopic PEDOT:PSS anode buffer layer [20–22]. In inverted OSCs, MoS_2 and $ZrSe_2$ nanosheets were used to improve the properties of ZnO CBL. Huang et al. achieved a significant enhancement in the efficiency of OSCs by utilizing MoS_2 nanosheet doped ZnO as the CBL [23]. The efficiency enhancement was attributed to the improvement in electron transport due to band alignment and interfacial smoothness of modified CBL. Li et al. increased the efficiency of PBDB-T:ITIC based OSCs from 10.5% to 12.09% using a $ZrSe_2$ nanosheet modified ZnO as the CBL [24]. A reduction in work function, passivation of oxygen defects on the ZnO surface and the selective trapping of holes by $ZrSe_2$ nanosheets were found to be responsible for the performance enhancement.

On the other hand, SnS_2, a promising MDC, is extensively studied for CBL applications in perovskite solar cells for its superior electrical properties, abundance, low cost and environment friendly nature [25,26]. Pramila et al. fabricated perovskite solar cells using a SnS_2-PCBM hybrid as the CBL and achieved higher efficiency and improved stability due to better energy level alignment, increased hydrophobicity and electrical compactness of the PCBM-SnS_2 CBL [25]. Yichuan et al. explored SnS_2 nanosheet modified SnO_2 as CBL and achieved high efficiency due to a reduction in the energy barrier between SnO_2 and the perovskite layer, the passivation of defects at the interface, and an improvement in the crystallization of the perovskite layer [26]. In spite of their promising properties like energy-level alignment, hydrophobicity, charge extraction efficiency, and ability to passivate interfacial defects as reported earlier, SnS_2 nanoplates have not been explored for the modification of the ZnO CBL in inverted OSCs.

In this study, we report the modification of the ZnO CBL using hydrothermally synthesized SnS_2 nanoplates for improving the properties of the ZnO/active layer interface in PTB7:$PC_{70}BM$ based OSCs. SnS_2 was selected due to its high electron mobility and suitable energy levels. The ZnO/SnS_2 composite CBL was expected to reduce the energy barrier for electron transport and simultaneously block the flow of holes from the active layer to the ITO cathode. The OSCs were fabricated in an inverted architecture and the concentration of SnS_2 nanoplate solution was optimized to achieve better photovoltaic performance. The SnS_2 nanoplate modification has led to a reduction in the work function, surface defect passivation, improved conductivity, and increased hydrophobicity. The performance enhancement mechanism is investigated using various material and device characterization techniques supported by theoretical simulations.

2. Experimental and simulation methods

2.1. Synthesis and characterization of SnS_2 nanoplates

SnS_2 nanoplates were synthesized using a hydrothermal method with tin (IV) chloride pentahydrate ($SnCl_4 \cdot 5H_2O$) and thioacetamide (C_2H_5NS) as the precursors. In this method, 2 mmol of $SnCl_4$. $5H_2O$ and 8 mmol of C_2H_5NS were dissolved in 20 mL of DI water and stirred for 30 min using a magnetic stirrer at room temperature. The solution was transferred into a 100 mL teflon-coated stainless-steel autoclave leading to a 20% filling ratio. The autoclave was kept in a hot air oven and the temperature was increased to 190°C at a rate of 5°C/min. The sample was heated at this temperature for 7.5 h and then allowed to cool naturally to room temperature. Subsequently, the yellow precipitate was collected by centrifugation at a speed of 6000 rpm for 15 min and then repeatedly washed with deionized water and ethanol to remove the impurities and then dried under vacuum at 60°C for 6 h [27]. The morphology of the synthesized SnS_2 nanoplates was examined using Field emission scanning electron microscopy (FE-SEM) (ZIESS, Gemini 1, Sigma 300) with an accelerating voltage of 3 kV and high resolution transmission electron microscopy (HR-TEM) (JEOL JEM 2100) operated at an accelerating voltage of 200 kV. The crystal structure of SnS_2 nanoplates was identified using powder X-ray diffractometer (XRD) (Rigaku Smartlab SE) with a Cu Kα radiation source. The diffraction pattern was recorded in the range of 10°-70° at a scan rate of 4.25°/min. Raman spectra of the samples were measured using a confocal Raman spectrometer (LabRAm HR Evo, Horiba) at an excitation wavelength of 532 nm and an excitation power of 5 mW.

2.2. Fabrication and characterization of inverted organic solar cells

Organic solar cells were fabricated with the structure indium tin oxide (ITO)/CBL/active layer/MoO_3/Ag using PTB7:$PC_{70}BM$ as the active layer and SnS_2 nanoplate modified ZnO as the CBL. Initially, patterned ITO substrates with a sheet resistance of 10-12 Ω/sq were cleaned thoroughly using the standard procedure. The ZnO precursor was prepared by using the sol-gel method. For the preparation, 110 mg of zinc acetate dihydrate, 31 mg of ethanolamine, and 1 mL of 2-methoxy ethanol were added in a 10 mL glass vial and magnetically stirred for 12 h. The prepared ZnO was spin-coated onto the plasma-treated ITO substrates at 4000 rpm for 40 s and annealed at 180°C for 12 min [28]. For the surface modification, various concentrations of pre-synthesized SnS_2 nanoplates in ethanol were spin-coated on top of the ZnO layer at 3000 rpm for 30 s and subsequently annealed at 100°C for 10 min. The active layer solution was prepared by dissolving PTB7 and $PC_{70}BM$ (1:1.5 wt ratio) in a mixture of chlorobenzene and 1,8-diiodooctane (97:3 v/v%) with a total concentration of 25 mg/mL. The solution was stirred overnight at 70°C and spin-coated on top of the CBL at 1300 rpm, and the film was dried at room temperature for 10 min for solvent evaporation. Finally, MoO_3 (7 nm) and Ag (100 nm) were thermally evaporated on top of the active layer through a shadow mask to create an active area of 9 mm^2. For the fabrication of PBDB-T:ITIC based OSCs, the active layer solution was prepared by dissolving PBDB-T and ITIC (1:1 wt ratio) in a mixture of chlorobenzene and 1,8 diiodooctane (99.5:0.5 v/v%) with a total concentration of 15 mg/ml. The solution was stirred for 12 h at 50°C and then spin coated on top of CBL at 1000 rpm followed by annealing at 160°C for 10 min.

The UV–Visible absorption spectra of the pristine and SnS_2 modified ZnO thin films on top of a glass substrate were measured using a PerkinElmer Lambda 365+ spectrophotometer. The photoluminescence spectra of the pristine and SnS_2 modified ZnO thin films on top of a glass substrate were measured using a PerkinElmer Fluorescence Spectrometer, LS55 at an excitation wavelength of 300 nm. The elemental composition of the pure and SnS_2 modified ZnO was investigated using X-ray photoelectron spectroscopy (XPS) (ULVAC-PHI, PHI5000 version probe III). The surface roughness of the CBLs was measured using an atomic force microscope (AFM) (Bruker's exclusive ScanAsyst). The contact angles on ZnO surface, before and after the modification with SnS_2 NPs, were measured using a contact angle meter (Holmarc, HO-IADCAM-01A). The current density-voltage (J-V) characteristics of the fabricated OSCs was measured using a precision source measure unit

two parallel R/CPE circuits, R1/CPE1 arising at higher frequencies corresponds to the bulk and R2/CPE2 appearing at lower frequencies represents the CBL/active layer interface [57]. The bulk resistance (R1) was observed to vary between 28 and 32 Ω indicating minute variation across all devices. Conversely, the interfacial resistance (R2) showed a significant change after modification of ZnO with SnS_2 nanoplates. The reference device displayed a high interfacial resistance of 923 Ω and which decreased to 565 Ω when the SnS_2 nanoplates of optimum concentration (0.05 mg/mL) were deposited on ZnO. When the SnS_2 nanoplate solution concentration was further increased to 0.1 mg/mL, the interfacial resistance increased to 781 Ω. The reduction in interfacial resistance is attributed to the passivation of surface defects and the suitable energy level alignment at the CBL/active layer interface.

To understand the reason behind the improvement in J_{SC} and *FF* values after incorporating SnS_2 nanoplates, exciton dissociation and charge collection efficiencies were calculated from the photocurrent density (J_{ph}) versus effective voltage (V_{eff}) plots. Here, J_{ph} is defined as the difference between the current densities under illumination (J_L) and dark (J_D). V_{eff} is defined as the difference between the voltage at which $J_{ph} = 0$ (V_0) and the applied voltage (V_A). Fig. 9b shows J_{ph} versus V_{eff} plots for the reference and modified devices at various SnS_2 concentrations. The exciton dissociation efficiency (η_{diss}) and the charge collection efficiency (η_{cc}) are defined as the ratio between J_{ph} and J_{sat} under short-circuit and maximum power output conditions, respectively. Here, J_{sat} is the saturation photocurrent density at a large reverse bias where all photo-generated excitons are dissociated and charge carriers are collected efficiently with negligible recombination losses. The η_{diss} and η_{cc} values of all devices were calculated and presented in Table 2. The reference device with pure ZnO CBL exhibited η_{diss} and η_{cc} values of 91.69% and 74.1%, respectively. When SnS_2 nanoplates were deposited on ZnO, η_{diss} and η_{cc} values increased to 93.43% and 78.03%, respectively indicating the significant role of SnS_2 nanoplates in improving the properties of ZnO/active layer interface in OSCs.

To verify the universality of the present modification strategy, OSCs were fabricated using a non-fullerene active layer system, PBDB-T:ITIC. The J-V characteristics of the OSCs obtained from the preliminary studies are shown in Fig. S10. The reference device with ZnO CBL exhibited a V_{OC} of 0.83 V, a J_{SC} of 14.14 mA/cm^2, and a FF of 53.59% leading to a PCE of 6.31%. Whereas, the modified device based on ZnO/SnS_2 CBL showed an improved PCE of 7.09% with V_{OC} of 0.83 V, a J_{SC} of 15.50 mA/cm^2, and a FF of 55.02%. These results confirm that the modification strategy reported in this study is applicable to both fullerene and non-fullerene active layer systems. Recently, several new materials such as natural dextran, antioxidants, fullerene-based self-assembled monolayers (SAMs), polyethylene glycol and small molecule electrolytes have been explored for the surface modification of ZnO CBL in OSCs leading to high efficiencies in the range 18-19% [42,58–61]. High PCE values exceeding 18% and improved device stability with T80 lifetimes more than 1500 h have been achieved by using natural dextran as a ZnO surface passivation layer [58]. Xia et al. demonstrated OSCs with PCE values above 19% utilizing fullerene-based SAMs for defect passivation and compatibility tuning of ZnO CBL [59]. These devices showed excellent stability by retaining 84% of their initial PCE even after 2000 h. More studies focusing on development of new materials suitable for improving the properties of ZnO/active layer interface will enable commercialization of OSCs.

Table 2
Exciton dissociation and charge collection efficiencies derived from $J_{ph}-V_{eff}$ curves.

	η_{diss}(%)	η_{cc}(%)
Reference	91.69	74.1
0.01 mg/mL	92.06	77.32
0.05 mg/mL	93.43	78.03
0.1 mg/mL	92.74	76.51

4. Conclusion

In summary, high purity SnS_2 nanoplates of average size 26 nm with hexagonal crystal structure were synthesized using hydrothermal method. The nanoplates were further utilized to improve the properties of ZnO CBL in PTB7:$PC_{70}BM$ based OSCs. The modified device with ZnO/SnS_2 composite CBL exhibited a relative PCE enhancement of 11.6% compared to the reference device based on pristine ZnO CBL. The performance enhancement is mainly attributed to the reduction in the work function of CBL from 5.4 eV to 5.2 eV and the passivation of ZnO surface defects as confirmed by the DFT and XPS results. The SnS_2 nanoplate modified ZnO exhibited enhanced hydrophobicity compared to bare ZnO leading to better interfacial contact with the active layer, thereby reducing the interfacial resistance from 923 Ω to 565 Ω. In addition, the modified device exhibited enhanced exciton dissociation and charge collection efficiencies compared to the reference device validating the observed improvement in J_{SC} and FF. The present study reveals that MDCs are potential candidates for improving the properties of ZnO CBL in OSCs.

Associated content

Calculated values of the lattice constant. EDS spectra and EDS colour mapping of hydrothermally synthesized SnS_2 nanoplates. XPS survey spectrum of ZnO and ZnO/SnS_2. The final configuration of the ZnO/SnS_2 interface for DFT calculations with and without defect. UV Visible transmittance spectra of ZnO film and ZnO/SnS_2 film with various concentrations of SnS_2 nanplates.

Author Information

Corresponding Authors.

Vari Sivaji Reddy - Department of Physics, National Institute of Technology Calicut (NITC), Kozhikode, Kerala India-673601, India https://orcid.org/0000-0001-8486-2086; Email: sivaji@nitc.ac.in.

Raghu Chatanathodi - Department of Physics, National Institute of Technology Calicut (NITC), Kerala, India-673601 https://orcid.org/0000-0001-9649-8285; E-mail: raghuc@nitc.ac.in.

Authors.

Adarsh Raj K P - Department of Physics, National Institute of Technology Calicut (NITC), Kozhikode, Kerala 673601, India, https://orcid.org/0009-0003-1745-5079,

Divya Vandananikal Sivarajan- Department of Physics, National Institute of Technology Calicut (NITC), Kozhikode, Kerala 673601, India, https://orcid.org/0009-0000-8511-3191.

Anoop C. Sathyadevan Nair - Department of Physics, National Institute of Technology Calicut (NITC), Kozhikode, Kerala 673601, India, https://orcid.org/0000-0002-2823-4998.

Abhijith Thazhathenair - Department of Physics, PSG Institute of Technology and Applied Research, Neelambur, Coimbatore, Tamil Nadu 641062, India; Department of Nanoscience and Technology, PSG Institute of Advanced Studies, Peelamedu, Coimbatore, Tamil Nadu 641004, India; https://orcid.org/0000-0001-5152-4478.

Funding sources

This work was supported by the Science and Engineering Research Board (SERB), India under Core Research Grant (CRG) (Project File No. CRG/2021/001795).

CRediT authorship contribution statement

Adarsh Raj K P: Data curation, Formal analysis, Investigation, Writing – original draft. **Divya Vandananikal Sivarajan:** Data curation, Formal analysis, Software, Writing – original draft. **Anoop C. Sathyadevan Nair:** Data curation, Formal analysis, Investigation.

Abhijith Thazhathenair: Data curation, Formal analysis, Writing – review & editing. **Raghu Chatanathodi:** Conceptualization, Formal analysis, Software, Supervision, Writing – review & editing. **Vari Sivaji Reddy:** Conceptualization, Formal analysis, Funding acquisition, Project administration, Supervision, Writing – review & editing.

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.

Acknowledgment

The authors thank the Science and Engineering Research Board (SERB) for partially supporting this work under Core Research Grant (CRG) (Project File No. CRG/2021/001795). Computational facilities provided by CCMS, NIT Calicut are gratefully acknowledged. The XRD facility at Dept. of Physics, NIT Calicut (FIST, Grant No.SR/FIST/PSI-113/2019) is gratefully acknowledged. DVS thanks Council of Scientific and Industrial Research (CSIR), India for providing fellowship under award number 09/0874(20082)/2024-EMR-I. AT acknowledges PSG Management Trustee and PSG Institute of Advanced Studies for providing the financial support through the Faculty Seed Research Grant. The authors also acknowledge Dr. Parameswaran P for valuable suggestions, Dr. Subramanyan N V for contact angle measurements, CeNSE, IISc for EQE facility, PSGIAS for AFM facility and, Nanotechnology Research Centre (NRC), SRMIST for XPS facility.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.physb.2026.419128.

Data availability

Data will be made available on request.

References

[1] T.M. Clarke, J.R. Durrant, Charge photogeneration in organic solar cells, Chem. Rev. 110 (2010) 6736–6767, https://doi.org/10.1021/cr900271s.
[2] Y. Cui, L. Hong, J. Hou, Organic photovoltaic cells for indoor applications: opportunities and challenges, ACS Appl. Mater. Interfaces 12 (2020) 38815–38828, https://doi.org/10.1021/acsami.0c10444.
[3] N. Wei, J. Chen, Y. Cheng, Z. Bian, W. Liu, H. Song, Y. Guo, W. Zhang, Y. Liu, H. Lu, J. Zhou, Z. Bo, Constructing multiscale fibrous morphology to achieve 20% efficiency organic solar cells by mixing high and low molecular weight D18, Adv. Mater. 36 (2024) 2408934, https://doi.org/10.1002/adma.202408934.
[4] C. Li, J. Song, H. Lai, H. Zhang, R. Zhou, J. Xu, H. Huang, L. Liu, J. Gao, Y. Li, M. H. Jee, Z. Zheng, S. Liu, J. Yan, X.-K. Chen, Z. Tang, C. Zhang, H.Y. Woo, F. He, F. Gao, H. Yan, Y. Sun, Non-fullerene acceptors with high crystallinity and photoluminescence quantum yield enable >20% efficiency organic solar cells, Nat. Mater. 24 (2025) 433–443, https://doi.org/10.1038/s41563-024-02087-5.
[5] A.C. Sathyadevan Nair, A. Rajan, K.P.A. Raj, A.M. Rajendran, M.R. Benny, K. Murali, P. Parameswaran, C.S. Suchand Sangeeth, R. Chatanathodi, V.S. Reddy, Fine tuning the work function of ZnO cathode buffer layers in organic solar cells by phenanthroline coordination, ACS Appl. Energy Mater. 7 (2024) 9011–9022, https://doi.org/10.1021/acsaem.4c02155.
[6] R. Po, C. Carbonera, A. Bernardi, N. Camaioni, The role of buffer layers in polymer solar cells, Energy Environ. Sci. 4 (2011) 285–310, https://doi.org/10.1039/C0EE00273A.
[7] S. Li, K. Bachagha, Application of buffer layer to improve the efficiency of organic solar cells, Energy Technol. 12 (2024) 2300822, https://doi.org/10.1002/ente.202300822.
[8] Z. Liang, Q. Zhang, L. Jiang, G. Cao, ZnO cathode buffer layers for inverted polymer solar cells, Energy Environ. Sci. 8 (2015) 3442–3476, https://doi.org/10.1039/C5EE02510A.
[9] H. Zheng, D. Zhou, L. Hu, Z. Xu, H. Xu, Y. Zhang, Y. Tong, B. Hu, Z. Li, L. Chen, Passivating the defects and modulating the surface energy of ZnO cathode interlayer for efficient nonfullerene organic solar cells, Sol. RRL 6 (2022) 2200871, https://doi.org/10.1002/solr.202200871.
[10] L. Li, H. Li, L. Nie, J. Chen, B. Chen, S. Wang, F. Nie, L. Tian, Inverted organic solar cells enabled by a ZnO/Organic electrolyte dual-layer electron transport layer with improved efficiency and stability, Langmuir 41 (2025) 32859–32865, https://doi.org/10.1021/acs.langmuir.5c04950.
[11] A. Kumar, A. Rana, N. Vashistha, K.K. Garg, M. Kumar, R.K. Singh, Defect density and performance influenced by ozone treatment of ZnO interface in inverted organic solar cell, Sol. Energy 225 (2021) 942–949, https://doi.org/10.1016/j.solener.2021.07.066.
[12] J. Yang, J. Lee, J. Lee, W. Yi, Oxygen annealing of the ZnO nanoparticle layer for the high-performance PbS colloidal quantum-dot photovoltaics, J. Power Sources 421 (2019) 124–131, https://doi.org/10.1016/j.jpowsour.2019.03.013.
[13] A. Pickett, A.A. Mohapatra, S. Ray, Q. Lu, G. Bian, K. Ghosh, S. Patil, S. Guha, UV–Ozone modified sol–gel processed ZnO for improved diketopyrrolopyrrole-based hybrid photodetectors, ACS Appl. Electron. Mater. 1 (2019) 2455–2462, https://doi.org/10.1021/acsaelm.9b00597.
[14] J. Li, J. Liu, X. Liu, R. Wang, J. Zhang, G. Tu, Lithium-ion-based conjugated polyelectrolyte as an interface material for efficient and stable non-fullerene organic solar cells, ChemSusChem 12 (2019) 1401–1409, https://doi.org/10.1002/cssc.201802939.
[15] S.B. Srivastava, R. Sharma, D. Appavoo, B. Lochab, S. Hahn, S. Yoo, S.P. Singh, Investigating the role of cathode buffer layers based on zinc oxide with surface-rich graded fullerene isomers in tuning the interfacial properties of organic solar cells, Sol. RRL 7 (2023) 2200797, https://doi.org/10.1002/solr.202200797.
[16] K.G. Gebremariam, F.G. Hone, A. Negash, Z. Genene, J. Dai, A.G. Waketola, G. T. Mola, W. Mammo, N.A. Tegegne, Self-assembled monolayer engineered ZnO electron transport layer to improve the photostability of organic solar cells, Energy Fuels 38 (2024) 13304–13314, https://doi.org/10.1021/acs.energyfuels.4c01558.
[17] W. Yang, S. Qu, S. Fu, Y. Shi, Z. Cao, Z. Guo, C. Huang, Y. Lei, J. Li, Self-doped quinacridone-fluorene alcohol-soluble conjugated polymer as an efficient cathode interlayer for organic solar cells, Opt. Mater. 173 (2026) 117864, https://doi.org/10.1016/j.optmat.2026.117864.
[18] S.A. Hosseini, A. Esfandiar, A. Iraji Zad, S.H. Hosseini-Shokouh, S.M. Mahdavi, High-photoresponsive backward diode by two-dimensional SnS2/Silicon heterostructure, ACS Photonics 6 (2019) 728–734, https://doi.org/10.1021/acsphotonics.8b01626.
[19] S. Manzeli, D. Ovchinnikov, D. Pasquier, O.V. Yazyev, A. Kis, 2D transition metal dichalcogenides, Nat. Rev. Mater. 2 (2017) 17033, https://doi.org/10.1038/natrevmats.2017.33.
[20] X. Gu, W. Cui, H. Li, Z. Wu, Z. Zeng, S. Lee, H. Zhang, B. Sun, A solution-processed hole extraction layer made from ultrathin MoS_2 nanosheets for efficient organic solar cells, Adv. Energy Mater. 3 (2013) 1262–1268, https://doi.org/10.1002/aenm201300549.
[21] X. Wang, P. Liu, B. Yap, R. Xia, W.-Y. Wong, Z. He, High-quality WS 2 film as a hole transport layer in high-efficiency non-fullerene organic solar cells, Nanoscale 13 (2021) 16589–16597, https://doi.org/10.1039/D1NR03728E.
[22] X. Gu, W. Cui, T. Song, C. Liu, X. Shi, S. Wang, B. Sun, Solution-processed 2D niobium diselenide nanosheets as efficient hole-transport layers in organic solar cells, ChemSusChem 7 (2014) 416–420, https://doi.org/10.1002/cssc.201300615.
[23] Y.-J. Huang, H.-C. Chen, H.-K. Lin, K.-H. Wei, Doping ZnO electron transport layers with MoS_2 nanosheets enhances the efficiency of polymer solar cells, ACS Appl. Mater. Interfaces 10 (2018) 20196–20204, https://doi.org/10.1021/acsami.8b06413.
[24] H. Li, B. Yu, H. Yu, An efficient and stable inverted structure organic solar cell using ZnO modified by 2D $ZrSe_2$ as a composite electron transport layer, Adv. Funct. Mater. 34 (2024) 2402128, https://doi.org/10.1002/adfm.202402128.
[25] P. Patil, D.S. Mann, U.T. Nakate, Y.-B. Hahn, S.-N. Kwon, S.-I. Na, Hybrid interfacial ETL engineering using PCBM-SnS2 for high-performance p-i-n structured planar perovskite solar cells, Chem. Eng. J. 397 (2020) 125504, https://doi.org/10.1016/j.cej.2020.125504.
[26] Y. Rui, T. Li, B. Li, Y. Wang, P. Müller-Buschbaum, Two-dimensional SnS_2 nanosheets as electron transport and interfacial layers enable efficient perovskite solar cells, J. Mater. Chem. C 10 (2022) 12392–12401, https://doi.org/10.1039/D2TC02452G.
[27] E. Zhao, L. Gao, S. Yang, L. Wang, J. Cao, T. Ma, In situ fabrication of 2D SnS2 nanosheets as a new electron transport layer for perovskite solar cells, Nano Res. 11 (2018) 5913–5923, https://doi.org/10.1007/s12274-018-2103-z.
[28] V. Papamakarios, E. Polydorou, A. Soultati, N. Droseros, D. Tsikritzis, A.M. Douvas, L. Palilis, M. Fakis, S. Kennou, P. Argitis, M. Vasilopoulou, Surface modification of ZnO layers via hydrogen plasma treatment for efficient inverted polymer solar cells, ACS Appl. Mater. Interfaces 8 (2016) 1194–1205, https://doi.org/10.1021/acsami.5b09533.
[29] P.E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50 (1994) 17953–17979, https://doi.org/10.1103/PhysRevB.50.17953.
[30] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (1996) 3865–3868, https://doi.org/10.1103/PhysRevLett.77.3865.
[31] S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, J. Comput. Chem. 27 (2006) 1787–1799, https://doi.org/10.1002/jcc.20495.
[32] L. Bengtsson, Dipole correction for surface supercell calculations, Phys. Rev. B 59 (1999) 12301–12304, https://doi.org/10.1103/PhysRevB.59.12301.
[33] J.D. Pack, H.J. Monkhorst, "special points for Brillouin-zone integrations"---a reply, Phys. Rev. B 16 (1977) 1748–1749, https://doi.org/10.1103/PhysRevB.16.1748.
[34] O. Dulub, L.A. Boatner, U. Diebold, STM study of the geometric and electronic structure of ZnO(.)-Zn, (.)-O, (,), and (.) surfaces, Surf. Sci. 519 (2002) 201–217, https://doi.org/10.1016/S0039-6028(02)02211-2.

[35] K. Rekha, M. Nirmala, M.G. Nair, A. Anukaliani, Structural, optical, photocatalytic and antibacterial activity of zinc oxide and manganese doped zinc oxide nanoparticles, Phys. B Condens. Matter 405 (2010) 3180–3185, https://doi.org/10.1016/j.physb.2010.04.042.
[36] M.Ø. Filsø, E. Eikeland, J. Zhang, S.R. Madsen, B.B. Iversen, Atomic and electronic structure transformations in SnS_2 at high pressures: a joint single crystal X-ray diffraction and DFT study, Dalton Trans 45 (2016) 3798–3805, https://doi.org/10.1039/C5DT04532K.
[37] V.N. Dhilshada, A. Chandran, S. Sen, M. Chattopadhyaya, Density functional theory-based modeling of the half-metallic g-C_3 N_4/CoN_4 heterojunction for photocatalytic water splitting reaction, Phys. Chem. Chem. Phys. 26 (2024) 21117–21133, https://doi.org/10.1039/D4CP00929K.
[38] K. Qi, S. Karthikeyan, W. Kim, F. Al Marzouqi, I.S. Al-Khusaibi, Y. Kim, R. Selvaraj, Hydrothermal synthesis of SnS2 nanocrystals for photocatalytic degradation of 2,4,6-trichlorophenol under white LED light irradiation, Desalination Water Treat. 92 (2017) 108–115, https://doi.org/10.5004/dwt.2017.21355.
[39] Y. Lei, J. Luo, X. Yang, T. Cai, R. Qi, L. Gu, Z. Zheng, Thermal evaporation of large-area SnS_2 thin films with a UV-to-NIR photoelectric response for flexible photodetector applications, ACS Appl. Mater. Interfaces 12 (2020) 24940–24950, https://doi.org/10.1021/acsami.0c01781.
[40] T. Sriv, K. Kim, H. Cheong, Low-frequency raman spectroscopy of few-layer 2H-SnS2, Sci. Rep. 8 (2018) 10194, https://doi.org/10.1038/s41598-018-28569-6.
[41] M. Kubovics, A. Trigo, A. Sánchez, G. Marbán, A. Borrás, J. Moral-Vico, A. M. López-Periago, C. Domingo, Role of graphene oxide aerogel support on the CuZnO catalytic activity: enhancing methanol selectivity in the hydrogenation reaction of CO_2, ChemCatChem 14 (2022) e202200607, https://doi.org/10.1002/cctc.202200607.
[42] S. Yang, H. Yu, The modification of ZnO surface with natural antioxidants to fabricate highly efficient and stable inverted organic solar cells, Chem. Eng. J. 452 (2023) 139658, https://doi.org/10.1016/j.cej.2022.139658.
[43] Q. Wang, H. Zhou, X. Liu, T. Li, C. Jiang, W. Song, W. Chen, Facet-dependent generation of superoxide radical anions by ZnO nanomaterials under simulated solar light, Environ. Sci. Nano 5 (2018) 2864–2875, https://doi.org/10.1039/c8en01008k.
[44] T. Yang, J. Wei, Y. Guo, Z. Lv, Z. Xu, Z. Cheng, Manipulation of oxygen vacancy for high photovoltaic output in bismuth ferrite films, ACS Appl. Mater. Interfaces 11 (2019) 23372–23381, https://doi.org/10.1021/acsami.9b06704.
[45] L. Saikia, D. Bhuyan, M. Saikia, B. Malakar, D.K. Dutta, P. Sengupta, Photocatalytic performance of ZnO nanomaterials for self sensitized degradation of malachite green dye under solar light, Appl. Catal., A 490 (2015) 42–49, https://doi.org/10.1016/j.apcata.2014.10.053.
[46] H. Jiang, T. Li, X. Han, X. Guo, B. Jia, K. Liu, H. Cao, Y. Lin, M. Zhang, Y. Li, X. Zhan, Passivated metal oxide n-Type contacts for efficient and stable organic solar cells, ACS Appl. Energy Mater. 3 (2020) 1111–1118, https://doi.org/10.1021/acsaem.9b02158.
[47] R.F.W. Bader, A quantum theory of molecular structure and its applications, Chem. Rev. 91 (1991) 893–928, https://doi.org/10.1021/cr00005a013.
[48] W. Sun, Y. Li, J.K. Jha, N.D. Shepherd, J. Du, Effect of surface adsorption and non-stoichiometry on the workfunction of ZnO surfaces: a first principles study, J. Appl. Phys. 117 (2015) 165304, https://doi.org/10.1063/1.4918921.
[49] J.-C. Deinert, Zinc Oxide Surfaces and Interfaces: Electronic Structure and Dynamics of Excited States, 2016. https://depositonce.tu-berlin.de/handle/11303/5786. (Accessed 22 January 2026).
[50] R.N. Shimizu, N.R. Demarquette, Evaluation of surface energy of solid polymers using different models, J. Appl. Polym. Sci. 76 (2000) 1831–1845, https://doi.org/10.1002/(SICI)1097-4628(20000620)76:12%3C1831::AID-APP14%3E3.0.CO;2-Q.
[51] A. Kozbial, Z. Li, C. Conaway, R. McGinley, S. Dhingra, V. Vahdat, F. Zhou, B. D'Urso, H. Liu, L. Li, Study on the surface energy of graphene by contact angle measurements, Langmuir 30 (2014) 8598–8606, https://doi.org/10.1021/la5018328.
[52] M. Annamalai, K. Gopinadhan, S.A. Han, S. Saha, H.J. Park, E.B. Cho, B. Kumar, A. Patra, S.-W. Kim, T. Venkatesan, Surface energy and wettability of van der Waals structures, Nanoscale 8 (2016) 5764–5770, https://doi.org/10.1039/C5NR06705G.
[53] S. Yang, S. Shi, H. Yu, The modification of ZnO with 2D g-C_3 N_5 as electron transport layer for high-performance and stable organic solar cells, ChemSusChem 18 (2025) e202500889, https://doi.org/10.1002/cssc.202500889.
[54] C. Sun, Y. Wu, W. Zhang, N. Jiang, T. Jiu, J. Fang, Improving efficiency by hybrid TiO_2 nanorods with 1,10-Phenanthroline as A cathode buffer layer for inverted organic solar cells, ACS Appl. Mater. Interfaces 6 (2014) 739–744, https://doi.org/10.1021/am404423k.
[55] H.W. Lee, S. Biswas, H. Choi, Y. Lee, H. Kim, Improving photostability of non-fullerene acceptor-based inverted organic solar cells using Ga-doped ZnO electron transport layer, Appl. Surf. Sci. 659 (2024) 159930, https://doi.org/10.1016/j.apsusc.2024.159930.
[56] J.-B. Jorcin, M.E. Orazem, N. Pébère, B. Tribollet, CPE analysis by local electrochemical impedance spectroscopy, Electrochim. Acta 51 (2006) 1473–1479, https://doi.org/10.1016/j.electacta.2005.02.128.
[57] Y. Zhang, Z. Zhang, G. Xie, Z. Su, Z. Deng, J. Liu, D. Wang, Y. Huang, J. Zhang, 16.5% polymer solar cells with 6-Aminocaproic acid-modified ZnO as a cathodic interface layer, Phys. Status Solidi (a) 219 (2022) 2100708, https://doi.org/10.1002/pssa.202100708.
[58] B. Zhang, Z. Pan, W. Li, Y. Zhao, X. Qin, A. Li, M. Lv, X. Qin, W. Guo, Z. He, E. Wang, Natural dextran as an efficient interfacial passivator for znO-based electron-transport layers in inverted organic solar cells, Adv. Energy Mater. 16 (2026) 2404297, https://doi.org/10.1002/aenm.202404297.
[59] T. Xia, Q. Li, K.-K. Liu, S. Ouyang, N. Zhang, L. Ke, G. Du, Y. Jiang, Q. Liu, H. Liu, Y. Li, Z. Guan, F.R. Lin, D. Lei, C.-S. Lee, X.C. Zeng, S.-W. Tsang, A.K.-Y. Jen, H.-L. Yip, Toward a robust ZnO interface via fullerene-based SAMs: defect passivation and compatibility tuning for high-performance inverted organic solar cells, Small 22 (2026) e13104, https://doi.org/10.1002/smll.202513104.
[60] Y. Liu, Y. Zhang, F. Zhang, Y. Zhang, M. Li, D. Wang, J. Zhou, D. Xu, X. Li, High-efficiency and stable inverted organic solar cells based on PEG-Modified ZnO electron transport layer, J. Mater. Sci. Mater. Electron. 37 (2025) 40, https://doi.org/10.1007/s10854-025-16415-1.
[61] R.F.B. Nasrun, D.H. Son, J.H. Kim, Role of tosylate anions in small molecule electrolytes enabling defect passivation by regulating zinc coordination of zinc oxide hybrid films for organic solar cells, Small Methods 10 (2026) e02425, https://doi.org/10.1002/smtd.202502425.