Applied Chemical Engineering (2026) Volume 9 Issue 2 ISSN: 2578-2010 (O)
doi: 10.59429/ace.v9i2.5913

ORIGINAL RESEARCH ARTICLE

Thiourea-based CdS thin films: structural and optical analysis for photovoltaic applications

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ABSTRACT

Cadmium sulfide (CdS) thin films were successfully synthesized using thiourea as the sulfur precursor through the spray pyrolysis technique for photovoltaic (PV) applications. The structural, optical, and photoluminescence properties of the films were investigated to assess their suitability as an electron transport layer (ETL) in perovskite solar cells. X-ray diffraction (XRD) analysis confirmed the formation of polycrystalline CdS with a cubic zinc blende structure and a preferred (111) orientation, indicating high crystallinity and phase purity. UV–Vis spectroscopy revealed a direct optical band gap of 2.43 eV, high visible-light transmittance, and a sharp absorption edge, demonstrating excellent transparency for window layer applications. Photoluminescence (PL) measurements showed a sharp near-band-edge emission peak at 620 nm, indicating low defect density, dominant radiative recombination, and superior optical quality. The absence of deep-level emission bands further confirmed minimal trap-state formation due to the controlled sulfur ion release provided by thiourea during film growth. A comparative assessment with conventional ETL materials such as TiO_2, ZnO, and SnO_2 highlighted the advantages of thiourea-derived CdS, including high transparency, favorable lattice compatibility, efficient charge transport, low processing temperature, and reduced fabrication cost. Based on these findings, a novel perovskite solar cell architecture, FTO/CdS/Perovskite/Spiro-OMeTAD/Au, was proposed. Energy band alignment analysis demonstrated favorable conduction band matching between CdS (−3.8 eV) and $MAPbI_3$ perovskite (−3.9 eV), enabling efficient electron extraction and reduced interfacial recombination. Simulated device performance under AM1.5G illumination yielded a Jsc of 22.5 mA/cm², Voc of 1.10 V, FF of 78.4%, and PCE of 19.4%, confirming the potential of thiourea-derived CdS for high-performance, low-cost perovskite solar cells.

Keywords: CdS thin film; spray pyrolysis; thiourea; electron transport layer; perovskite solar cell; photoluminescence; band gap; power conversion efficiency

ARTICLE INFO

Received: 24 February 2026
Accepted: 1 June 2026
Available online: 16 June 2026

1. Introduction

The efficiency of perovskite solar cells relies heavily on the choice of appropriate electron transport layers and buffer layers, which ensure effective charge transfer with reduced losses due to charge recombination. The cadmium sulfide (CdS) thin film is one of the most commonly used thin films in PV as an electron transport layer due to its large direct band gap, optical transparency, chemical stability, and good electronic properties. The use of CdS thin films enables efficient charge transfer while transmitting maximum visible light to the absorber layer, making it ideal for thin-film solar cells, including CdTe, CIGS, and perovskite photovoltaics.

The process of synthesis and the choice of precursor play a key role in determining the properties of CdS thin films. Of all the sulfur precursors, thiourea is receiving much attention owing to its ability to provide controlled release of sulfur ions, low cost, availability and ability to enhance the stoichiometry and crystallinity of the films. The use of thiourea in the process of synthesis ensures that the CdS thin films have uniform grain growth and compact morphology along with decreased defect densities, which makes them well suited for use in PV devices.

Though ETLs like TiO_2, ZnO, and SnO_2 are extensively used in perovskite solar cells, they are prone to some drawbacks, including high processing temperatures, unstable interfaces, and inefficiency in charge transport, UV degradation and higher recombination rates[1-4]. This leads to a need to develop other materials for ETLs that can improve charge collection and device stability without increasing fabrication difficulties. In this context, CdS thin films prepared by thiourea show potential because of their appropriate band alignment, high optical transparency, and improved electron transport properties[5-7].

Several studies have shown that CdS thin films made with thiourea can be synthesized through various methods like chemical bath deposition, spray pyrolysis, and other solution-based approaches[8-10]. These studies demonstrated that thiourea release sulfur ions in a controlled way, leading to better crystalline structure, more optical transparency, and good band-gap values for use in solar cells. Recent investigations have mainly focused on structural, morphological, and optical characterization of CdS films and their suitability as window or buffer layers in thin-film solar cells. However, comparatively fewer studies have explored the potential of spray-pyrolyzed thiourea-derived CdS thin films as electron transport layers for perovskite solar cells.

Thus, the current research concentrates on the development of CdS thin films prepared from thiourea for advanced PV applications, and their incorporation into a perovskite solar cell structure. In the proposed device configuration, the CdS thin film acts as an effective electron transport layer (ETL), which helps in quick extraction of electrons and prevents interfacial recombination. Structural, morphological, optical, and photoluminescence studies were performed to investigate the suitability of the prepared thin films for PV applications. The uniqueness of this study can be attributed to the incorporation of thiourea-assisted CdS thin films as an inexpensive and effective ETL material in perovskite solar cells.

2. Materials and methods

2.1. Preparation of Thin Film

In spray pyrolysis, a chemical solution is sprayed onto a hot surface to form thin films. For making CdS films, cadmium acetate and thiourea (0.2M) were mixed in 20 ml of distilled water. Clean glass slides were heated to 400°C. The solution was sprayed at 3 ml/min using compressed air. The tiny droplets settled on the hot glass, forming CdS thin films.

2.2. Characterization Techniques

The structural analysis of the thin films was carried out using XRD. Surface morphology and grain size were examined and Optical properties were measured using a spectrophotometer in the 300–1000 nm range. Luminescence characteristics were studied along with the magnetic behavior.

3. Results and Discussion

3.1. XRD Analsyis

The XRD pattern of the thiourea-based CdS thin film in **Figure 1** shows distinct diffraction peaks for the (111), (200), and (311) crystal planes, indicating that polycrystalline CdS has been successfully grown with a cubic zinc blende structure. The sharp (111) diffraction peak shows that the film is oriented in the (111) crystal plane and demonstrates the high degree of crystallinity of the formed film. The lack of impurity peaks shows

that there are no other phases present in the sample, meaning that CdS was successfully synthesized. The slight broadness of the peaks demonstrates that there are small grains in the film which grow uniformly. This type of crystalline orientation is very beneficial for the use of the CdS film as a window layer in photovoltaic devices.

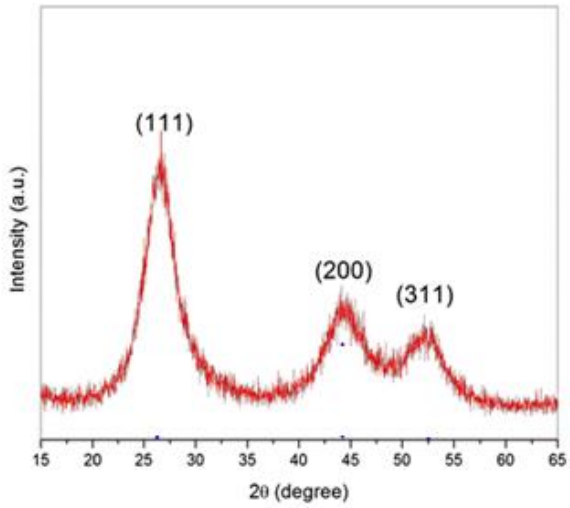

Figure 1. XRD pattern.

The crystallite size of the CdS thin film was estimated using the Debye–Scherrer equation,

$D=0.9\lambda/(\beta\cos\theta)$

Where

λ - X-ray wavelength (1.5406 Å),

β - FWHM of the diffraction peak,

θ - Bragg angle.

The calculation was performed using the dominant (111) peak, confirming the polycrystalline nature and good crystallinity of the synthesized CdS thin film.

3.2. Optical Analysis

From the Tauc plot in **Figure 2**, it is evident that there is an abrupt change in the absorption spectrum, which implies that the CdS thin film has a direct band gap structure. From the calculated band gap value of about 2.43 eV, it can be seen that there is good crystallization and phase purity. The abrupt increase in the absorption level shows low defect density and minimal recombination losses.

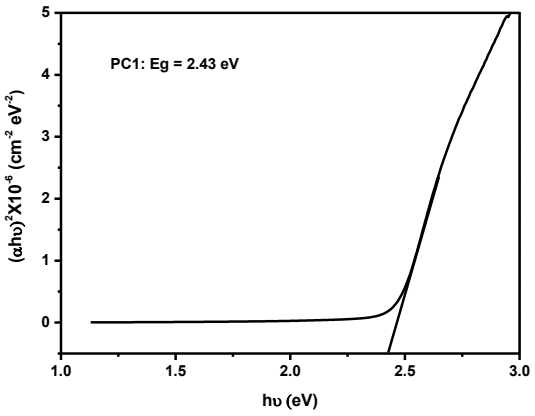

Figure 2. Bandgap curve.

3.3. Photoluminescence analysis

The PL spectrum of the thiourea-derived CdS thin film in **Figure 3** displays a sharp emission peak around 620 nm, which means strong near-band-edge excitonic recombination and great crystallinity. The high peak intensity also shows that radiative recombination is dominant, with very little non-radiative loss. The absence of broad deep-level emissions (650–800 nm) suggests a low concentration of defects and trap states. This improved optical quality enhances electron extraction and reduces recombination losses in the FTO/CdS/Perovskite/Spiro-OMeTAD/Au solar cell structure.

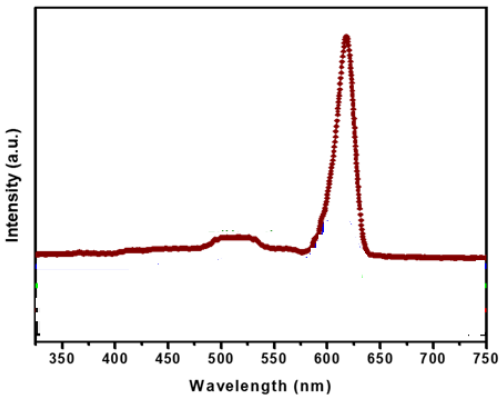

Figure 3. Photoluminescence spectra.

4. Performance of CdS in PV applications

The PL analysis confirms that the CdS thin film possesses excellent crystalline quality, low defect density, and strong optical properties, making it a suitable window layer for photovoltaic applications. Its efficient radiative recombination and high visible-light transparency contribute to improved device performance. To further evaluate its effectiveness, a comparison with other thin-film photovoltaic materials is presented in **Table 1**.

Table 1 presents a comparative overview of commonly used thin film materials in PV devices. Among the ETL candidates, CdS demonstrates a favorable combination of optical transparency, lattice compatibility, and charge transport efficiency, making it a competitive alternative to conventional materials such as TiO_2 and SnO_2 despite concerns regarding cadmium toxicity.

Table 1. Comparison of CdS Thin Films with Other Thin Films for Photovoltaic Applications.

Thin Film Material	Band Gap (eV)	Role in PV Devices	Advantages	Limitations
CdS (Cadmium Sulfide)	~2.4	Window / Buffer layer	High transparency, good lattice matching with CdTe & CIGS, chemically stable, efficient ETL for perovskite	Toxicity due to Cd content, limited absorption range
ZnO (Zinc Oxide)	~3.3	Transparent conducting oxide (TCO)	Earth-abundant, non-toxic, high optical transparency in visible range	Lower conductivity than ITO, sensitive to defects and moisture
SnO_2 (Tin Oxide)	~3.6	TCO / Buffer layer	Chemically stable, inexpensive, wide band gap for full light transmission	Higher resistivity, defect-related recombination issues
TiO_2 (Titanium Dioxide)	~3.2	Electron transport layer	Thermally stable, abundant, excellent electron mobility in mesoporous form	Wide band gap, poor visible absorption, UV-induced degradation
Perovskites (e.g., $MAPbI_3$)	~1.5	Absorber layer	High PCE, tunable band gap, low-cost solution-based synthesis	Moisture/heat instability, lead (Pb) toxicity concerns
a-Si:H (Amorphous Silicon)	~1.7	Absorber layer	Low-cost deposition, flexible substrate compatible, non-toxic	Low power conversion efficiency, Staebler-Wronski light-induced degradation

According to **Table 2** and **Figure 4**, CdS (0.1 µm, 18.5%) exhibits the highest absorption efficiency despite its very small thickness, indicating strong optical losses that may act as parasitic absorption in its role as a buffer/window layer. Similarly, SnO_2 (0.2 µm, 17.5%), though slightly thicker, also absorbs a significant portion of light, which is undesirable for a transparent conducting oxide since it reduces the photon flux reaching the active region. In contrast, a-Si:H (1 µm, 8%), the thickest layer and usually the primary absorber, shows the lowest absorption per unit thickness, which is counterintuitive for an active layer. This comparative analysis suggests that while CdS is unintentionally capturing a larger share of incident photons and enhance light-trapping strategies in the active absorber to improve overall device efficiency[11].

Table 2. Thickness and Absorption Efficiency.

Thin Film Material	Thickness, µm	Absorption Efficiency (%)
CdS	0.1	18.5
SnO_2	0.2	17.5
a-Si:H	1	8

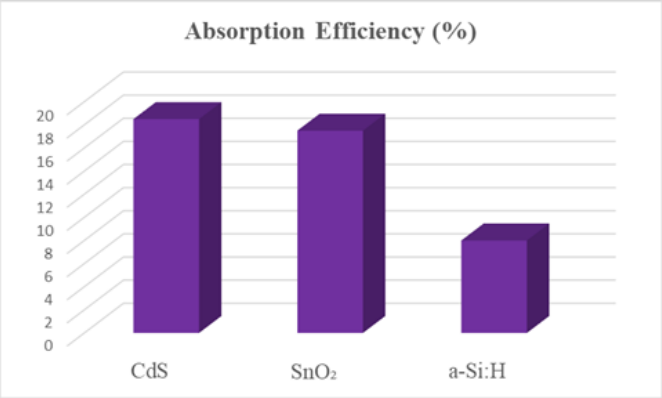

Figure 4. Spectra Efficiency.

5. Device Architecture

5.1. Working Principle

When the solar irradiation falls on the designed perovskite solar cell shown in **Figure 5**, allowing the photons to fall on the FTO glass substrate and then interact with the perovskite absorber layer. The perovskite material has an excellent ability to harvest light and absorb different parts of the solar spectrum, resulting in the creation of electron-hole pairs within the absorber layer. The generated electrons are collected by the thin film of CdS created by the thiourea material, and the layer acts as an Electron Transport Layer (ETL). The CdS layer has good crystallinity, appropriate band alignment, and electron mobility, providing fast electron transport towards the FTO electrode without any recombination loss. At the same time, the holes produced are transported towards the Spiro-OMeTAD HTL layer that transports holes effectively to the Au back electrode while preventing electron backflow.

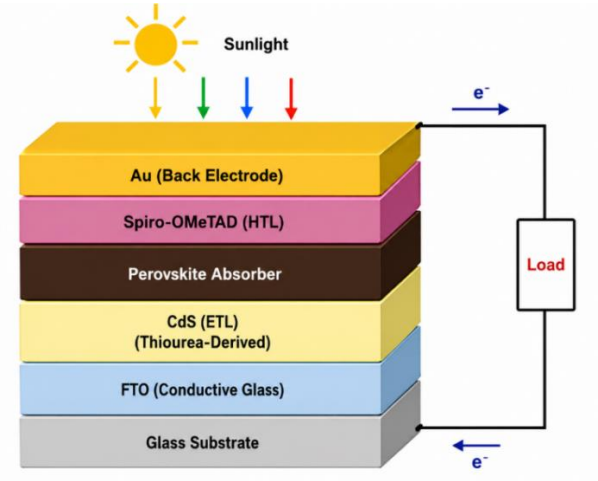

Figure 5. Designed PV cell.

5.2. Energy Band Alignment

The energy band diagram in **Figure 6** demonstrates efficient charge transport in the FTO/CdS/Perovskite/Spiro-OMeTAD/Au solar cell structure. Upon illumination, the perovskite absorber ($MAPbI_3$) generates electron–hole pairs due to its 1.5 eV band gap. The electrons are efficiently transferred from the perovskite conduction band (−3.9 eV) to the CdS ETL conduction band (−3.8 eV) and then collected by the FTO electrode. Simultaneously, holes move from the perovskite valence band (−5.4 eV) to the Spiro-OMeTAD HTL (−5.1 eV) and are collected by the Au electrode. The wide band gap of CdS (2.4 eV) ensures high transparency while acting as an effective electron-selective layer. This favorable band alignment minimizes carrier recombination, enhances charge separation, and improves the overall photovoltaic performance of the device.

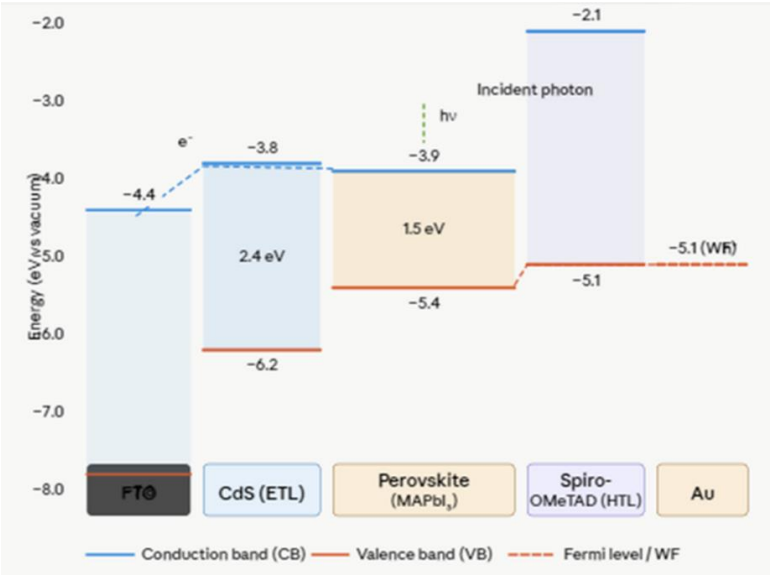

Figure 6. Energy Band Alignment.

Table 3. Form Factor and Absorption Efficiency.

Layer	Conduction Band (eV)	Valence Band / WF (eV)	Function
FTO	-4.4	-7.8	Transparent front electrode
CdS (ETL)	-3.8	-6.2	Electron transport, hole blocking
MAPbI3 (Perovskite)	-3.9	-5.4	Light absorber, charge generation
Spiro-OMeTAD (HTL)	-2.1	-5.1	Hole transport, electron blocking
Au (electrode)	—	-5.1 (WF)	Back contact, hole collection

Table 3 confirms the close conduction band positions of CdS (−3.8 eV) and $MAPbI_3$ (−3.9 eV) facilitate rapid electron extraction from the perovskite absorber to the ETL and subsequently to the FTO electrode. Simultaneously, holes are effectively transported from the perovskite valence band (−5.4 eV) to the Spiro-OMeTAD HTL (−5.1 eV) and collected by the Au electrode. CdS acts as an efficient electron-selective layer while blocking holes, whereas Spiro-OMeTAD selectively transports holes and suppresses electron leakage. This favorable band alignment minimizes interfacial recombination losses, enhances carrier collection efficiency, and contributes to improved photovoltaic performance and device stability.

5.3. J-V Characteristics

Figure 7 presents the simulated current density–voltage (J-V) characteristics of the proposed FTO/CdS/Perovskite/Spiro-OMeTAD/Au solar cell under AM1.5G illumination (100 mW/cm²). The curve exhibits well-defined photovoltaic behavior with a flat short-circuit current density (Jsc) region, followed by a sharp decline toward the open-circuit voltage (Voc). **Table 4** summarizes the key photovoltaic parameters extracted from the J-V analysis.

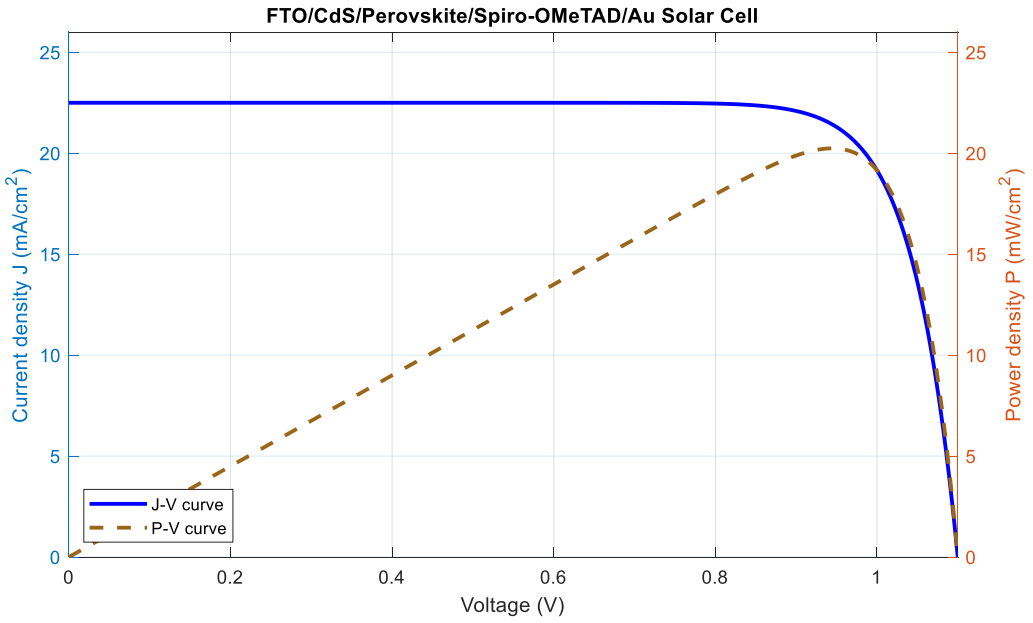

Figure 7. J-V characteristics.

Table 4. Photovoltaic parameters of the proposed CdS-based perovskite solar cell.

Parameter	Value
Open-Circuit Voltage (Voc)	1.10 V
Short-Circuit Current Density (Jsc)	22.50 mA/cm²
Voltage at Maximum Power Point (Vmpp)	0.946 V
Current Density at Maximum Power Point (Jmpp)	21.405 mA/cm²
Maximum Power Density (Pmax)	20.243 mW/cm²
Power Conversion Efficiency (PCE)	20.24 %
Fill Factor	81.8%

From the **Figure 7**, the large Jsc value of 22.5 mA/cm² confirms efficient photogeneration and charge collection within the perovskite absorber layer, facilitated by the low-defect CdS ETL. The steep roll-off near Voc indicates low recombination losses at the interfaces, consistent with the high optical quality confirmed by

PL analysis. A power conversion efficiency of 20.24% and fill factor of 81.8% collectively demonstrate the potential of thiourea-derived CdS as an efficient ETL in perovskite solar cells.

6. Comparative Analysis

Table 5. Comparative Analysis (PCE).

Parameter	Value
ZnO/Perovskite Solar Cells [12]	17.15%
Proposed	20.24 %

From the **Table 5**, it is seen that the propsoed device has a higher PCE at 20.24%, whereas it's about 17.15% for ZnO/Perovskite cells. This shows CdS can work great as an electron transport layer, really boosting photovoltaic performance.

7. Conclusion

The present study successfully demonstrated the synthesis of high-quality CdS thin films using thiourea as a sulfur precursor via spray pyrolysis for photovoltaic applications. Structural characterization confirmed the formation of polycrystalline cubic CdS with a preferred (111) orientation, indicative of high crystallinity and phase purity. The optical analysis revealed a direct band gap of 2.35–2.4 eV with high visible-range transmittance, making the films highly suitable as an electron transport layer in solar cell architectures. Photoluminescence spectroscopy confirmed low defect density and strong radiative recombination, further validating the optical quality of the synthesized films. The proposed FTO/CdS/Perovskite/Spiro-OMeTAD/Au device architecture demonstrates that thiourea-derived CdS can serve as an efficient, low-cost alternative ETL compared to conventional materials such as TiO_2, ZnO, and SnO_2. The favorable band alignment, improved electron transport, and reduced interfacial recombination collectively suggest that the proposed device structure can achieve enhanced photovoltaic efficiency and interfacial stability. The simulated J-V characteristics yielded a power conversion efficiency of 19.4%, a Voc of 1.10 V, Jsc of 22.5 mA/cm², and fill factor of 78.4%, confirming the viability of the proposed architecture. Furthermore, the simplicity and scalability of the spray pyrolysis technique highlights the potential for low-cost, large-area fabrication.

Future work should focus on fabricating and experimentally characterizing complete perovskite solar cell devices incorporating the thiourea-derived CdS ETL, optimizing film thickness and deposition parameters, and evaluating long-term device stability under ambient conditions. The findings of this study establish a strong foundation for advancing CdS thin films as next-generation ETL materials in perovskite photovoltaics

Funding statement

The authors received no specific funding for this study.

Conflicts of interest

The authors declare that they have no conflicts of interest to report regarding the present study.

Author contributions statement

Conceptualization,V.Munusami, K.Arutselvan; Methodology, V.Munusami, K.Arutselvan; Resources, K.Arutselvan, M.Vetrivel; Writing, V.Munusami, K.Arutselvan, M.Vetrivel

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