

Article

Preparation of Efficient MoS_2 Photocatalysts for Hydrogen Generation Through Sulfurization of MoO_3 Thin Films via Chemical Vapor Deposition

Sana Zulfiqar ¹, Tanvir Hussain ¹, Joun Ali Faraz ¹, Khaleel Ahmad ^{2,3,*}, Soumaya Goudria ⁴, Daniel Breaz ⁵ and Luminita-Ioana Cotirla ⁶ 

¹ Department of Physics, University of Management and Technology, Lahore 54770, Pakistan; sanazulfiqarali@gmail.com (S.Z.); tanvir.hussain@umt.edu.pk (T.H.); joun.faraz@umt.edu.pk (J.A.F.)

² Center for Theoretical Physics, Khazar University, 41 Mehseti Str., Baku AZ1096, Azerbaijan

³ Department of Mathematics and Statistics, The University of Lahore, Lahore 54770, Pakistan

⁴ Department of Physics, College of Science, Princess Nourah bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia; sgoudria@pnu.edu.sa

⁵ Department of Mathematics, "1 Decembrie 1918" University of Alba Iulia, 510009 Alba Iulia, Romania; dbreaz@uab.ro

⁶ Department of Mathematics, Technical University of Cluj-Napoca, 400114 Cluj-Napoca, Romania; luminita.cotirla@math.utcluj.ro

* Correspondence: khaleel.ahmad@math.uol.edu.pk

Abstract

The transition to clean and renewable energy sources is of prime importance in addressing environmental challenges related to the consumption of fossil fuels. Hydrogen, being a clean fuel with a high energy density, has huge potential, especially when it can be obtained through solar-driven PEC water splitting. Herein, MoS_2 photocatalysts were synthesized by sulfurizing MoO_3 thin films, using a CVD technique. The deposited MoO_3 films by thermal evaporation at 450 °C were further sulfurized at 500 °C, 550 °C, and 600 °C. XRD results confirmed the successful conversion of MoO_3 into MoS_2 . The optical properties showed a bandgap reduction from 2.50 eV to 1.30 eV, which leads to better absorption of light in the visible region. The photoelectrochemical experiment shows that the S- MoO_3 -600 °C thin film has the best performance, and the solar-to-hydrogen conversion efficiency reaches 0.11385% at an applied bias of 1.0 V versus Ag/AgCl, which is about 189 times higher than that of the pristine MoO_3 thin film.

Keywords: photocatalysis; MoS_2 ; water splitting; renewable energy; hydrogen generation



Academic Editor: Jiefang Zhu

Received: 25 December 2025

Revised: 10 February 2026

Accepted: 27 February 2026

Published: 4 March 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

1. Introduction

The present energy system remains largely reliant on fossil fuels such as coal, oil, and gas [1]. Although these energy resources are economically feasible, their burning leads to a massive emission of greenhouse gases such as carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) in the atmosphere, which are primarily responsible for global warming, acid rain, and other deleterious environmental effects. With a projected future demand for energy likely to reach a massive 50 TW by 2050, it is unsustainable to continue relying on a non-renewable and polluting source of energy such as fossil fuels. Hence, a need arises to design efficient and clean substitutes for fueling future energy demand [2–4]. Among all, solar energy is a very promising option considering its abundance, universality, and environment friendly nature. To tap this energy, efficient conversion and storage methods

are equally important. Among all proposed methods for efficient conversion of solar energy, photoelectrochemical (PEC) water splitting is considered most efficient, in which water is split into hydrogen and oxygen using solar light [5]. This hydrogen can be used either in a fuel cell or in an internal combustion engine with very high efficiency because hydrogen possesses a higher energy density than gasoline, in addition to being a very efficient energy carrier that can easily be used in fuel cells, gas turbines, and other industrial devices [6,7].

Among the oxide-based photoanodes, hematite ($\alpha\text{-Fe}_2\text{O}_3$) and bismuth vanadate (BiVO_4) are considered to be the most promising materials for photoelectrochemical water splitting because of their abundance on earth, stability, and favorable bandgap energies. ($\alpha\text{-Fe}_2\text{O}_3$) has a bandgap of 2.1 eV, which allows it to absorb visible light. However, its actual photoelectrochemical performance is impeded by its extremely short hole diffusion length (2–4 nm), low electrical conductivity, sluggish oxygen evolution reaction rates, and high onset potentials, which result in strong charge recombination losses. As a result, efficient water splitting in Fe_2O_3 photoanodes requires complex nanostructuring, high doping levels, or the use of co-catalysts [8]. BiVO_4 is considered to be one of the most promising oxide-based photoanodes for photoelectrochemical water splitting because of its moderate bandgap value of 2.4 eV, which allows it to absorb visible light, and its favorable valence band position for the oxygen evolution reaction. Additionally, BiVO_4 has a longer hole diffusion length and superior charge separation properties compared to hematite, resulting in higher photocurrent densities under solar illumination. However, BiVO_4 suffers from similar restrictions to that of hematite with regard to poor electron mobility, severe surface recombination, and slow kinetics of water oxidation (OER). In addition, therefore, BiVO_4 requires doping, heterojunction formation, and addition of co-catalysts [9,10].

Overall, PEC water splitting efficiency mostly depends on the semiconducting photo-catalyst employed. Good charge carrier mobility, chemical stability in chemical solution, and a proper bandgap for absorption of solar light are all requirements of ideal materials. Because of their high oxidation capacity and photostability, although metal oxides such as MoO_3 exhibit high oxidation capability and excellent photostability [11], their relatively large bandgaps hinder the use of visible light. In this regard, the use of heterostructures with narrow bandgaps like chalcogenides MoS_2 is an effective way to overcome these challenges. MoS_2 , a transition metal dichalcogenide, is renowned for its layered crystal structure, adjustable electronic properties, and strong absorption in the visible region, which make it a promising material for enhanced PEC water splitting [12–15].

2. Results and Discussion

2.1. Structural Properties

Figure 1 depicts the XRD patterns of MoO_3 -450 °C, S-MoO_3 -500 °C, S-MoO_3 -550 °C, and S-MoO_3 -600 °C thin films. X-ray diffraction (XRD) analysis revealed that the MoO_3 thin film synthesized at 450 °C exhibited an amorphous phase, as no distinct diffraction peaks were observed. In contrast, the sulfurized samples prepared at 500 °C, 550 °C, and 600 °C displayed clear diffraction peaks, indicating the formation of crystalline phases. The S-MoO_3 -500 °C showed three major diffraction peaks at 26.5°, 37.7°, and 54.4° belonging to the (-111), (-211), (-312) planes, respectively of a monoclinic MoO_3 phase (JCPDS card 32-0671).

The intense diffraction peak at $2\theta = 14.45^\circ$ observed for the samples sulfurized at 550 °C and 600 °C corresponds to the (002) plane marked with an asterisk of hexagonal MoS_2 , arising from the interlayer stacking of S–Mo–S layers and indicating preferential orientation along the c-axis. The absence of this peak at 500 °C suggests no sulfurization was achieved at this temperature; only sulfur was transported on the MoO_3 thin film, shown by the low sulfur atomic percentage observed in EDX analysis. The (002) peak is the preferred

orientation, which is a commonly intense peak in bulk MoS_2 powder consistent with the hexagonal phase of MoS_2 (JCPDS Card No. 00-037-1492) [16]. XRD patterns of films that were sulfurized at 550 °C and 600 °C confirm the phase transformation and also indicate the presence of MoO_3 peaks, which indicates that the upper layer was changed from MoO_3 to MoS_2 , while the lower layers are still MoO_3 , which is an indication of the formation of a heterostructure.

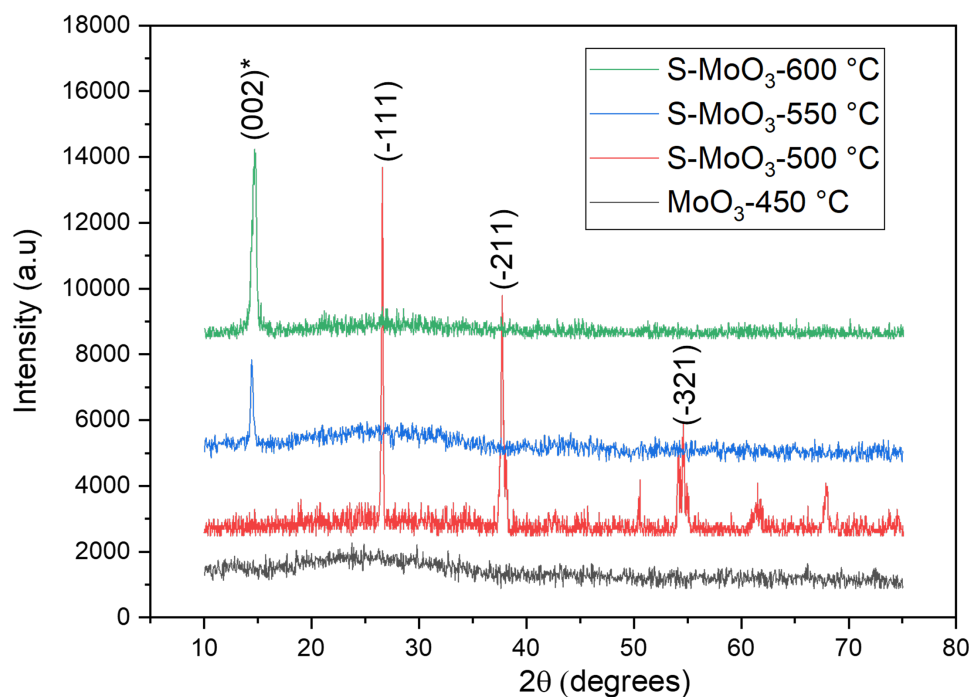


Figure 1. XRD patterns of MoO_3 -450 °C, MoO_3 -500 °C, S- MoO_3 -550 °C, and S- MoO_3 -600 °C.

2.2. Morphological Properties

Figure 2 shows the SEM images illustrating the surface morphology of the as-deposited MoO_3 -450 °C thin films and their sulfurized counterparts prepared at 500 °C, 550 °C, and 600 °C. The pristine MoO_3 -450 °C film exhibits a relatively flat, layered structure with limited surface texturing, which corresponds to its low photocurrent density and negligible STH efficiency due to the small active surface area. Sulfurization at 500 °C produces fine particles, indicating initial sulfur incorporation, but the surface nanostructuring remains weak, resulting in only a modest photocurrent improvement. At 550 °C, a more uniform granular morphology is observed, which improves film continuity yet still provides limited active sites for efficient charge transfer [17]. For the S- MoO_3 -600 °C sample, a well-defined nanostructured morphology emerges, characterized by triangular and flake-like domains consistent with crystalline MoS_2 growth. Such triangular features are widely reported for layered transition metal dichalcogenides and are associated with energetically favorable crystal facets and anisotropic growth kinetics. This nanostructuring increases the density of exposed edge sites and enhances the electrochemically active surface area, both of which are critical for interfacial charge transfer and catalytic reactions [18–20].

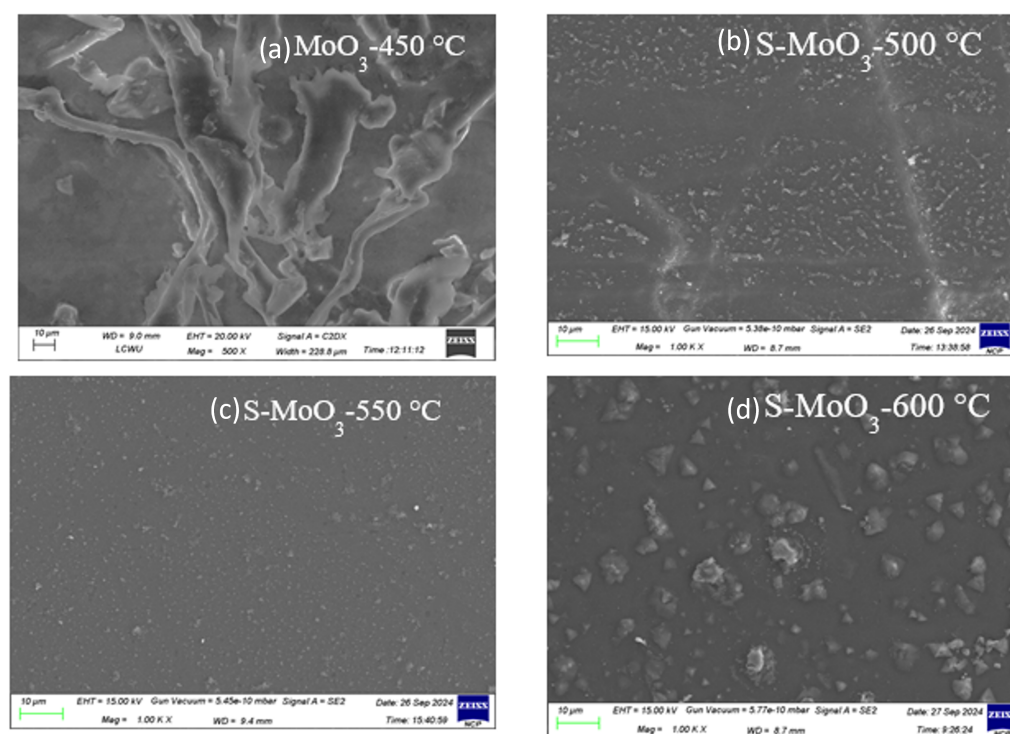


Figure 2. SEM images of (a) MoO_3 -450 °C, (b) MoO_3 -500 °C, (c) S-MoO_3 -550 °C, and (d) S-MoO_3 -600 °C.

2.3. EDX Analysis

Figure 3 shows the EDX spectra of the prepared films. It was employed to analyze their elemental composition and to confirm the extent of sulfurization of MoO_3 . At 450 °C, molybdenum and oxygen were detected along with other elements whose peaks originate from the substrate, verifying the formation of pure MoO_3 . At 500 °C and 550 °C, a minor amount of sulfur (1.7 % and 0.9 %, respectively) was observed, indicating the onset of sulfurization. A significant increase in sulphur content to 34.7 % was observed at 600 °C, accompanied by a decrease in oxygen content. This composition change confirms the successful transformation of MoO_3 into MoS_2 at elevated temperatures. The peaks originating from other than molybdenum, oxygen, and sulphur are from the substrate. EDX analysis only confirms the presence of sulphur along with the molybdenum and oxygen. The relative atomic percentages of Mo, O, and S obtained from EDX spectra of pristine and sulfurized MoO_3 thin films at different sulfurization temperatures are given in Table 1.

Table 1. Relative atomic percentages of Mo, O, and S obtained from EDX spectra of pristine and sulfurized MoO_3 thin films at different sulfurization temperatures.

Sample	Mo (at.%)	O (at.%)	S (at.%)
MoO_3 -450 °C	3.70	96.3	—
S-MoO_3 -500 °C	5.50	92.8	1.70
S-MoO_3 -550 °C	1.50	97.6	0.90
S-MoO_3 -600 °C	17.4	96.3	34.7

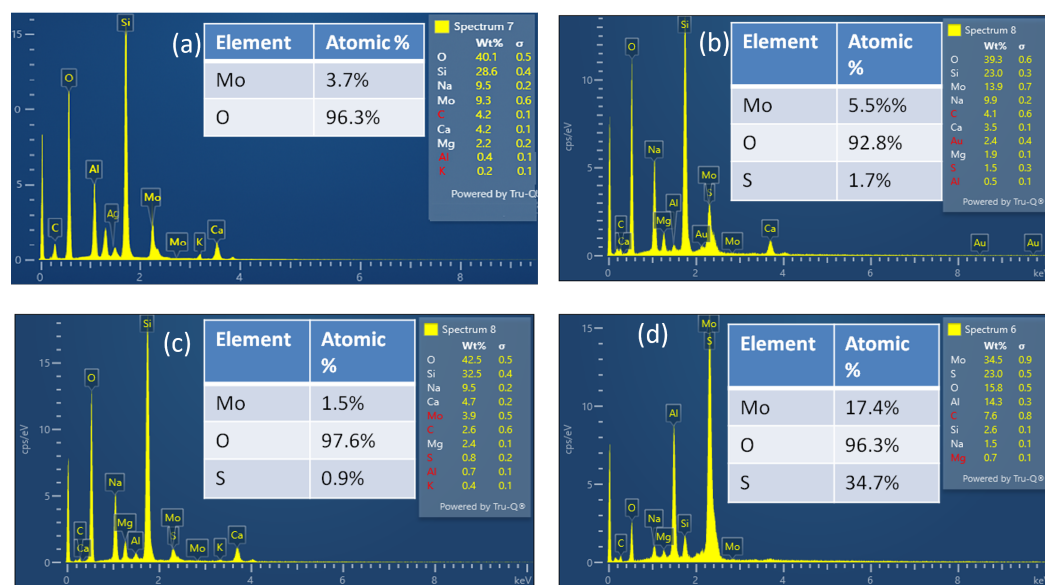


Figure 3. EDX spectra of (a) MoO_3 -450 °C, (b) S- MoO_3 -500 °C, (c) S- MoO_3 -550 °C, and (d) S- MoO_3 -600 °C.

2.4. Optical Properties

The absorption coefficient (α) was calculated using the following relation [21]:

$$\alpha = \frac{1}{d} \ln \left(\frac{1}{T} \right). \quad (1)$$

Here, d is the film thickness, and T is the transmittance. The film thickness for each sample was determined using a surface profilometer. Moreover, to estimate the optical bandgap, both direct and indirect transitions were analyzed using the Tauc plot relation:

$$(E\alpha)^{1/k} = \beta(E - E_g). \quad (2)$$

where $k = 1/2$ for indirect bandgap transitions, β is a constant, and E_g is the bandgap energy. Keeping in view that MoO_3 is an indirect bandgap semiconductor. The optical properties of the as-prepared and sulfurized MoO_3 thin films were investigated using Tauc plot analysis to estimate the optical bandgap energy (E_g). The Tauc plots, derived from UV-Vis transmittance spectra, indicated a clear trend of bandgap narrowing with increasing sulfurization temperature. Figure 4 shows the Tauc plots for the MoO_3 -450 °C, S- MoO_3 -500 °C, S- MoO_3 -550 °C, and S- MoO_3 -600 °C films. The MoO_3 oxide thin film annealed at 450 °C had a bandgap of 2.50 eV, which usually restricts the absorption of visible light. However, sulfurization at 500 °C, 550 °C, and 600 °C decreased the bandgap values to 1.80 eV, 1.35 eV, and 1.30 eV, respectively. The ability to tune the bandgap with sulfurization is important for solar-driven water splitting because it enables more efficient use of the solar spectrum which usually absorbs a small portion of visible light. A narrower bandgap enhances the absorption of photons and increases electron-hole pair generation under solar irradiation [22]. Particularly, the formation of MoS_2 at higher sulfurization temperatures with a bandgap of 1.30 eV aligns well with the optimal range for photocatalytic water splitting. Thus, the optical analysis confirms that controlled sulfurization of MoO_3 is an effective strategy for engineering the band structure to improve light harvesting and hydrogen generation efficiency in photoelectrochemical systems.

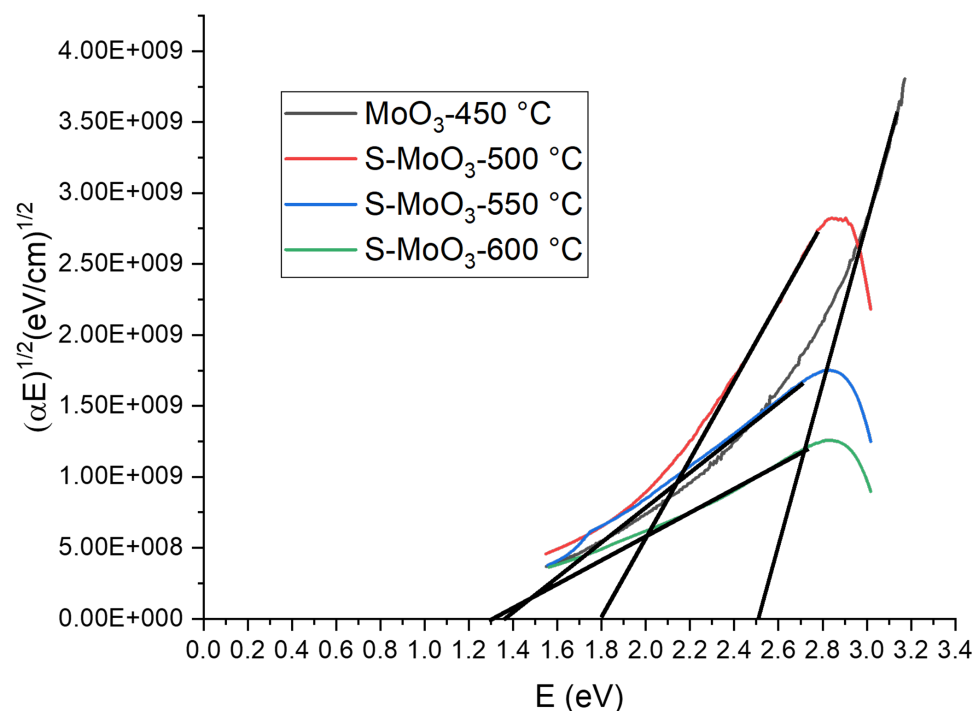


Figure 4. Tauc Plots for the MoO_3 -450 °C, MoO_3 -500 °C, S-MoO_3 -550 °C, and S-MoO_3 -600 °C films.

2.5. Photoelectrochemical Performance

The photoelectrochemical properties of the prepared samples were measured by measuring the linear sweep voltammetry (LSV) under dark and under light conditions by measuring the current response. The current was measured by applying the voltage vs reference electrode Ag/AgCl from -1.0 to 1.0 V. Figure 5 depicts the LSV graphs of the prepared photocatalysts. It was observed that all the prepared samples showed better photocurrent density under light, which indicates that the generation of electron–hole pairs contributes to the current response. It was observed that photocurrent response was increased by sulfurization of the MoO_3 thin film, which indicates that more solar light is observed and more electron–hole pairs are generated, which contributes to enhancing the oxidation and reduction reaction. SEM images also reveal that the formation of triangular nanostructure at 600 °C is favorable for the oxidation reaction, which is the bottleneck of the water splitting reaction. The photocurrent response of MoS_2 prepared by temperature-dependent sulfurization through CVD was compared with the already reported values of MoS_2 prepared with different techniques, which are summarized in Table 2.

Table 2. Comparison of various photocatalysts and their photoelectrochemical performance.

Photocatalyst	Method	Electrolyte	Photocurrent Density (mA cm^{-2})	Applied Potential	Ref.
Pristine MoS_2	Ultrasonication	0.5 M Na_2SO_4	0.26	0.62 V vs. Ag/AgCl	[23]
MoS_2/ZnSe heterojunction	CVD	0.5 M Na_2SO_4	0.22	0.8 V vs. Ag/AgCl	[24]
MoS_2/CdS heterostructure	Chemical Bath deposition	0.5 M $\text{Na}_2\text{S}/\text{Na}_2\text{SO}_3$	2.50	0 V vs. Ag/AgCl	[25]
$\text{MoS}_2/\text{BiVO}_4$ heterostructure	Hydrothermal	1 M Na_2SO_4	0.63	1.23 V vs. RHE	[26]
S-MoO_3 -600 °C	CVD	0.5 M Na_2SO_4	0.49	1.0 V vs. Ag/AgCl	—

MoS_2 is attractive for photocatalytic water splitting because its bandgap lies in the visible region; its band edges are well-positioned for HER/OER; and it has long carrier lifetimes and abundant active sites [27–30]. The efficiency of conversion from solar light to hydrogen generation was estimated from the following equation [31].

$$\text{STH}\% = \frac{(1.23 - V_{\text{applied}}) I_{\text{ph}} (\text{mA cm}^{-2}) \times 100}{P (\text{mW cm}^{-2})}. \quad (3)$$

V_{Applied} represents the voltages applied between the working and Ag/AgCl reference electrode; I_{ph} represents the photocurrent; and P represents the solar intensity at the earth's surface (100 mW/cm^2). This improved capability is due to a larger absorption window for the solar spectrum, which generates more electron–hole pairs, and a higher reaction rate resulting from the optimized nanostructure morphology. The values of photocurrent density and estimated STH% conversion efficiencies are given in the Table 3.

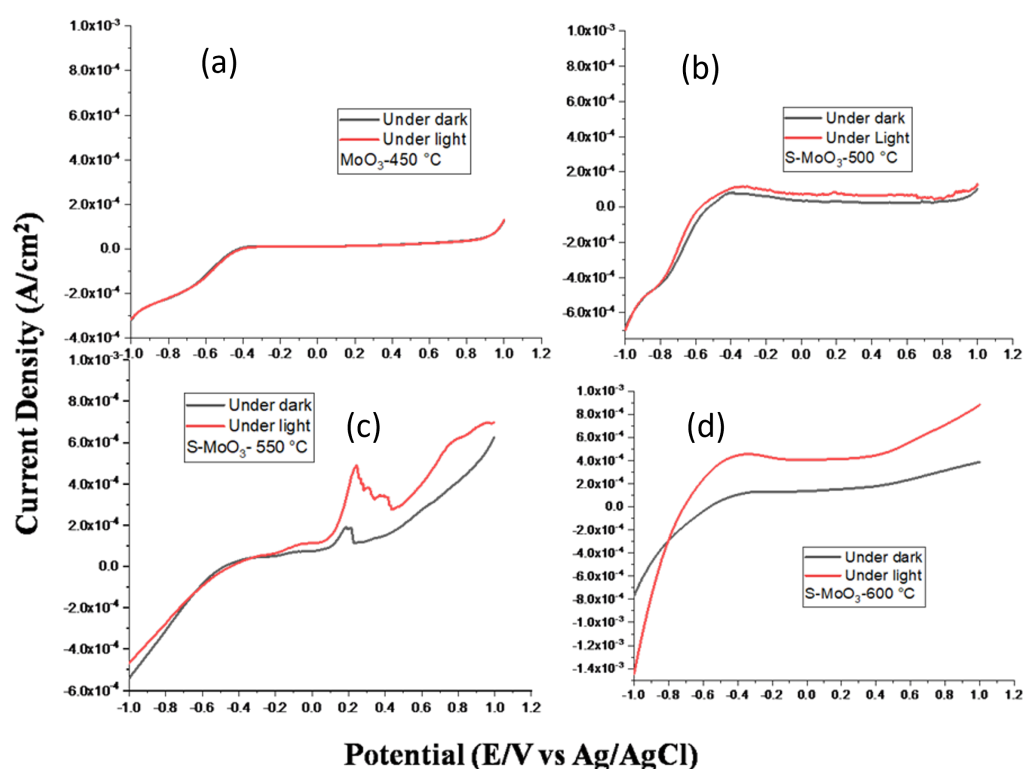


Figure 5. LSV graphs of (a) MoO_3 -450 °C, (b) S-MoO_3 -500 °C, (c) S-MoO_3 -550 °C, and (d) S-MoO_3 -600 °C films under dark and under light conditions.

Table 3. Values of photocurrent density and STH% efficiency of MoO_3 -450 °C, MoO_3 -500 °C, S-MoO_3 -550 °C, and S-MoO_3 -600 °C films.

Sample Name	Photocurrent Density (A cm^{-2})	STH (%)
MoO_3 -450 °C	2.62×10^{-6}	0.00060
S-MoO_3 -500 °C	2.78×10^{-5}	0.00639
S-MoO_3 -550 °C	7.18×10^{-5}	0.01651
S-MoO_3 -600 °C	4.95×10^{-4}	0.11385

3. Methodology

3.1. Photocatalyst Preparation

Thin films of MoO_3 were synthesized by thermal evaporation from molybdenum trioxide powder (purity 99.5 % Sigma Aldrich, Darmstadt, Germany) onto glass and ITO substrates at 450 °C in a tube furnace at a base pressure of 1.5×10^{-2} mbar in a vacuum tube furnace. For this purpose, 2 g MoO_3 powder was placed in a crucible; substrates were placed at the top of the crucible and placed at the centre of the tube furnace. The temperature of the furnace was set to 450 °C, and at a temperature of around 450 °C, the MoO_3 sublimates and condenses on the substrates and forms MoO_3 films.

Further, these films were sulfurized under a controlled atmosphere by chemical vapor deposition (CVD). The sulfurization step involved placing sulfur powder (99.5% purity from Sigma Aldrich) in a quartz boat upstream, approximately 300 mm from its center in the low temperature section of a furnace, where sulfur vapor could be consistently produced at 150–200 °C under equilibrium conditions. MoO_3 films that resulted from deposition were then placed in the middle heating zone of the furnace, which is used to precisely maintain the temperature for the sulphurization process. The quartz tube was flushed with high-purity pure argon for 15 min before heating to remove any residual moisture and/or oxygen that could lead to unwanted oxidation during the sulfurization process. Sulfurization was carried out at three different temperatures, namely, 500 °C, 550 °C, and 600 °C, to study the temperature-dependent evolution of the MoS_2 phase. During sulfurization, the system was kept in an inert gas, argon, at a flow rate of 500 sccm to move the sulfur vapour.

The gradual increase in furnace temperature occurred at a rate of 10 °C/min and was raised until the desired sulfurization temperature was reached. The system will then remain at that temperature for one hour so that the sulfur species will diffuse adequately into the MoO_3 lattice structure and aid in the transition from one phase to another. Once that hour has passed, the entire system will then cool to ambient temperature under an argon gas environment, which will preserve the film morphology as well as prevent the re-oxidation of the sample surface. The resultant thin films are labeled MoO_3 -450 °C, S- MoO_3 -500 °C, S- MoO_3 -550 °C, and S- MoO_3 -600 °C.

3.2. Characterization

Structural analysis of the prepared films was carried out using an X-ray diffractometer (Bruker D2-Phaser, Billerica, MA, USA). The scanning range was set from 10° to 75° 2θ with a scan rate of 2° min⁻¹. Surface morphology was examined using a Nova NanoSEM 450 scanning electron microscope (SEM, Hillsboro, OR, USA). Elemental composition was determined via energy-dispersive X-ray spectroscopy (EDX) attached to the SEM system. Optical properties were measured using a Jasco 770 UV-Vis spectrophotometer (Japan Spectroscopic Company, Tokyo, Japan), while film thickness was estimated using a surface profilometer.

3.3. Photoelectrochemical Measurement

Photoelectrochemical (PEC) measurements were performed using a three-electrode configuration connected to a Gamry 3000 potentiostat (Warminster, PA, USA). A Ag/AgCl electrode served as the reference electrode, and a platinum wire acted as the counter electrode. The prepared MoO_3 and sulfurized MoO_3 thin films were used as working electrodes. A 0.5 M Na_2SO_4 aqueous solution (pH = 7) was used as the electrolyte. Photocurrent responses were recorded under illumination using a xenon lamp (100 mW/cm²) as the light source. Linear sweep voltammetry (LSV) measurements were conducted under

both dark and illuminated conditions. The sulfurization process and CVD configuration are schematically illustrated in Figure 6.

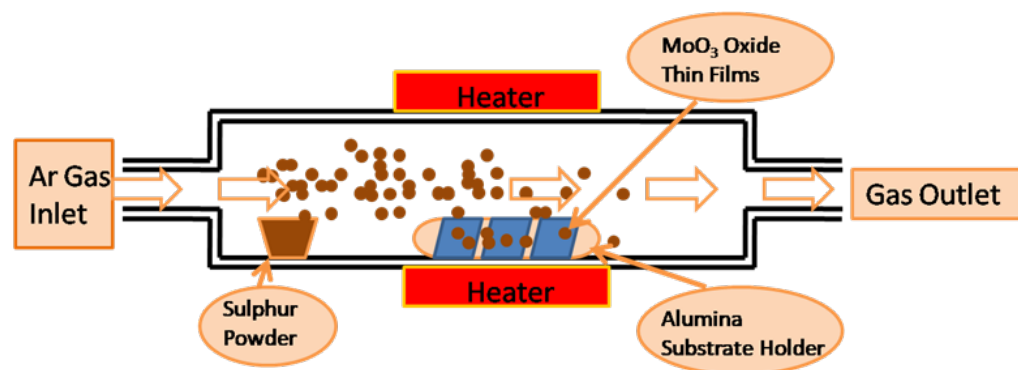


Figure 6. Schematic of CVD setup for sulfurization of MoO_3 thin films.

4. Conclusions

In this study, molybdenum disulfide (MoS_2) thin films were successfully synthesized by the sulfurization of MoO_3 by chemical vapor deposition (CVD), aiming to engineer a photocatalyst with a suitable bandgap for efficient solar hydrogen generation. The systematic sulfurization at varying temperatures demonstrated a clear structural, morphological, and optoelectronic evolution from amorphous MoO_3 to crystalline MoS_2 . XRD analysis confirmed the formation of the hexagonal MoS_2 phase at 550 °C and 600 °C, as evidenced by the dominant (002) peak. SEM and EDX analyses supported this transformation by showing changes in surface morphology and increased sulfur incorporation, respectively. Optical measurements revealed a substantial reduction in bandgap from 2.50 eV (MoO_3 -450 °C) to 1.30 eV (S- MoO_3 -600 °C), enabling broader visible light absorption and enhancing the material's photocatalytic potential. The S- MoO_3 -600 °C sample showed the highest photocurrent density compared to the other samples, and the solar light to hydrogen conversion efficiency of the S- MoO_3 -600 °C was 0.11385% at a 1.0 V applied bias versus Ag/AgCl. Notably, this represents a 189-fold increase compared to the pristine MoO_3 -450 °C film, indicating the effectiveness of the sulfurization in optimizing the photocatalyst. In short, the results confirm that CVD-based sulfurization of a metal oxide, like MoO_3 , is a scalable and tunable approach through which to develop an efficient photocatalyst with an ideal bandgap and band edge position for the PEC water splitting process. This strategy offers a promising route toward sustainable hydrogen production through solar energy conversion.

Author Contributions: Conceptualization, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; methodology, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; software, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; validation, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; formal analysis, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; investigation, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; resources, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; data curation, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; writing—original draft preparation, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; writing—review and editing, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; visualization, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; supervision, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; project administration, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C.; funding acquisition, S.Z.; T.H.; J.A.F.; K.A.; S.G.; D.B. and L.-I.C. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: Dataset available on request from the authors.

Acknowledgments: The authors extend their appreciation to the Princess Nourah bint Abdulrahman University Researchers Supporting Project number (PNURSP2026R184), Princess Nourah bint Abdulrahman University, Riyadh, Saudi Arabia.

Conflicts of Interest: The authors declare no conflict of interest.

References

- Lewis, N.S.; Nocera, D.G. Powering the planet: Chemical challenges in solar energy utilization. *Proc. Natl. Acad. Sci. USA* **2006**, *103*, 15729–15735.
- Wang, B.; Feng, X.; Liu, Y.; Wang, X.; Liu, E.; Zhao, Y.; Li, Z. Ultrafast Electron Transfer Coupled with a Proton Relay in an Anisotropic Dual S-Scheme Heterojunction for Overcoming Kinetics Mismatch in H₂O₂ Photosynthesis. *Adv. Sci.* **2025**, *12*, e22285.
- Wang, C.; Chen, P.; Li, H.; Cheng, X.; Zhang, J.; Ni, M. Photoelectrocatalytic hydrogen evolution combined with organic waste water treatment by red mud derived catalysts. *J. Power Sources* **2026**, *661*, 238600.
- Lu, Y.; Zhao, Y.; Wang, S.; Hu, B. Exploring charge-transfer of 2D borophene in carbon nitride: Boosting uranium photoreduction. *Desalination* **2026**, *619*, 119488.
- Chen, B.; Qiu, F.; Xia, L.; Xu, L.; Jin, J.; Gou, G. In Situ Ultrasonic Characterization of Hydrogen Damage Evolution in X80 Pipeline Steel. *Materials* **2024**, *17*, 5891.
- Tong, J.; Wan, Y.; Cui, J.; Lim, S.; Song, N.; Lennon, A. Solution-processed molybdenum oxide for hole-selective contacts on crystalline silicon solar cells. *Appl. Surf. Sci.* **2017**, *423*, 139–146.
- Xiang, Z.; Zhang, Q.; Zhang, Z.; Xu, X.; Wang, Q. Preparation and photoelectric properties of semiconductor MoO₂ micro/nanospheres with wide bandgap. *Ceram. Inter.* **2015**, *41*, 977–981.
- Kay, A.; Cesar, I.; Grätzel, M. New benchmark for water photooxidation by nanostructured α -Fe₂O₃ films. *J. Am. Chem. Soc.* **2006**, *128*, 15714–15721.
- Sivula, K.; Le Formal, F.; Grätzel, M. Solar water splitting: Progress using hematite (α -Fe₂O₃) photoelectrodes. *ChemSusChem* **2011**, *4*, 432–449.
- Park, Y.; McDonald, K.J.; Choi, K.S. Progress in bismuth vanadate photoanodes for use in solar water oxidation. *Chem. Soc. Rev.* **2013**, *42*, 2321–2337.
- Abdi, F.F.; Van De Krol, R. Nature and light dependence of bulk recombination in Co-Pi-catalyzed BiVO₄ photoanodes. *J. Phys. Chem. C* **2012**, *116*, 9398–9404.
- Li, J.; Guo, Q.; Jin, H.; Wang, K.; Xu, D.; Xu, G.; Xu, X. Low-temperature solution-processed MoO_x as hole injection layer for efficient quantum dot light-emitting diodes. *RSC Adv.* **2017**, *7*, 27464–27472.
- Li, Z.; Liao, D.; Tian, G.; Fan, X.; Chai, X.; Chang, W.; Zhang, C. Determination of Mn valence states in nanocatalysts during sustainable syngas conversion. *J. Am. Chem. Soc.* **2025**, *147*, 32548–32559.
- Wang, Q.H.; Kalantar-Zadeh, K.; Kis, A.; Coleman, J.N.; Strano, M.S. Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nat. Nanotechnol.* **2012**, *7*, 699–712.
- Gunawan, M.; Priest, M.; Gunawan, D.; Nie, S.; Satriyatama, A.; Vongsvivut, J.; Amal, R. Differentiating the role of Ni and Fe in NiFeOx co-catalyzed BiVO₄ photoanode for water oxidation. *Energy Environ. Sustain.* **2025**, *1*, 100019.
- Jiang, F.; Xiong, J.; Zhou, W.; Liu, C.; Wang, L.; Zhao, F.; Xu, J. Use of organic solvent-assisted exfoliated MoS₂ for optimizing the thermoelectric performance of flexible PEDOT: PSS thin films. *J. Mater. Chem. A* **2016**, *4*, 5265–5273.
- Zhan, Y.; Liu, Z.; Najmaei, S.; Ajayan, P.M.; Lou, J. Large area vapor phase growth and characterization of MoS₂ atomic layers on SiO₂ substrate. *Small* **2012**, *8*, 966–971.
- Lee, Y.H.; Zhang, X.Q.; Zhang, W.; Chang, M.T.; Lin, C.T.; Chang, K.D.; Lin, T.W. Synthesis of large-area MoS₂ atomic layers with chemical vapor deposition. *arXiv* **2012**, arXiv:1202.5458.
- van der Zande, A.M.; Huang, P.Y.; Chenet, D.A.; Berkelbach, T.C.; You, Y.; Lee, G.H.; Hone, J.C. Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. *Nat. Mater.* **2013**, *12*, 554–561.
- Voiry, D.; Mohite, A.; Chhowalla, M. Phase engineering of transition metal dichalcogenides. *Chem. Soc. Rev.* **2015**, *44*, 2702–2712.
- Al-Kuhaili, M.F.; Kayani, A.; Durrani, S.M.A.; Bakhtiari, I.A.; Haider, M.B. Band gap engineering of zinc selenide thin films through alloying with cadmium telluride. *ACS Appl. Mater. Interfaces* **2013**, *5*, 5366–5372.
- Hussain, T.; Al-Kuhaili, M.F.; Durrani, S.M.A.; Qayyum, H.A. Influence of angle deposition on the properties of ZnTe thin films prepared by thermal evaporation. *Ceram. Int.* **2018**, *44*, 10130–10140.
- Sitara, E.; Nasir, H.; Mumtaz, A.; Ehsan, M.F.; Sohail, M.; Iram, S.; Bukhari, S.A.B. Efficient photoelectrochemical water splitting by tailoring MoS₂/CoTe heterojunction in a photoelectrochemical cell. *Nanomaterials* **2020**, *10*, 2341.
- Rahmoune, A.; Babahani, O. Performance analysis of tungsten disulfide (WS₂) as HTL for MoS₂ solar cell with ZnSe ETL and graphene as window layer. *J. Opt.* **2024**, *54*, 1–21.

25. Liu, Y.; Yu, Y.X.; Zhang, W.D. MoS₂/CdS heterojunction with high photoelectrochemical activity for H₂ evolution under visible light: The role of MoS₂. *J. Phys. Chem. C* **2013**, *117*, 12949–12957.
26. Li, R.; Cai, M.; Xie, Z.; Zhang, Q.; Zeng, Y.; Liu, H.; Lv, W. Construction of heterostructured CuFe₂O₄/g-C₃N₄ nanocomposite as an efficient visible light photocatalyst with peroxydisulfate for the organic oxidation. *Appl. Catal. B Environ.* **2019**, *244*, 974–982.
27. Faraz, J.A.; Hussain, T.; Bilal, M.; Ahmad, K.; Cotirla, L.I. Photoelectrochemical Water Splitting by SnO₂/CuO Thin Film Heterostructure-Based Photocatalysts for Hydrogen Generation. *Nanomaterials* **2025**, *15*, 1748.
28. Caballero, R.; Condé, V.; León, M. SnS thin films grown by sulfurization of evaporated Sn layers: Effect of sulfurization temperature and pressure. *Thin Solid Film.* **2016**, *612*, 202–207.
29. Eda, G.; Maier, S.A. Two-dimensional crystals: Managing light for optoelectronics. *ACS Nano* **2013**, *7*, 5660–5665.
30. Hinnemann, B.; Moses, P.G.; Bonde, J.; Jørgensen, K.P.; Nielsen, J.H.; Hørch, S.; Nørskov, J.K. Biomimetic hydrogen evolution: MoS₂ nanoparticles as catalyst for hydrogen evolution. *J. Am. Chem. Soc.* **2005**, *127*, 5308–5309.
31. Dom, R.; Kim, H.G.; Borse, P.H. Efficient hydrogen generation over (100)-oriented ZnO nanostructured photoanodes under solar light. *CrystEngComm* **2014**, *16*, 2432–2439.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.