

Growth and Characterization of Copper Zinc Tin Sulfide (CZTS), Molybdenum Disulfide (MoS₂) MoS₂, and CZTS/MoS₂ Nanocomposite Photocatalysts for Water Cleaning

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Abstract

Copper Zinc Tin Sulfide (CZTS) is a non-toxic, earth-abundant, and environmentally friendly semiconductor used in energy harvesting and photocatalysis due to its favorable optical band gap (~1.5 eV) and absorption coefficient (~10⁴ cm⁻¹). The low band gap of CZTS causes free charge carriers to recombine. Two-dimensional materials, such as molybdenum disulfide (MoS₂) can be composited with CZTS to enhance carrier mobility and optical absorption properties across the solar spectrum, providing a promising solution for solar energy applications. In the present study, CZTS, MoS₂, and hybrid CZTS/MoS₂ nanocomposite were successfully synthesized using a facile hydrothermal method and systematically analyzed to investigate their structural, optical, photoluminescent, morphological characteristics, and photocatalytic dye degradation application. X-ray diffraction analysis confirmed the kesterite structure of CZTS and the hexagonal phase of MoS₂, revealing diffraction patterns indicating both phases and confirming the formation of a heterojunction. The average crystallite sizes were determined to be approximately ~24 nm, ~40 nm, and ~27 nm for CZTS, MoS₂, and CZTS/MoS₂ nanocomposite, respectively. Field Effect Scanning Electron Microscopy images demonstrated spherical and layered morphologies for CZTS and MoS₂, respectively, while the composite showed a cohesive and uniform distribution of CZTS nanoparticles across the MoS₂ nanosheets. UV-Vis spectroscopy revealed increased light absorption and a decreased band gap in the CZTS/MoS₂ composite, indicating better photon harvesting compared to individual materials. The photoluminescence study revealed a significant decrease in light emission from the CZTS/MoS₂ nanocomposite, indicating effective charge separation and reduced recombination. This enhances photocatalytic activity and demonstrates the potential of CZTS/MoS₂ nanocomposites for photocatalytic and environmental applications.

Categories: Catalysis and Reaction Engineering, Materials Engineering, Nano Materials

Keywords: czts/mos2 nanocomposite, dye degradation, hydrothermal, xrd, czts

Introduction

Environmental pollution constitutes a significant global challenge, adversely affecting ecosystems, human health, and water quality. Organic dyes, heavy metal ions, and microbial contamination are especially perilous pollutants due to their toxicity, persistence, and potential for bioaccumulation. These pollutants are primary contributors to water contamination, which presents considerable threats to both the ecosystem and population health [1]. Consequently, the advancement of extremely effective and economical techniques for the treatment and elimination of these dyes is critically important. Various techniques have been systematically explored for the removal of dyes from wastewater, including ultrafiltration, adsorption, coagulation/flocculation, precipitation, and microbial applications [2]. Photocatalysis has emerged as a viable solar-driven technology for the degradation of various contaminants among sophisticated alternatives for treatment. Photocatalysis is a versatile technology that facilitates the treatment of wastewater, the creation of self-cleaning surfaces, and the remediation of environmental issues by utilizing the renewable and abundant solar energy [3]. Numerous techniques for wastewater treatment can be classified as physical and chemical processes, which only transform organic pollutants into different phases, whereas photocatalysis significantly contributes to their conversion into carbonaceous products [4]. A photocatalyst improves the purification of contaminated water into clean water while simultaneously enhancing the reaction rate in its presence. Organic contaminants in water could be remedied with the use of semiconductor photocatalysts. Semiconducting photocatalysts possess significant potential for the remediation of organic pollutants in water. The interaction between the organic contaminants and the catalyst surface enhances photocatalytic performance [5]. The morphology, atomic arrangements, and coordination are some of the most significant variables that have an effect on the photocatalytic activity [6]. An optimal photocatalyst must demonstrate outstanding photo-responsiveness, utilize a wide range of solar wavelengths, be economically viable, and have remarkable

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stability [7]. Recent improvements have primarily focused on hetero-structured and doped nanomaterials, characterized by synergistic combinations of metals or semiconductors that improve catalytic efficiency. Because of their higher recyclability, optimum energy levels, and improved charge transfer, these composite materials frequently perform better than single-component materials, making them extremely effective for pollutant degradation. The degradation of organic contaminants has been studied with several types of photocatalysts. TiO_2 and ZnO serve as highly effective photocatalysts for the photocatalytic decomposition of organic contaminants [8]. Metal sulfides, such as CdS and nickel-based photocatalytic materials, demonstrate an efficient photo response across the entire ultraviolet to visible spectrum of the optical band [9]. However, the primary limitation of these materials is that their absorption spectrum is confined exclusively to the UV range. Consequently, to optimize the utilization of the solar spectrum, it is needed that we develop semiconductor materials with a bandgap within the visible range. Thermoelectric, photovoltaic, and photocatalytic applications demonstrate interest in chalcogenide materials such as CuInSe , PbTe , $\text{Cu}_2\text{InGa}(\text{Se,S})_4$, Bi_2Te_3 , CdTe , and others. But because indium (In) and tellurium (Te) are rare and cadmium (Cd) is toxic, there is more focus on creating chalcogenide materials that are inexpensive, abundant, and environmentally friendly [10,11]. The quaternary chalcogenide semiconductor Cu_2XSnS_4 (CXTS) [X=Zn, Co, Mn, Ni], which belongs to the $\text{I}_2(\text{Cu}_2)\text{-II-IV-VI}_4$ group and is earth abundant, is less toxic and has been found to be appropriate for both photocatalytic and electrocatalytic applications [8]. Copper zinc tin sulfide (CZTS) has garnered considerable interest due to its notable advantages, including reduced toxicity, affordability, and the abundance of its constituent constituents [12]. Along with its electronic and optical characteristics, which include a high absorption coefficient ($\sim 10^4 \text{ cm}^{-1}$), an ideal direct band gap (between 1.4 and 1.6 eV), a thermodynamically stable structure, an intrinsic p-type conductivity, and a 3-dimensional (3D) symmetry of charge carrier transport, it is primarily made up of earth-abundant and non-toxic elements (like Cu, Sn, and Zn) [13]. The presence of a low band gap results in a tendency for the free charge carriers to recombine with one another. The photocatalytic efficiency of semiconductor materials can be improved by integrating noble metals, like gold (Au) and platinum (Pt), which acts as cocatalysts, or by making composites with 2-dimensional (2D) materials such as transition metal dichalcogenides (TMDCs) [14]. These 2D materials, with their high charge carrier mobility and extensive surface area, dissociate electron-hole pairs more effectively than bare 3D nanomaterials [15]. Among the transition metal dichalcogenides, molybdenum disulfide (MoS_2) is the dominant nanomaterial due to its high charge carrier mobility ($\sim 200 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$), surface with no dangling interactions, and unsaturated d-orbitals of the transition metal [14]. The production of composite CZTS- MoS_2 utilizes the benefits of 2D materials, such as a high surface-to-volume ratio and enhanced carrier mobility, with the advantageous properties of CZTS nanoparticles, which exhibit significant optical absorption across the solar spectrum [16]. The present study reports the synthesis of CZTS and CZTS- MoS_2 nanocomposite via the hydrothermal method. A comprehensive structural, morphological, surface chemical analysis, and optical characterization of these nanomaterials has been studied. The prepared sample was utilized as a photocatalyst to decompose crystal violet dye to examine the photocatalytic efficiency of CZTS- MoS_2 nanocomposite.

Materials And Methods

Materials

The reagents utilized in the analysis, which included copper (II) acetate monohydrate ($\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$) and zinc acetate pentahydrate ($\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 5\text{H}_2\text{O}$) from Rankem, stannous chloride dihydrate ($\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$) from CDH, ethylene diamine ($\text{C}_2\text{H}_8\text{N}_2$) from SRL, and thiourea ($\text{CH}_4\text{N}_2\text{S}$) from Merck were used. Commercially prepared molybdenum disulfide (MoS_2) nanopowder (98% purity, SRL) was used as received without any further purification or modification. All chemical reagents were of analytical grade and used directly in the synthesis process.

Synthesis of CZTS and CZTS- MoS_2 nanocomposite

All chemical reagents utilized in the production and characterization of the photocatalyst were used directly, without additional purification. In this study, two comparable samples, pure CZTS and CZTS- MoS_2 nanocomposite, were synthesized using the hydrothermal technique, as illustrated in Figure 1. In an ordinary synthesis, 30 ml of a solvent consisting of a mixture of ethylene diamine and deionized water (volume ratio 1:9) was added to $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ (0.04 M), $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (0.02 M), and $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 5\text{H}_2\text{O}$ (0.02 M). The mixture was dissolved under continuous magnetic stirring, with ethylene diamine serving as a stabilizing and chelating agent. Thiourea (0.16 M) was separately dissolved in 30 ml of the same solvent mixture and added dropwise to the above precursor solution. The resulting solution was then placed in a 100 ml Teflon-lined stainless-steel autoclave, and subjected to a temperature of 180°C for 24 hours in a hot air oven. the selection of 180°C is critical because hydrothermal synthesis carried out below this temperature can lead to the formation of secondary impurity phases, such as Cu_{2-x}S or ZnS , which may adversely influence the phase purity, crystallinity, and optical characteristics of CZTS. Maintaining the temperature at 180°C ensure complete sulfurization of the metal precursors and supports the formation of the phase-pure kesterite CZTS structure. After natural

cooling to the room temperature, the obtained precipitate was centrifuged, repeatedly washed several times with using ethanol and distilled water. After that, the samples were dried at 80°C overnight (Figure 1). The CZTS-MoS₂ composite was prepared by incorporating 3 wt.% of pre-prepared MoS₂ into the CZTS precursor solution, which was subsequently placed in an autoclave, and heated at 180°C for 24 hours.



FIGURE 1: Schematic diagram of the synthesis process for CZTS and CZTS-MoS₂ nanocomposite

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

Characterization

The powder X-ray diffraction (XRD) technique has been used for analyzing the crystalline characteristics of prepared CZTS and CZTS-MoS₂ nanocomposites. For the measurement, a Rigaku X-ray diffractometer equipped with a Cu K α source ($\lambda = 1.54 \text{ \AA}$) was employed. The X-ray source operates at a voltage of 40 kV within a 2θ range of 20°-80°. A Perkin Elmer Lambda 365 UV-Visible Spectrophotometer, operating within the 200-800 nm range, was used to analyze the optical properties of the synthesized CZTS and CZTS-MoS₂ nanocomposites. The optical band gap values were determined using Tauc plot analysis. A Renishaw Raman spectroscope coupled with an argon ion laser functioning at a 514.5 nm wavelength was used to perform Raman spectroscopy of the synthesized samples. The photoluminescence (PL) analysis was conducted using a spectrofluorophotometer (SHIMADZU RF-6000) with an excitation wavelength set at 510 nm. Using a Field-Emission Scanning Electron Microscope (FE-SEM, TESCAN MAGNA) at a 15 kV acceleration voltage, the surface morphology of the samples was analyzed. The elemental composition of the samples was analyzed using Energy Dispersive X-ray Spectroscopy (EDX).

Photo-catalytic dye degradation experiment

The photocatalytic efficiency of CZTS and the CZTS-MoS₂ nanocomposite have been examined using the photocatalytic decomposition of crystal violet dye in a water-based solution under visible light irradiation. To assess the degradation of dye, a 100 ml stock solution was prepared at 100 ppm. A dye solution with a concentration of 20 ppm was prepared by mixing 20 ml of the stock solution with 80 ml of distilled water. In the typical procedure, 20 mg of CZTS-MoS₂ was incorporated into 100 ml of an aqueous crystal violet dye solution. A 300 W J-type linear halogen lamp is employed for irradiation. The degradation procedure began with a 20-ppm dye solution being stirred by a magnetic stirrer for 30 minutes in total darkness once adsorption-desorption equilibrium was reached. To optimize dye degradation, 3 ml samples were taken at regular intervals of 10 minutes, and the catalyst was separated from the liquid via centrifugation. The absorption spectra of the liquid were obtained using a UV-Vis. spectrophotometer to assess the degradation of crystal violet dye in the solution. The absorbance of the supernatant for crystal violet dye was measured at 582 nm.

Results And Discussion

XRD measurements

The X-ray diffraction pattern of prepared CZTS and CZTS-MoS₂ nanocomposite, captured at room temperature, is shown in Figure 2. The synthesized CZTS phase exhibits a kesterite structure (tetragonal), verified by XRD peaks at $2\theta = 28.5^\circ, 33.3^\circ, 47.4^\circ, 56.1^\circ, 69.2^\circ$, and 76.5° , corresponding to the (112), (200), (220), (312), (008), and (332) lattice planes, respectively, as per JCPDS card no. 26-0575. The XRD peaks corresponding to MoS₂ (hexagonal structure) (JCPDS card no. 37-1492) lattice planes (002), (100), (101), (102) (103), (006), (105), (106), (110), (008), (108), (205) and (116) are observed at 2θ values of $14.30^\circ, 32.67^\circ, 33.53^\circ, 36.02^\circ, 39.58^\circ, 44.25^\circ, 49.61^\circ, 56.13^\circ, 58.29^\circ, 60.16^\circ, 70.01^\circ, 72.17^\circ$ and 75.96° , respectively. CZTS-MoS₂ nanocomposite exhibits peaks in its X-ray diffraction patterns that correspond to the tetragonal phase of CZTS and the hexagonal phase of MoS₂ [17].

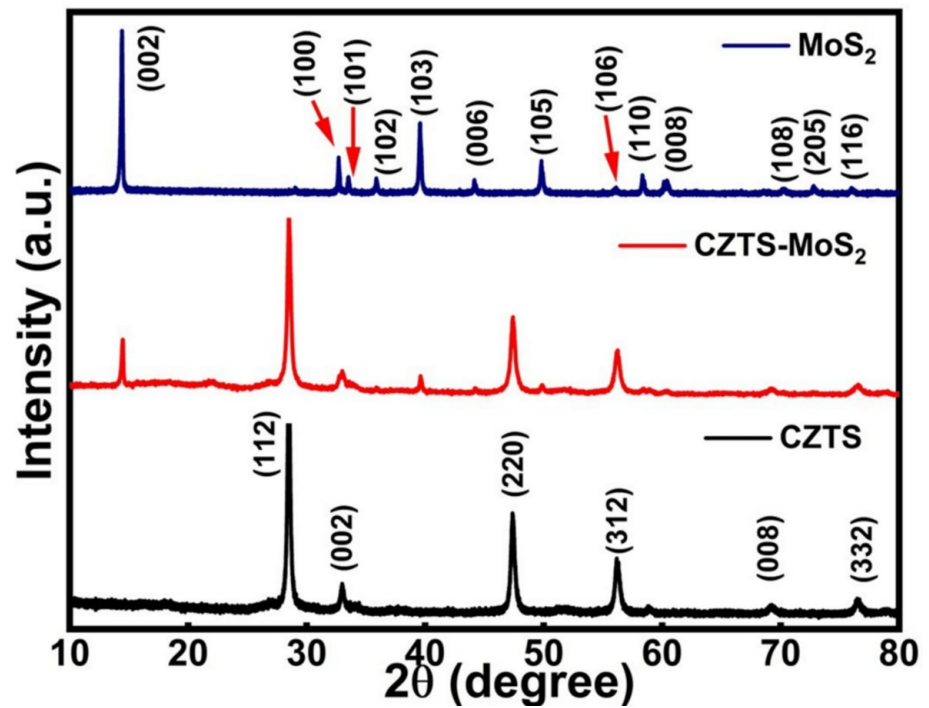


FIGURE 2: Powder XRD patterns of CZTS, MoS₂, and CZTS-MoS₂ composite

XRD, X-ray diffraction; CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

The Debye-Scherrer formula was used to calculate the average crystallite size D (nm) from the full width at half maximum (FWHM) of XRD peaks [10].

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (1)$$

Here, k is Scherrer's constant (assumed to be 0.9), λ stands for the wavelength of the X-ray source, θ refers to the Bragg diffraction angle, and β denotes the FWHM of the peak. The crystallite sizes of CZTS, MoS₂, and CZTS-MoS₂ nanocomposite have been found to be 24 nm, 40 nm, and 27 nm, respectively. The Williamson-Hall analysis was applied to the XRD data to investigate factors responsible for the improved crystallinity of the synthesized samples. It is possible that the intrinsic strain plays a significant part in determining the structurally appropriate ties by causing changes in the size of the crystallites.

$$\beta \cos \theta = \frac{k\lambda}{D} + 4\epsilon \sin \theta \quad (2)$$

Macrostrain (ϵ) of the CZTS nanoparticles can be estimated using the relation

$$\epsilon = \frac{\beta \cos \theta}{4} \quad (3)$$

In this equation, ϵ denotes the strain, D stands for the average crystallite size, λ refers to the wavelength, θ is the Bragg diffraction angle, and β represents the full width at half maxima of the XRD peak. The Williamson-Hall (W-H) plots for all the hydrothermally synthesized samples are shown in Figure 3. Utilizing Equations (2) and (3), we have determined parameters such as strain and crystallite size for the synthesized sample. Table 1 shows the crystallite size of samples calculated through the Williamson-Hall approach as well as Scherrer's formula. The estimated crystallite sizes for CZTS (24 nm) and MoS₂ (40 nm) affect their photocatalytic properties. The small size of CZTS increase its surface-to-volume ratio, thereby increasing the number of active sites, whereas the larger size of MoS₂ enhances charge extraction due to a reduced presence of defects. The CZTS-MoS₂ nanocomposite, possessing an effective crystallite size of 27 nm, integrates the reactive sites of CZTS with the interfacial charge separation capabilities of MoS₂, thereby enhancing the photocatalytic response to visible light.

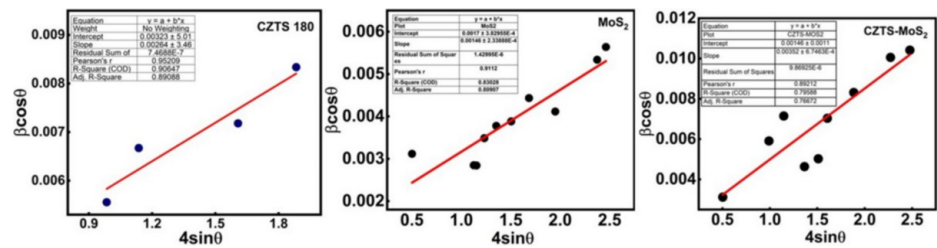


FIGURE 3: W-H plots of synthesized CZTS, CZTS-MoS₂, and MoS₂

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

Sample name	Scherrer crystallite size (nm)	William-Hall crystallite size (nm)	Strain (ϵ) $\times 10^{-3}$
CZTS	24	20	2.34
MoS ₂	40	48	1.46
CZTS/MoS ₂	27	35	3.57

TABLE 1: Crystallite size and strain of the samples, calculated by the Scherrer equation and the Williamson-Hall equation

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

Raman analysis

Raman spectroscopy is a widely utilized analytical technique for examining vibrational, rotational, and other low-frequency modes in molecules, atoms, and ions. Raman spectra for CZTS, MoS₂, and CZTS-MoS₂ nanocomposites were recorded at room temperature over the 200-700 cm⁻¹ range to verify their phase purity (Figure 4). The Raman spectra of CZTS reveal a prominent peak at 333.2 cm⁻¹, attributed to the A₁ vibration mode. The A₁ vibration mode primarily originates from the vibrations of S atoms within the kesterite lattice and is used as the principal peak for identifying CZTS, aligning with the associated XRD pattern [10]. The Raman analysis of MoS₂ showed a prominent peak at 405.5 cm⁻¹, attributed to the A_{1g} vibrational mode, along with a secondary, less intense peak at 378.8 cm⁻¹, corresponding to the E_{12g} mode characteristic of MoS₂. The E_{12g} mode involves the sulfur atoms vibrating in opposite directions within the plane, relative to the molybdenum atom, while the A_{1g} mode is associated with sulfur atoms moving out of the plane in opposite directions. The frequency difference (Δk) between these two modes is closely associated with the number of layers and can be utilized to ascertain the thickness of MoS₂ materials [18]. The frequency difference between the E_{12g} and A_{1g} modes is $\Delta k = 26.7$, indicating that the MoS₂ has more than six layers. The Raman spectra of CZTS-MoS₂ nanocomposites displayed characteristic peaks associated with both CZTS and MoS₂ [19]. The CZTS principal dominant peak (A₁ mode) decreased a substantial amount of intensity when composited with MoS₂.

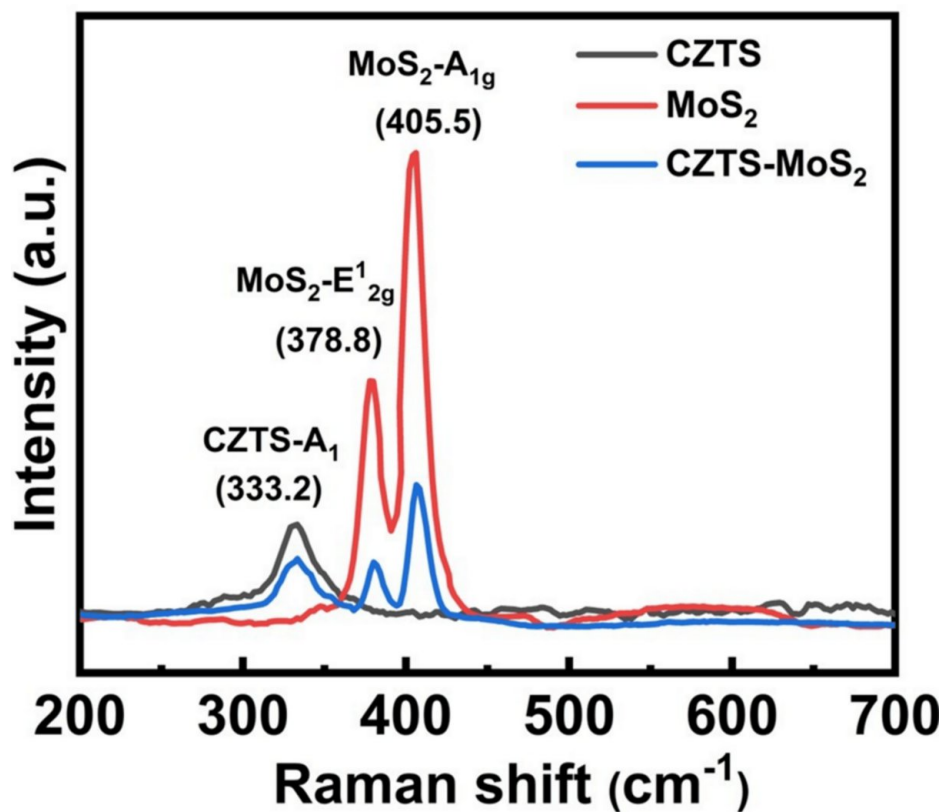


FIGURE 4: Raman spectra of hydrothermally synthesized CZTS and CZTS-MoS₂ nanocomposite

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

UV-Visible spectroscopy analysis

The optical absorption spectra and bandgap energy of CZTS nanoparticles are analyzed by UV-visible spectroscopy throughout the 200-800 nm range of wavelength. Figure 5(a) displays the UV-Vis. absorbance spectra of the synthesized CZTS and CZTS-MoS₂ nanocomposites, exhibiting substantial absorption across the 200-800 nm range, indicative of the optical quality of the generated samples. The band gap energy of the nanostructure was evaluated through analysis of the Tauc plot [20].

$$\alpha h\nu = A(h\nu - E_g)^n \quad (4)$$

Where A is a proportionality constant, α represents the absorption coefficient, ν indicates the frequency, h signifies Planck's constant, E_g refers to the band gap, and n can assume values of 2 or 1/2, corresponding to allowed indirect and direct transitions, respectively. We have used $n = 1/2$ since CZTS exhibits direct allowed transitions. The Tauc plot (Figure 5b) is derived by graphing $(\alpha h\nu)^2$ against $h\nu$. The linear segment of the graph is extrapolated to the zero point of $(\alpha h\nu)^2$. The calculated band gap values derived from the intercepts are 1.64 eV for CZTS and 1.69 eV for CZTS-MoS₂, respectively.

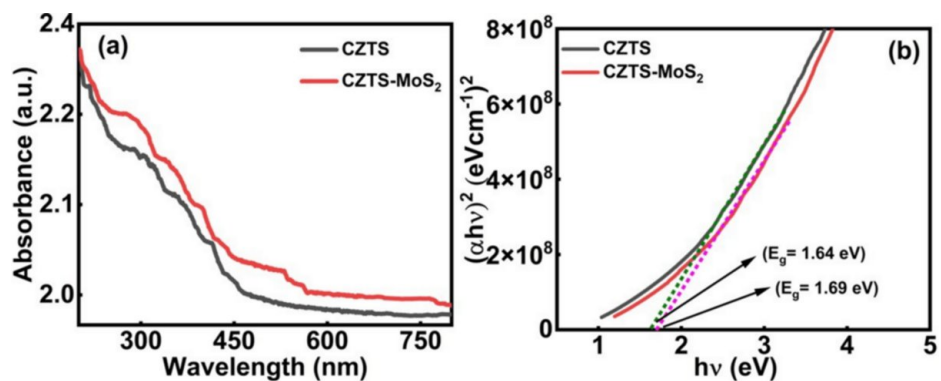


FIGURE 5: (a) UV-vis absorbance spectra and (b) corresponding Tauc plots of CZTS and CZTS-MoS₂ nanocomposite

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

Photoluminescence (PL) spectra

The PL spectra are widely used for investigating the separation dynamics of electron-hole pairs in catalysts. The PL emission arises due to the recombination of free charge carriers, specifically electrons and holes. It is well known that an increased PL intensity may be determined from a higher recombination rate of charge carriers. A reduced intensity in the PL spectrum suggests a lower rate of electron-hole pair recombination. On the other hand, if the intensity is greater, it indicates that the amount of recombination is higher. When compared to the photoluminescence results of the CZTS-MoS₂ nanocomposite, it is shown that there is less electron-hole pair recombination in CZTS. Figure 6 illustrates that the photoluminescence emission intensity of the CZTS-MoS₂ nanocomposite is superior to that of CZTS, indicating a reduced recombination rate of electrons and holes in CZTS-MoS₂. The decreased PL intensity of the CZTS-MoS₂ nanocomposite relative to pure CZTS is ascribed to enhanced charge separation enabled by the heterointerface between the two semiconductors. The advantageous band alignment facilitates the effective transmission of photogenerated electrons in CZTS to the MoS₂ layers, which serve as electron-accepting and high-mobility transport channels. Simultaneously, the associated holes persist in the valence band of CZTS, facilitating spatial charge separation and inhibiting their radiative recombination. The extended carrier lifetime increases the probability of interfacial redox reactions, therefore enhancing the overall photocatalytic efficiency of the CZTS-MoS₂ system.

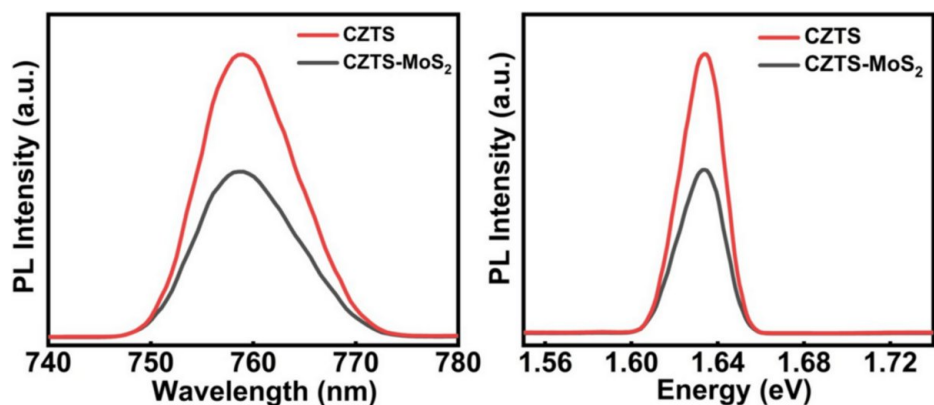


FIGURE 6: Photoluminescence spectra of CZTS and CZTS-MoS₂

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

Morphological analysis

Field Effect Scanning Electron Microscopy (FESEM) was used to analyze the surface morphology of CZTS and CZTS-MoS₂ nanocomposite. Figure 7a and b exhibit the FESEM images of the hydrothermally synthesized CZTS and CZTS-MoS₂ nanocomposite. As observed in Figure 7a, the sample shows uniformly dispersed polygonal nanoparticles, while some particle agglomeration is also apparent in the structure.

The CZTS showed approximately spherical particles of uniform size, whereas the CZTS-MoS₂ nanocomposite exhibited larger particles with irregular morphology, likely due to the aggregation of CZTS particles within the MoS₂ layers. The average grain size was found to be 0.57 μm for CZTS and 0.50 μm for the CZTS-MoS₂ nanocomposite, respectively.

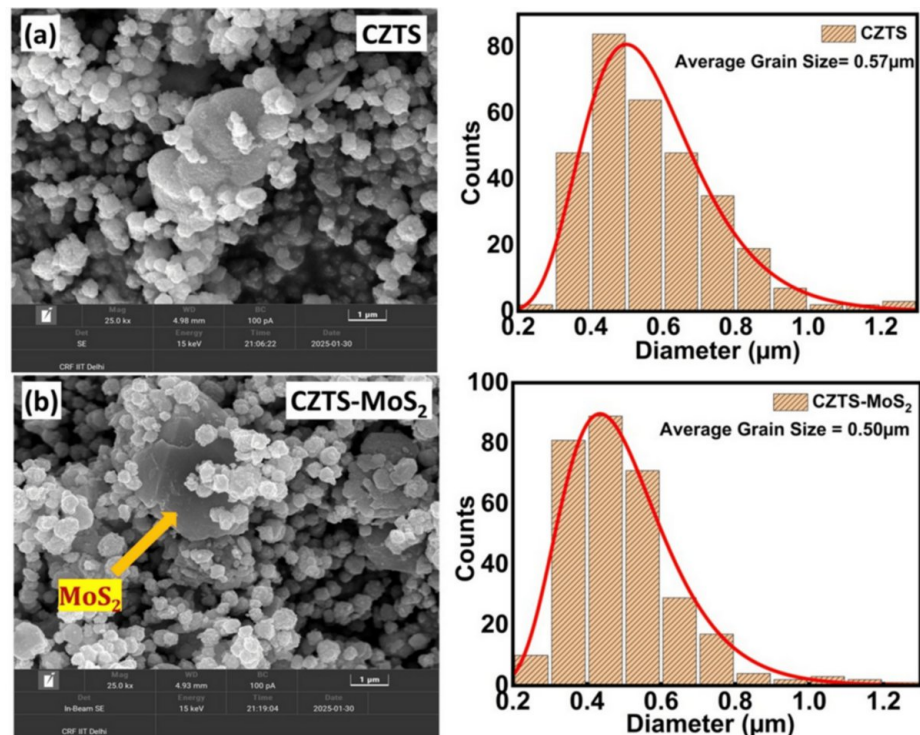


FIGURE 7: FESEM images of hydrothermally synthesized (a) CZTS and (b) CZTS-MoS₂ nanocomposite

FESEM, Field Effect Scanning Electron Microscopy; CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

The EDX technique was used to determine the elemental composition. This is used to verify the existence of copper (Cu), tin (Sn), zinc (Zn), molybdenum (Mo), and sulfur (S). During the synthesis procedure, the optimal stoichiometric ratios of $\text{Cu}/(\text{Zn} + \text{Sn}) = 1$ and $\text{Zn}/\text{Sn} = 1$ for the metal precursors were selected [21]. The EDX analysis showed a slight change in the composition of CZTS and CZTS-MoS₂ nanocomposite (Figure 8). The measured composition ratios of $\text{Cu}/(\text{Zn} + \text{Sn})$ were 0.99 and 1.08, while the Zn/Sn ratios were 1.04 and 0.96 for the CZTS and CZTS-MoS₂ nanocomposite, respectively.

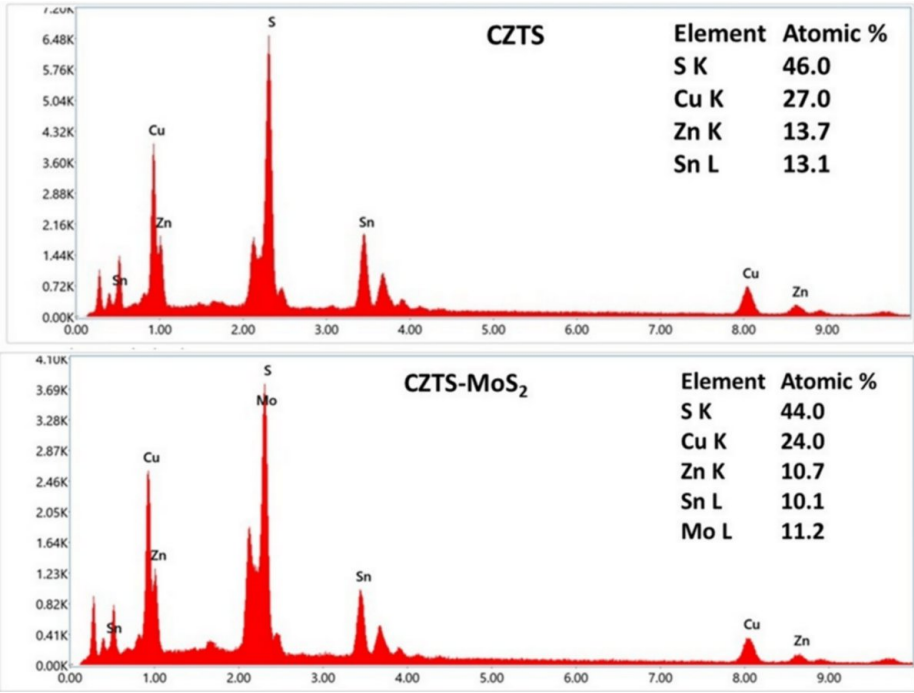


FIGURE 8: EDX analysis of CZTS and CZTS-MoS₂ nanocomposite

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide; EDX, Energy Dispersive X-ray Spectroscopy

Photocatalytic degradation of crystal violet dye

In a simple photoreactor that was powered by a halogen lamp with a power output of 300 W, the CZTS-MoS₂ nanocomposite that had been synthesized was tested to determine its capacity for photocatalysis. The purpose was to decompose the crystal violet dye. A total of 20 mg of the CZTS-MoS₂ catalyst was incorporated into a 100 ml solution containing 20 ppm of dye. The photodegradation of crystal violet dye has been observed by measuring its concentration at an absorption wavelength of 582 nm. The Lambert-Beer law states that there is a direct correlation between the concentration of a solution and its absorbance outcomes. A decreasing dye concentration in the solution is shown by the decrease in absorbance with longer illumination time. Figure 9a illustrates the absorbance spectra of the crystal violet dye solution as a function of reaction time for CZTS-MoS₂. The spectra reveal that prior to the oxidation process, the absorption spectrum of crystal violet in an aqueous solution exhibited a significant peak at 582 nm within the visible range [22].

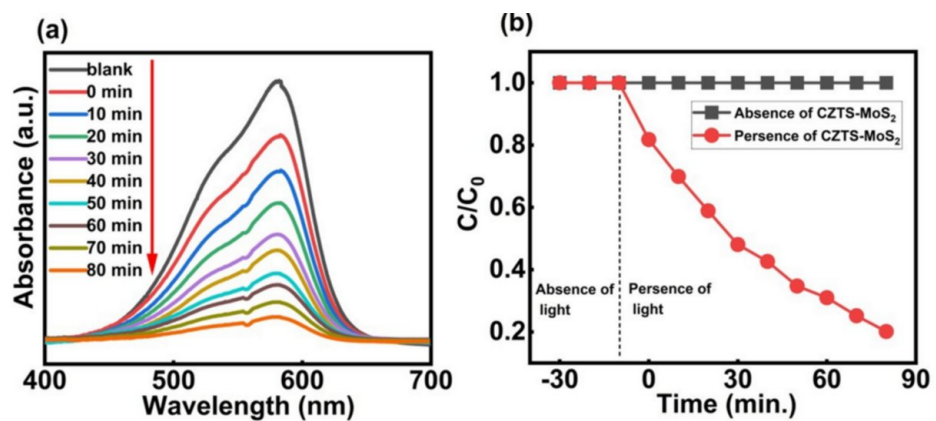


FIGURE 9: (a) Absorbance spectra of crystal violet dye solution at different reaction time and (b) Photocatalytic degradation under illumination of visible light for CZTS-MoS₂

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

The percentage of degradation or degradation efficiency is computed using the following equation

$$\% \text{ of Degradation} = \left(1 - \frac{C}{C_0}\right) \times 100 \quad (5)$$

Here C_0 represents the initial absorption of crystal violet dye at time $t = 0$, while C reflects the absorption at time t after catalyst injection. The degradation efficiency is calculated to be approximately 79.9% for the CZTS-MoS₂ nanocomposite when exposed to light for 80 minutes (Figure 10b). However, while comparable MoS₂-CZTS systems have demonstrated faster degradation kinetics (e.g., Mondal and Saha reported $k \approx 0.283 \text{ min}^{-1}$ and complete methylene blue degradation in 15 minutes) [16], the differences stem from dye chemistry, light source intensity, and material morphology. Crystal violet is more stable and reacts slowly than methylene blue, which is photosensitive and degrades faster under visible light. The previous study used high-intensity visible light and ultrathin MoS₂ nanosheets with higher contact area, but our study used a 300 W halogen lamp and a larger structure via a simpler synthesis technique. The apparent rate constant is affected by photon flux, catalyst shape, starting dye concentration, and adsorption behavior. The lower kinetic value found in this study is in line with the parameters of our experiment and the natural properties of the crystal violet dye system.

Kinetics of crystal violet dye photodegradation

The kinetics of photocatalytic degradation was examined to better understand the degradation process. The degradation of crystal violet dye follows pseudo first-order kinetics. The rate constant (k) can be calculated using this relationship [23].

$$\log \frac{C}{C_0} = -kt \quad (6)$$

Where, C_0 and C represent the dye concentrations at the initial times $t = 0$ and at a later time t , respectively, while k denotes the pseudo-first-order rate constant.

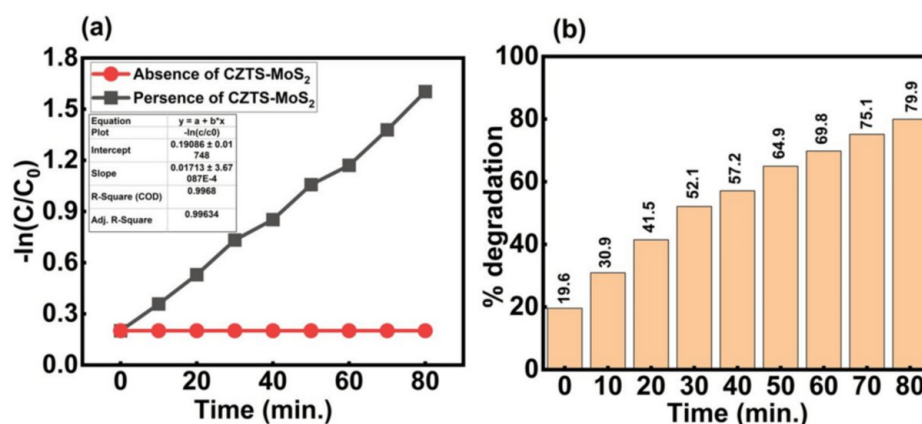


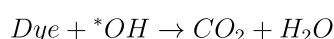
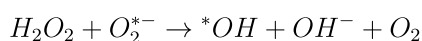
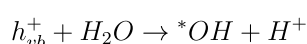
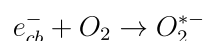
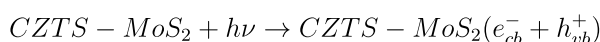
FIGURE 10: (a) Kinetics plot and (b) degradation % vs time plot of crystal violet dye by CZTS-MoS₂ nanocomposite

CZTS, Copper Zinc Tin Sulfide; MoS₂, molybdenum disulfide

The relation between $-\log(C/C_0)$ and irradiation duration is shown visually in Figure 10. With the help of this plot, we can calculate the pseudo-first-order rate constant (k) for the CZTS-MoS₂ nanocomposite. In optimal condition, a pseudo-first-order rate constant of 0.0171 min^{-1} was determined. Adsorption and photodegradation are both methods that may be used to remove crystal violet dye; however, at lower concentrations, adsorption is more significant than photodegradation.

Photo-catalytic dye degradation mechanism

The photocatalytic process for crystal violet dye using the CZTS-MoS₂ catalyst under light irradiation is shown in the following equations. Electron-hole pairs are created when the incident photon interacts with the photocatalyst. When electrons are excited to the conduction band, they leave behind vacancies (holes) in the valence band enabling oxidation and reduction reactions to occur [5]. The electrons (e^-) and holes (h^+) can move toward the surface of the catalyst, where they engage in redox reactions with other species. This process helps to prevent the recombination of the initially generated electrons and holes. Holes (h^+) in the valence band readily react with surface-adsorbed H₂O molecules to generate hydroxyl radicals ($^{\bullet}\text{OH}$), while electrons in the conduction band interact with O₂ to produce superoxide anion radicals (O₂ ^{$\bullet -$}). These reactive oxygen species play a dominant role in the degradation of the crystal violet dye by attacking its aromatic rings and chromophoric groups, leading to the formation of smaller intermediates and eventual mineralization. The synergistic charge separation at the CZTS-MoS₂ interface and the continuous generation of reactive oxygen species (ROS) ($^{\bullet}\text{OH}$ and O₂ ^{$\bullet -$}) collectively enhance the photocatalytic efficiency of the composite catalyst. The hydroxyl radicals ($^{\bullet}\text{OH}$) may subsequently form hydrogen peroxide (H₂O₂). The H₂O₂ can further react with O₂ ^{$\bullet -$} to produce $^{\bullet}\text{OH}$. These reactive hydroxyl species are primarily responsible for the degradation of the dye [24].



The superoxide radicals and hydroxide radicals are both primary agents responsible for the photodegradation of organic dye pollutants [25]. The synthesized CZTS-MoS₂ nanocomposite has enhanced photocatalytic activity owing to its homogeneity and microscopic size, which provides a high surface area-to-volume ratio and inhibits agglomeration, hence enhancing the effective surface area accessible for the reaction [26].

Conclusions

In conclusion, CZTS and CZTS-MoS₂ nanocomposites were synthesized hydrothermally and characterized by XRD, UV-Vis. spectroscopy, FE-SEM/EDX, Raman spectroscopy, and photoluminescence analysis. The CZTS-MoS₂ nanocomposite was superior to pure CZTS in visible light absorption, band gap (1.69 eV), charge carrier recombination, and exhibiting a greater active surface area. The CZTS-MoS₂ nanocomposite exhibited a degradation efficiency of 79.9% within 80 minutes when utilizing crystal violet dye and visible-light irradiation, with a pseudo-first-order kinetics rate constant of 0.0171 min⁻¹. Enhanced activity arises from the synergy between 2D MoS₂ sheets and CZTS nanoparticles, which facilitates improved charge separation, reduced electron-hole recombination, and enhanced active site density. The findings to the study suggest that the study, the CZTS-MoS₂ nanocomposite acts as an eco-friendly photocatalyst, effectively facilitating the degradation of organic dye pollutants under visible light illumination. This study develops economical, high-efficiency chalcogenide-based nanocomposites for wastewater and environmental remediation.

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

Concept and design: Mohd Z. Ansari, Neha Neha

Acquisition, analysis, or interpretation of data: Mohd Z. Ansari, Neha Neha

Critical review of the manuscript for important intellectual content: Mohd Z. Ansari

Supervision: Mohd Z. Ansari

Drafting of the manuscript: Neha Neha

Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue.

Animal subjects: All authors have confirmed that this study did not involve animal subjects or tissue.

Conflicts of interest: In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** All authors have declared that no financial support was received from any organization for the submitted work. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

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