SYNTHESIS AND CHARACTERIZATION OF CZTS NANOPARTICLES BY USING HYDROTHERMAL TECHNIQUE

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Abstract:
In this comprehensive study, our primary focus revolved around the meticulous synthesis and thorough characterization of CuZnSnS (CZTS) nanoparticles utilizing the hydrothermal technique as the key methodological approach. The production of the CZTS nanoparticles was meticulously carried out through a meticulously devised hydrothermal synthesis route, followed by a detailed characterization involving sophisticated techniques such as UV-Vis spectroscopy and FTIR analysis. The utilization of UV-Vis spectroscopy played a pivotal role in unraveling crucial insights into the inherent optical properties exhibited by the finely crafted CZTS nanoparticles, shedding light on their light-absorption capabilities and potential photovoltaic applications. On the other hand, FTIR analysis served as a valuable tool in delving into the intricate details of the chemical composition and bonding characteristics inherent to the synthesized CZTS nanoparticles, thus providing crucial information that enhances our understanding of their structural makeup on a molecular level.
However, despite the invaluable insights garnered through this study, further in-depth investigations and meticulous assessments are deemed essential to fully unveil the latent potential harbored by these CZTS nanoparticles in driving innovation across various practical realms, marking a crucial stepping stone towards the realization of their promising applications in real-world scenarios.
Keywords: CuZnSnS (CZTS) nanoparticles, UV-vis spectroscopy, FTIR

1. Introduction:

In recent years, the search for green semiconducting photovoltaic absorber materials has led to the emergence of a potential candidate known as Cu_2ZnSnS_4 (CZTS) with a kesterite structure (He et al., 2021). CZTS offers several advantages, including optimal direct band gap, high absorption coefficient, intrinsic p-type conductivity, thermodynamic stability, and the use of earth-abundant and non-toxic elements (Wang et al., 2023) (Zhao et al., 2022). The efficiency of CZTS solar cells has been found to be higher than that of conventional materials like CdTe and Cu(In,Ga)Se_2 (Zaki et al., 2022) (Shrivastava & VERMA, 2023). However, the efficiency of CZTS cells is still below the theoretical limit, suggesting untapped potential (Apostolopoulou et al., 2018).

Apart from its application in thin film solar cells, CZTS has also been explored for other uses such as charge-transfer layers, sensors, thermoelectric devices, and water splitting. CZTS has shown promise as a photocathode for solar-assisted water splitting and has demonstrated excellent photoreactivity and photocatalytic performance (Alirezazadeh & Sheibani, 2020) . It has been extensively studied for air purification, water remediation of pollutants and wastes, and has shown different properties based on its size and morphology (Kannan & Manjulavalli, 2015).

Various techniques have been developed for the synthesis of CZTS, including vacuum and non-vacuum thin film deposition methods, as well as the direct production of nanocrystals (Sinha et al., 2023). Among the wet-chemical processes, the hydrothermal/solvothermal synthesis of CZTS nanocrystals has gained popularity due to its controlled production capabilities without the need for specific vessel conditions (Semalti et al., 2021). This approach has been preferred over the hot injection method (Henríquez et al., 2023).

Congo red (CR), a synthetic dye used in the textile industry and medical tests, has harmful effects on human health and is a known carcinogen. Therefore, efforts have been made to eliminate CR from aqueous effluents (Zaman et al., 2019).

In this study, CZTS nanoparticles were synthesized using the hydrothermal technique. The structural, morphological, surface chemical, optical, and optoelectronic properties of the synthesized sample were characterized (Dwivedi et al., 2020).

Overall, the use of CZTS as a potential material for next-generation solar cells and its applications in various fields, as well as the synthesis and characterization of CZTS nanoparticles, are discussed. The study also focuses on the use of CZTS as a photocatalyst for the degradation of the harmful Congo red dye, emphasizing the novelty of this research.

2. Experimental:

2.1 Materials

Cu_2ZnSnS_4(CZTS) nanoparticles were synthesized by thehydrothermal method using copper dichloride twice hydrated ($CuCl_2 \cdot 2H_2O$, 99.0%, Chemicals of India), zinc dichloride ($ZnCl_2$99% India Glycols Ltd),tin dichloride twice hydrated ($SnCl_2 \cdot 2H_2O$, 99%, Lab Chemical Manufacturers In Delhi) and sodium sulfide, hydrated nine times($Na_2S \cdot 9H2O$, 98% India Glycols Ltd). Ethyleneglycol (99%, India Glycols Ltd) was used for the deposition of thin films. Europiumnitride six times hydrated ($Eu(NO_3)3 \cdot 6H_2O$, 99.99% Lab Chemical Manufacturers In Delhi) was used for photoelectrochemical measure-ments (PEC).

2.2 Synthesis of CuZnSnS Nanoparticles by Using Hydrothermal Technique:

CZTS nanoparticle powder was synthesized by carefully preparing a precise mixture of $CuCl_2 \cdot 2H_2O$, $ZnCl_2$, $SnCl_2 \cdot 2H_2O$, and $Na_2S \cdot 9H_2O$ in a molar ratio of 2:1:1:4, which was then combined with deionized water. The solution underwent magnetic stirring and sonication for 30 minutes to ensure complete dissolution. Next, the solution was transferred to a stainless steel autoclave and heated at 260 °C for 24 hours for the hydrothermal reaction. After cooling to room temperature, the resulting black precipitate, indicating CZTS nanoparticle powder formation, was collected. The collected powder went through washing steps using deionized water and ethanol, involving centrifugation at 12000 rpm for 10 minutes to remove impurities.

Finally, the CZTS nanoparticle powder was dried at 80 °C for 2 hours to achieve desired physical characteristics for future applications.

2.3 Characterization

The optical properties were studied by UV-VIS molecular absorption spectra through the transmittance spectrum, using a SHIMADZU UV-2600 Spectrophotometer with a PC connection. The measurement range was from 400 nm to 900 nm at room temperature, with a scanning speed of 0.2 nm s^{-1}, and 10 mg of CZTS nanoparticles suspended in ethanol were prepared. The vibration spectra were recorded using an Avtar 370, Thermo Nicolet, Fourier transform infrared (FT-IR) spectrophotometer equipped with a DTGS detector with 4 cm^{-1} resolution, and samples prepared with KBr discs for this study.

3. Results and Discussion:

3.1 Characterization

3.1.1 UV-Vis Absorption

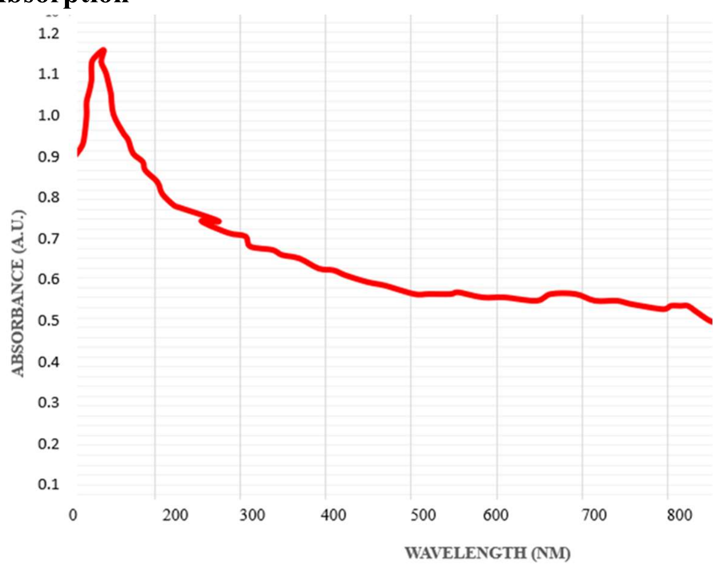

Fig 3.1. UV-visible spectrum of as synthesized Cu_2ZnSnS_4.

UV vis absorption spectra of CZTS nanoparticles (Figure 3.1) exhibit slight variations and demonstrate absorption at different wavelengths. This data aids in studying the optical properties and material characteristics of the sample effectively.

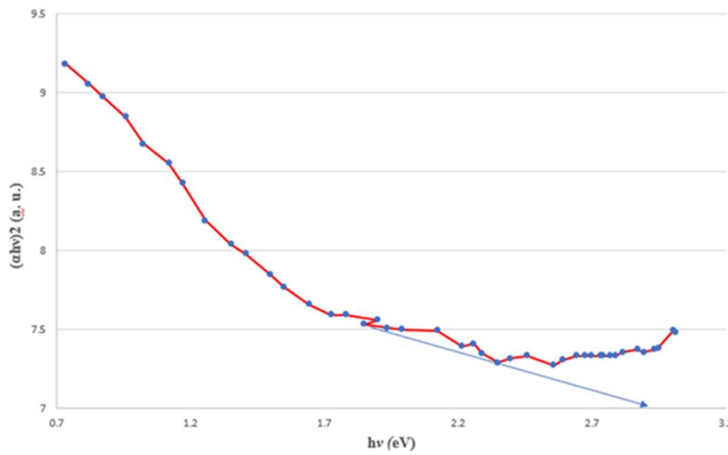

Fig3.2. Tauc plot of as synthesized Cu_2ZnSnS_4.

3.1.2 FTIR

The vibrational stretching of different bonds in CZTS was studied using FTIR spectrophotometer. Various peaks with maxima representing transmission spectra were observed. The peak at 2976 cm-1 corresponded to O-H stretching due to water absorption on the CZTS surface. A strong peak at 2895 cm-1 indicated the presence of a C-H group. An aldehyde group was observed at 1392 cm-1. C-O stretching vibration showed an intense peak at 1249.87 cm-1. The peak at 1055.06 cm-1 was attributed to the presence of S=O, i.e., sulfoxide group. Lastly, a small and strong peak at 445.56 cm-1 indicated a C-Cl Halo compound.

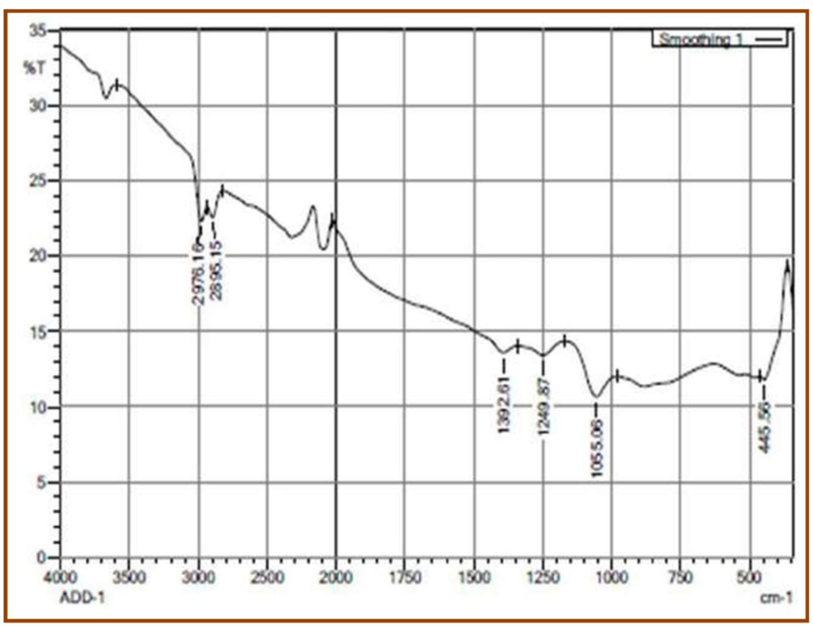

Fig3.3 FTIR Spectra of CZTS

4. Conclusion:

In this research paper, a novel synthesis approach was employed to successfully produce Cu2ZnSnS4 nanostructures utilizing the hydrothermal method, showcasing efficient manufacturing techniques in the field of nanotechnology. Upon detailed analysis of the optical properties of the synthesized nanostructures, it was revealed that the material exhibited a distinct energy bandgap of approximately 1.42 eV, shedding light on its potential applications in solar cell technology and other optoelectronic devices. Moreover, the investigation into the sensor characteristics of the Cu2ZnSnS4 nanostructures yielded intriguing results, notably a remarkable maximum sensitivity of 83.63% coupled with an impressive response time of 0.78 seconds, both crucial parameters for evaluating the efficacy of the sensor material. Furthermore, the recovery time of the sample, conducted at a temperature of 150 °C, was determined to be 15.8 seconds, showcasing the material's ability to swiftly return to its initial state after sensing an external stimulus, essential for real-world sensing applications where rapid response is imperative. This comprehensive analysis underscores the promising prospects of Cu2ZnSnS4 nanostructures in the realm of sensor technology and paves the way for further exploration into their diverse functionalities and potential practical applications.

5. future prospective

Cu_2ZnSnS_4 (CZTS) nanoparticles synthesized via hydrothermal methods exhibit promising properties for various applications. The CZTS nanoparticles show a bandgap of 1.5 eV, ideal for solar photocatalytic degradation. Additionally, CZTS nanoparticles have demonstrated efficient photocatalytic degradation of organic dyes under solar simulation light irradiation, with high degradation rates. Furthermore, the structural, morphological, and optical characteristics of CZTS nanoparticles have been extensively studied, highlighting their potential for photovoltaics and photocatalysis. The unique properties of CZTS nanoparticles, such as their bandgap and photocatalytic efficiency, suggest a bright future for their application in sustainable energy generation and environmental remediation.

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