

Doping effect on properties of CdZnS nanoparticles

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In current work, Nanoparticles of cadmium zinc sulfide (CdZnS) and copper zinc sulfide (Cu: CdZnS) were synthesized through a capping-agent-free chemical co-precipitation method. This article focuses on the optical characteristics, elemental analysis, and surface morphology of CdZnS and Cu: CdZnS. these properties of prepared materials were investigated using a variety of techniques, including X-ray diffraction (XRD), scanning electron microscopy, energy dispersive X-ray, and ultraviolet–visible absorption. The results show both pure and doped CdZnS have cubic structure. The energy gap of CdZnS was equal to 3.14 eV and 3.4 eV for Cu doped CdZnS. According to the results the prepared nanoparticles are suitable for photodegradation applications.

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1. Introduction

Owing to their high optical absorption coefficient, heterostructures based on II–VI group compounds have long been recognized as excellent materials for thin-film solar cells devices applications. To produce hetero-junction photovoltaic systems, Group II–VI compounds can be employed to generate ternary and quaternary mixtures with a direct primary band gap assignment across the full alloy composition range and high absorption coefficients. As a result, work on the material and device properties of group II–VI compounds has increased both experimentally and theoretically [1,2]. There are numerous uses for the wide bandgap metals chalcogenide group II–VI semiconductors NP, including solar cell, sensor, lasers and light emitting diodes [3]. The size of the NPs can be changed to change the band gap. The quantum confinement effect is said to be the reason for the situation. In this way, the energy levels become separate so that the band gap widens when the particle size gets smaller [4]. New potential for tuning optical characteristics from the ultraviolet to the near infrared have recently been opened up due to the creation of ternary semiconductors [5]. In recent years, Cadmium zinc sulfide (CdZnS) alloy composites have piqued technological interest due to the fact that the energy gap can be controlled and the lattice properties can be changed [6]. Cadmium zinc sulfide (CdZnS) has good electrical conductivity and a well and tunable absorptions in the visible spectrum of solar energies. As a result, they've been widely exploited as photocatalytic degradation materials with large band gaps [7,8]. Metal-doped semiconductors have been getting a lot of attention because they could be used in a lot of different applications [9]. Optical properties of semiconductors can be improved [10] and the intermediary bands [11] are capable to custom in bandgap of semiconductors in process of doping. Also, the metal-doped semiconductors might make the chemical steadiness better by putting the holes into the acceptors energy levels and making them less active on photo corrosion. In latest years, nanocrystals that doped with transition metals ions have been examined intensively since they don't basically have all the nanocrystals advantages but too own extra advantages such as larger Stokes shifts to avoiding self-absorption/energy transfer, larger lifetimes of excited state and

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improved thermal and chemical stability [12-15]. Doping CdZnS with transition metals such as Cu, Ag, and Mn can introduce discrete energy levels into the band gap [16]. A significant role is played by the synthesis process in the manufacture of nanoparticles of the desired size and structure. In some cases, material with an amorphous structures can be converted into crystalline forms through the application of the suitable processing techniques [17]. Many technique have been used to prepare CdZnS nanoparticles like mild aqueous route [18], thermal evaporation [19], exploding wire technique [20] and co precipitation method [21].

In the present work, we use the co precipitation method to prepare pure and doped trinary CdZnS nanoparticles and study their structural, surface and optical properties for their possible applications in the environment.

2. Experimental part

2.1. Preparation of CdZnS nanoparticles

Co precipitation of CdZnS nanoparticles in a solution of 0.5M/ 20ml cadmium chloride CdCl₂ and 0.5M/20ml Zinc nitride [Zn(NO)₃] is utilized to provide a Cd and Zn ions source. The solution's pH was brought down to 10 by adding ammonia solution, and the total volume was 100 ml. 20 ml of thiourea at a concentration of 0.5 M was added gradually to the aforementioned solution. after which the concoction was heated at 70 degrees Celsius for 60 minutes on a hot plate.

At last, impurities are removed by centrifuging the particles and washing them in distilled water and methanol. CdZnS NPs preparation was placed in the oven at 80 degrees Celsius for 12 hours, resulting in a yellowish powder.

2.2. Preparation of CdZnS:Cu nanoparticles

Following the same protocol as before, Cu (1%) doped CdZnS NPs were synthesized by adding a 0.05 M aqueous solution of CuCl₂ to a solution of 0.5 M/ 20 ml of cadmium chloride CdCl₂ and 0.5 M/20 ml of Zinc nitride [Zn(NO)₃].

CdZnS and CdZnS X-ray diffraction (XRD) studies:

Cu-K radiation at a wavelength of 1.5418 nm is used to conduct Cu NPs. The surfaces morphologies were studied with a scanning electron microscopy. When measuring absorption and the band gap from 350 nm to 1000 nm, a UV-VIS spectrophotometer is utilized.

3. Results and discussion

XRD measurement was used to examine the structure characteristics of CdZnS and Cu:CdZnS nanoparticles. As illustrated in Figure 1, the XRD patterns of CdZnS and Cu doped CdZnS nanoparticles produced at room temperature using the co precipitation technique are displayed in detail. Figure 1 shows the diffraction peaks of nanoparticles before and after doping with Cu. It is noted in the figure that CdZnS nanoparticles show one broad peak at 26, and after doping with Cu, completely new peaks appeared indicating the formation of the CdZnS:Cu. These diffraction peaks are identical to the peaks obtained by [6,22]. The angles of diffraction, intensities and d interatomic spacing of prepared materials are shown in table 1. SEM examination was used to study the morphology and form of CdZnS and Cu doped CdZnS nanoparticles. For CdZnS and Cu:CdZnS 1 NPs, Figure 6a and b show typical SEM images. The element compositions of the nanoparticles forms of CdZnS and CdZnS: Cu were determined using an energy dispersive spectroscopy instrument. The peaks observed in the EDX spectrum (shown in Figs. 2a and b) are related with the elements Cd, Zn, S, and Cu, respectively. The results of Fig. 5b demonstrated that Cu contents was successfully alloyed into CdZnS nanoparticles.

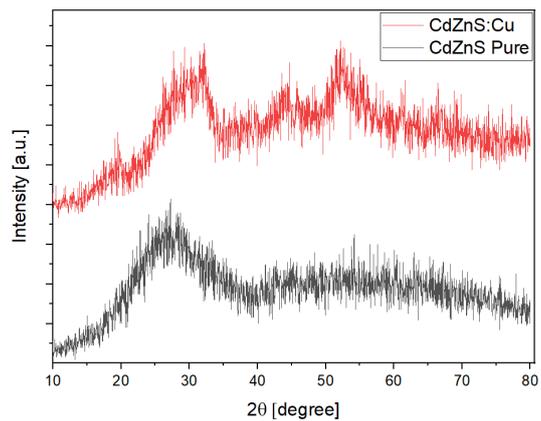


Fig. 1. diffraction patterns from XRD for both samples.

Table 1. The angles of diffractions, intensities and d interatomic spacing of prepared materials.

Samples	Position [°2Th]	Heights [counts]	FWHM [°2Th]	d [Å]
CdZnS	26.0322	31.87	4.0000	3.29584
CdZnS:Cu	19.0644	4.92	1.6613	4.65151
	27.6426	24.92	3.7513	3.11410
	31.9854	34.51	1.6712	2.79585
	44.5462	11.10	4.0000	2.03234
	52.4142	23.14	2.4273	1.74427

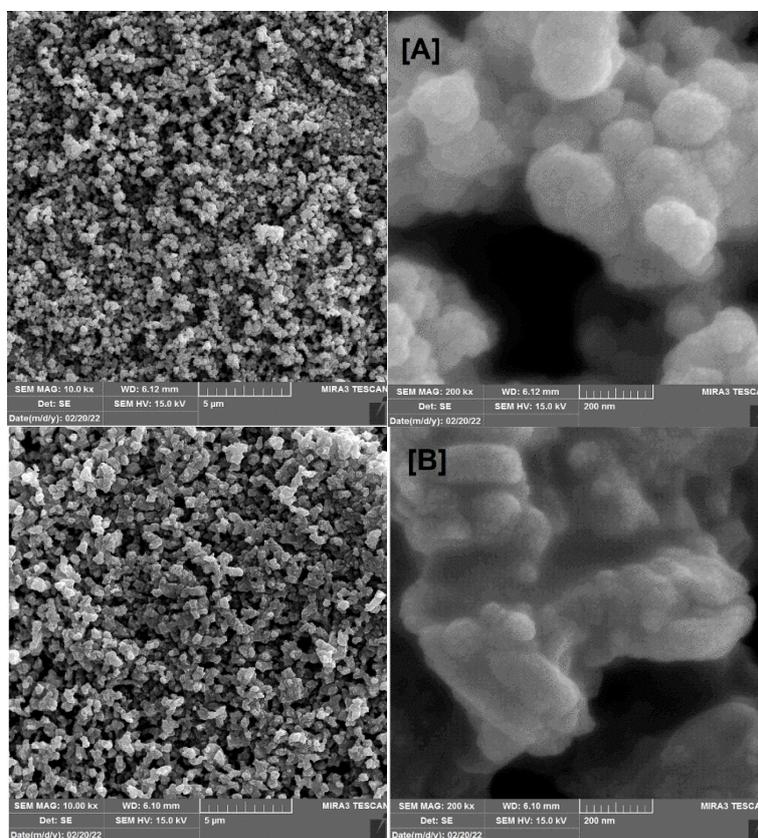


Fig. 2. FE SEM images for CdZnS and CdZnS:Cu NPs.

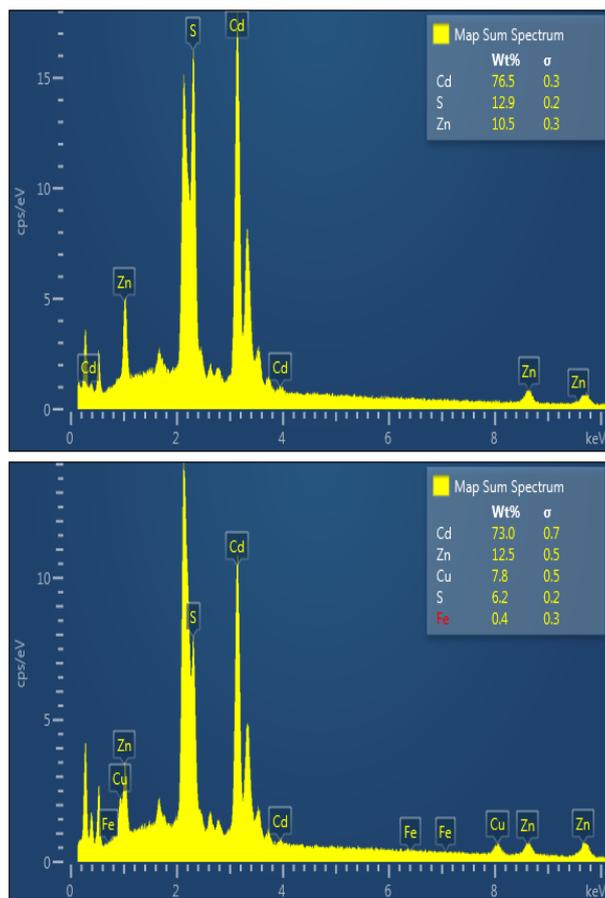


Fig. 3. EDX patterns from SEM for CdZnS and CdZnS:Cu NPs.

Figure 4 depicts the mapping and EDX pattern of CdZnS and Cu:CdZnS nanoparticles, as well as their morphology. Figure 4 a depicts a mapping for calculating the elemental distributions of Cd, Zn, and S. In addition to Cd, Zn and S elements are found in the Cd region, as shown on the colored map.

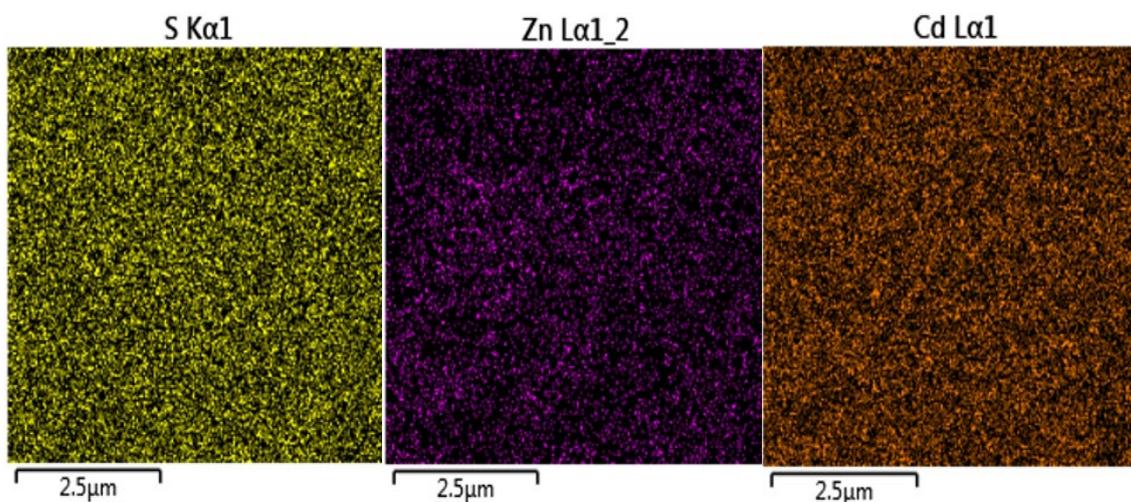


Fig. 4a. Mapping for CdZnS and NPs.

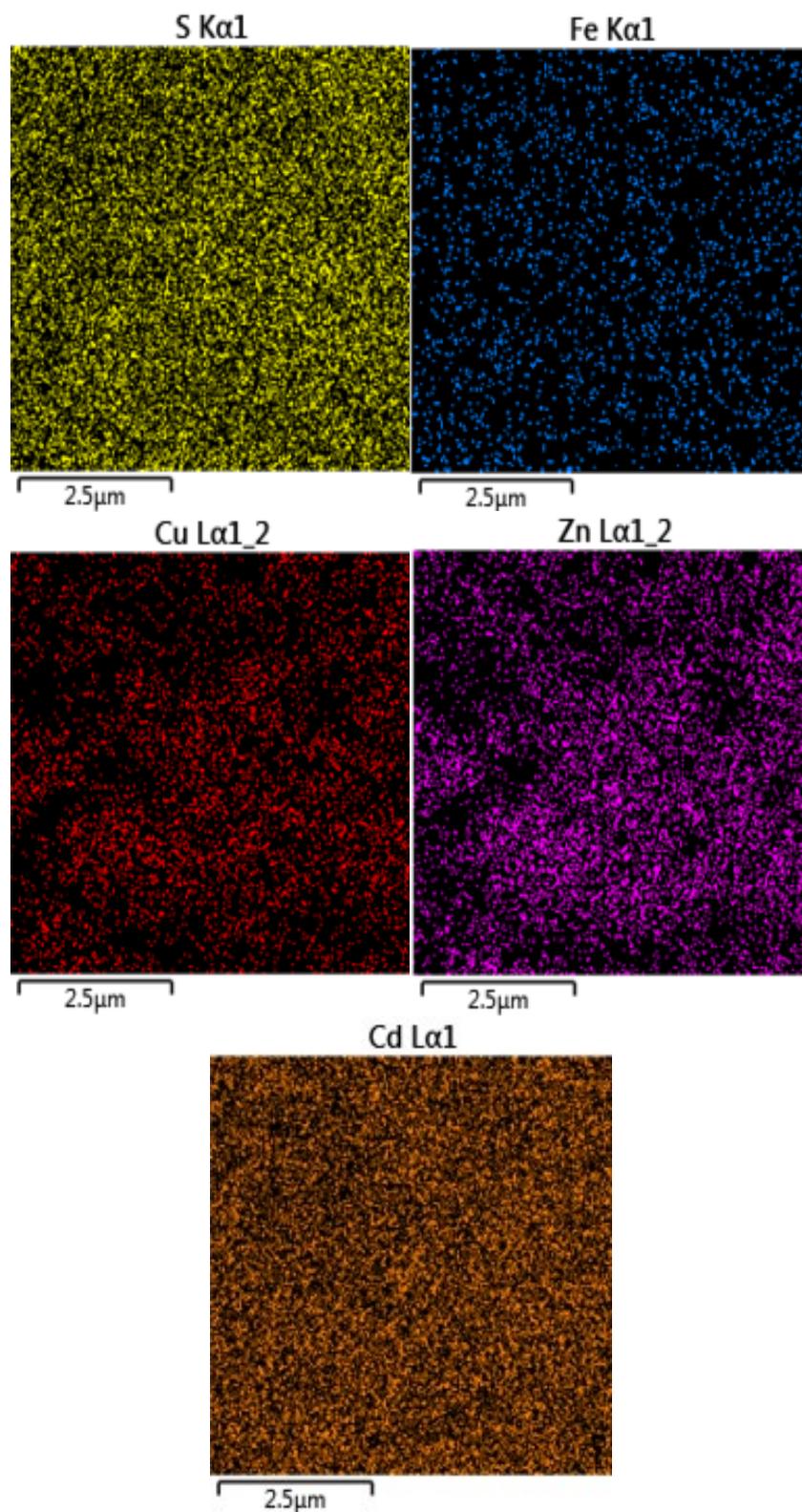


Fig. 4b. Mapping for CdZnS:Cu NPs.

Optical absorption measurements were conducted by dissolving CdZnS and Cu: CdZnS NPs in ethanol. The optical absorption spectrum of CdZnS and Cu doped CdZnS nanoparticles in ethanol are shown in Figure 5a and b. Using Fig. 5 as an example, we may find out the wavelength at which the NP are absorbed, as well as the energy of the band gaps that correspond to this

wavelength. Increasing the Cu content was found to decrease CdZnS NP size, which is directly associated to a higher bandgap value. Perhaps the bulk of the CdS is experiencing the effect of quantum confinement. In order to understand how quantum confinement influences impurity, we need to know the size of the host crystal [23]. Adding copper to CdZnS NPs causes the band gap (3.19 eV) to expand (3.4 eV). From what we can see, alloying drastically alters a material's band gap assignment.

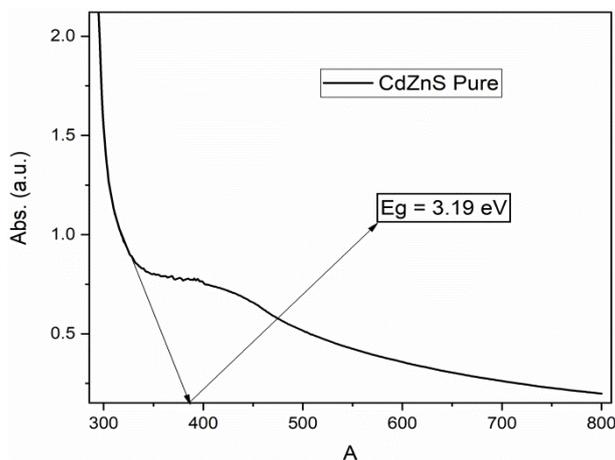


Fig. 5a. Absorption spectrum and corresponds bandgap for CdZnS NPs.

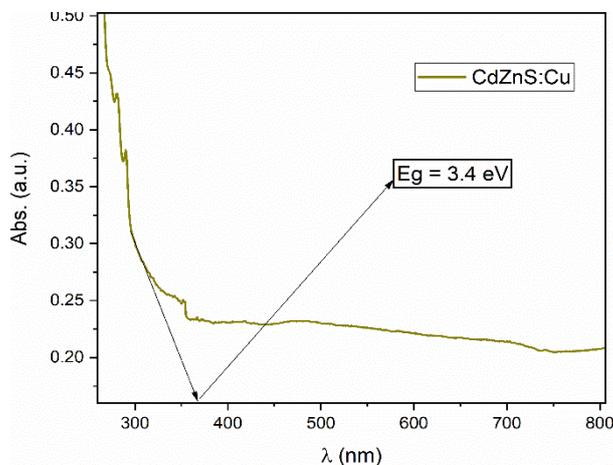


Fig. 5b. Absorption spectrum and corresponds bandgap for CdZnS NPs.

4. Conclusions

CdZnS and CdZnS:Cu nanoparticles have been synthesized by chemical co-precipitation technique. XRD pattern reveals the formation of cubic structure of CdZnS and CdZnS:Cu with the peak shift toward higher angle, which confirms the incorporation of copper. The energy gap decreases after doping with copper.

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