

Study The Optical Properties of Quantitative Points of Manganese (Mn)-Infected CdSe Prepared by Sol-gel

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Abstract: We prepared one of the selenium salts in order to use it in the preparation of cadmium selenide in the chemical way and alloy it in a different proportions of manganese Mn and then we deposited CdSe manganese-alloyed on glass slides and we did a structural characterization of it XRD and studied the light properties of it (Abs-Pl) & (UV-VIS) Samples of CdSe cadmium selenide (-manganese-Mn) were prepared by Sol-Gel method (5%, 3%, 1%) and deposited on glass substrates in order to obtain thin films, by taking the absorption spectrum and found that the samples were of high absorbency within the domain (300-500) nm Energy gaps for pure and similar thin CdSe films were measured using visible UV spectroscopy, and their value was within the range (2-5) eV. From a study of fluorescence spectroscopy, it was found that the best excitation wavelength was at $\lambda=340\text{nm}$. It would give the best fluorescence spectrum with high intensity and wide pulse starting from (450-500) at Wavelength of $\lambda=480\text{nm}$, indicating that the samples are subject to *stux* transitions. Our aim of research is to study the structural and optical properties of CdSe and the effect of its alloy with manganese (Mn).

Keywords: absorption spectrum, cadmium selenide, fluorescence spectrum, thin films.

INTRODUCTION

In 2009, a group of researchers (Nguyen Van Hung, Nguyen Van Min, Pham Thu Nga, Trinh Duc Thien, Khong Cat Cuong) presented research about preparing quantitative points in a sol-gel way where the size of the quantum point was calculated by experimental equations (Shearar equation and Brass equation) where quantitative points were obtained 4nm. In 2011, the two researchers (Alexandra A.P. Mansur, Herman S. Mansur) presented research about the preparation of quantitative points from stable CdSe using the functional clique (PVA) in a watery middle at room temperature. Using spectrum UV-vis for determine the size of quantum points (2nm), the size of the points was observed to increase over time. In 2017 the researcher (Aliya binti Hamizi) presented search about preparing different sizes of quantitative points of CdSe and the effect of alloyed it to manganese Mn.

1.1. The CdSe:

is a semiconductor of the n-type, and it is one of the most famous compounds of the second and sixth semiconductors group [1]. It is found in nature as a red crystalline powder. It has a crystalline structure in the form of a cube as shown in Fig.1

IMPORTANCE AND OBJECTIVES OF THE RESEARCH

The importance of research in preparing quantitative points of CdSe precipitated on glass substrates and manganese-like Mn ratios (1% .3% .5%) in a chemical way and studying the effect of impurity on their optical properties

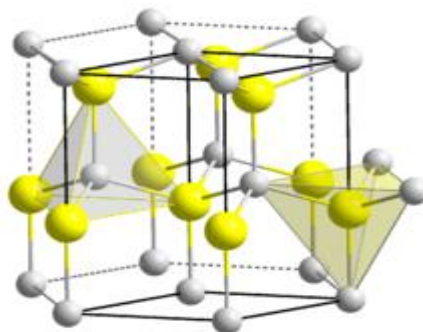


Figure.1: shows the crystalline structure of cadmium selenide.

The slight difference in atomic distribution leads to large differences in the properties of electronic structures and the energy gap and is in the crystalline structure within the domain (3.45– 3.79) eV [3]

Cadmium selenide shows high transparency within a wide area of the spectrum, and its energy gap is direct, it is a promising material used in the manufacture of optical and optical devices and diode laser valves, in addition to a variety of applications in high-efficiency solar cells [2].

PILOT STUY

We used a sensitive thermometer to determine the appropriate amounts of used materials then mix it with a magnetic mixer for a few minutes To dissolve CdSe fully and the elements merge together and after the dissolution of CdSe with distilled water, we alloy it with manganese in a different proportions (1%-3%-5%) and we studied its optical properties using the absorption spectrometer (UV-Vis) and spectrometer (Abs-PI).

3.1. Method of preparation:

Prepare the solution of selenium (Na_2SeSO_3):

1. Dissolve 25.2 gr of $\text{Na}_2(\text{SO}_3)$ in 200 ml of distilled water.
2. put on a magnetic mixer for 5 minutes with continuous stirring until the sodium sulfite is completely dissolved as a transparent solution is formed.
3. 7.89gr of selenium metal is added to the previous solution. The color of the solution changes to black.
4. The previous solution is placed on a magnetic mixer for 5 minutes until the solution becomes homogeneous and then the solution is placed within a three-headed glass block.
5. then a reversible distillation of the previous solution is carried out with heating at Grade 80 for 12 hours until selenium is completely dissolved and a transparent Na_2SeSO_3 (a) solution tends to brown (red wine).
6. The previous solution cools to room temperature called solution A.

Preparing cadmium solutions:

1. 12.6 gr of Cadmium chloride $\text{CdCl}_2 \cdot 2 \text{H}_2\text{O}$ is dissolved in 100 ml of distilled water.
2. placed on a magnetic mixer for five minutes as cadmium chloride solution of 0.1 mol / L concentration is formed in transparent color symbolized by solutionB.

Prepare quantitative points of CdSe impurity by manganese at 1%. 3% 5%: Quantitative points of selenium cadmium impurity by manganese were prepared in aqueous medium with different concentrations as follows: 1-Mix 1 ml of solution (A) (Na_2SeSO_3) with a 0.1 mol / L concentration of with 3ml of solution (B) $\text{CdCl}_2 \cdot 2\text{H}_2\text{O}$ by adding

0.126gr (1%) Mn (CH₃COO)₂ 2- add polyethelencol dissolved with 20 ml of distilled water in a test tube and form Orange solution from selenium-cadmium over time the color of the solution turns into a dark red color, and this indicates the growth of the molecule size over time. In the same way, we prepare the remaining solutions with an increase in the percentage of Mn (3% -5%).

3.2. Measurements and discussion:

3.2.1. X-Ray Diffraction (XRD) X-Ray Spectroscopy:

XRD device performs an analysis of crystalline solids using X-rays to identify the properties of the material such as determining the crystalline form of the material and measuring the shape and size of the crystal and determining the distance between the internal layers of the crystal.

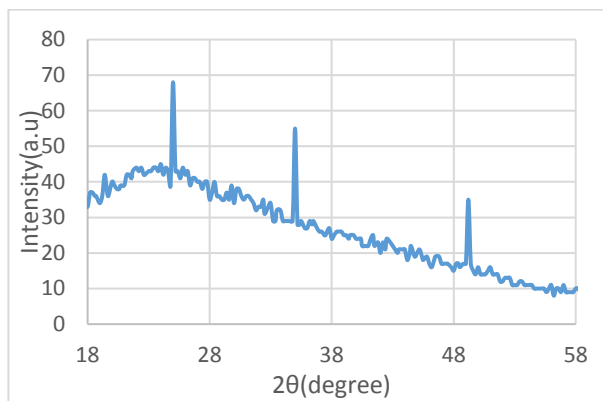


Figure.2: shows the X-ray diffraction spectrum for pure CdSe.

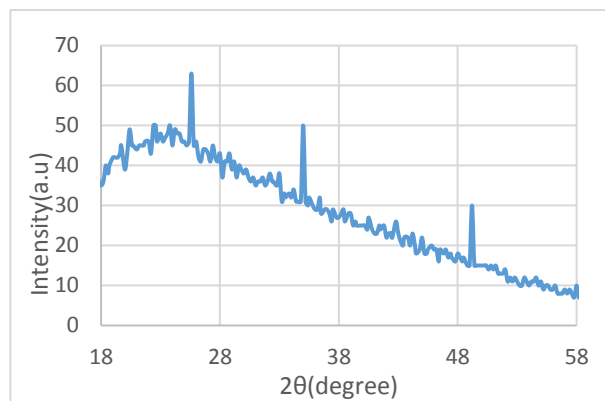


Figure.3: shows the x-ray diffraction spectrum for CdSe with manganese by 1%.

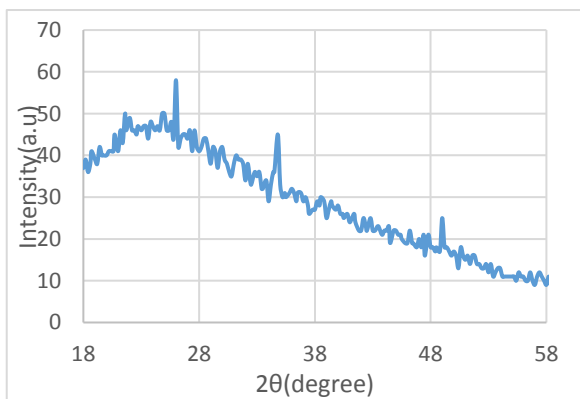


Figure.4: shows the x-ray diffraction spectrum of CdSe with manganese by 3%.

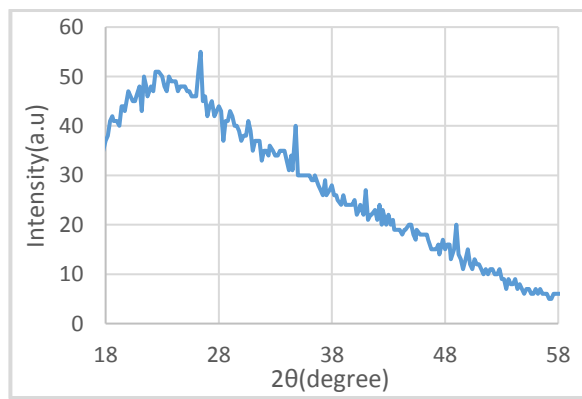


Figure.5: shows the x-ray diffraction spectrum of CdSe with manganese by 5%.

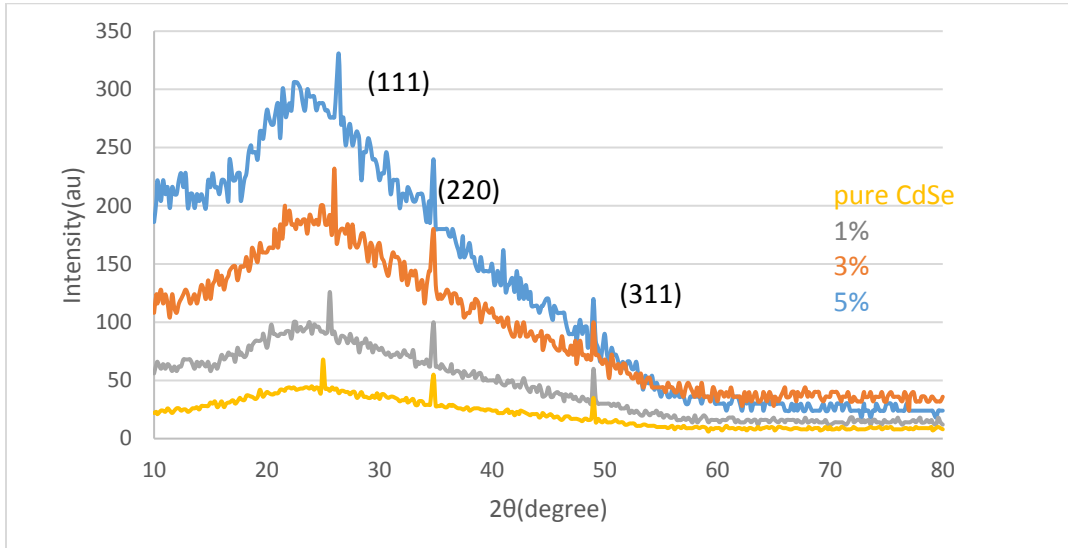


Figure.6: shows the x-ray diffraction spectrum of pure CdSe and impure by manganese in ratios (1%, 3%, 5%).

In order to know the structure of the prepared compound, the prepared samples were studied by X-Ray X-ray machine - an elevator made of copper material within an angular field (80° - 20°) where it was found that the structure of the prepared samples of the CdSe compound (QDs) at different rates of manganese with different rates FCC Frosted Cube Installation Three peaks were observed at $2\theta = (25)$, (34.8) and (49)

In conformity with (JCPDS) it is clear that they are compatible with crystalline levels (111), (220) and (311) respectively, and this corresponds to the cubic structure Figures (2), (3), (4) and (5) show the X-ray diffraction spectrum of samples prepared for pure and impurity by manganese CdSe in percentages 1%, 3%, and 5%. Depending on the X-ray diffraction spectra (2), (3), (4) and (5), the crystalline levels can be determined according to the required directions and the crystal dimension of the network can be calculated using the Bragg

$$d_{hkl} = \frac{n\lambda}{2 \sin \theta} \quad (1)$$

Where d_{hkl} is the distance between parallel crystalline levels according to the direction hkl , θ diffraction angle, x-ray wavelength ($\lambda = 1.5401 \text{ \AA}$), n diffraction ranks The relationship between the cell unit constants and the distance between parallel crystal levels in addition to the cell unit size is given in relation to the cubic structure

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad (2)$$

Depending on the relations (1) and (2), cell unit constants and cell size for the prepared samples can be calculated at each manganese impurity ratio as shown in Table (1). The crystallization volume can be set by the Debye-Scherer method. It depends on the relationship Debye-Scherer given as [10].

$$D = \frac{k \lambda}{\beta_{hkl} \cos \theta} \quad (3)$$

β_{hkl} mid-intensity width of the diffraction peak corresponding to the level hkl , K Shearer constant and equal to 0.94 in the case of spherical particles, $\lambda = 1.5401 \text{ \AA}$ X-ray Wavelength

The network emotion can also be calculated from the relation:

$$\varepsilon = \frac{\beta_{hkl}}{4 \tan \theta} \quad (4)$$

The crystallization scale is used to calculate the intensity of the dislocations in the crystal network, which is defined as the length of the dislocation lines in one volume of the material in relation to:

$$\delta = \frac{15\varepsilon}{\alpha D} \quad (5)$$

Table.1: Structural parameter of pure and doped Mn 1% ,3% ,5% CdSe films.

samples	2θ (deg)	hkl	Crystal Grid Constant a (Å°)	Crystal dimension d (nm)	Crystallization scale D (Å°)	Agitation ε (lin ⁻² .m ⁻⁴)	Dislocation δ (lin.m ⁻²)
Without Mn	25	111	6.16	3.56	42.50	0.000395	2.26
1%	25.3	111	6.01	3.47	42.52	0.000384	2.31
3%	26	111	5.92	3.42	42.61	0.000377	2.34
5%	26.5	111	5.83	3.37	42.65	0.000371	2.38

3.2.2. UV / VIS absorption spectrum:

Using the UV / VIS spectroscopy, the absorption spectra of the samples prepared within the wave range (400-800) nm, as shown in Figures (6-7-8-9-10):

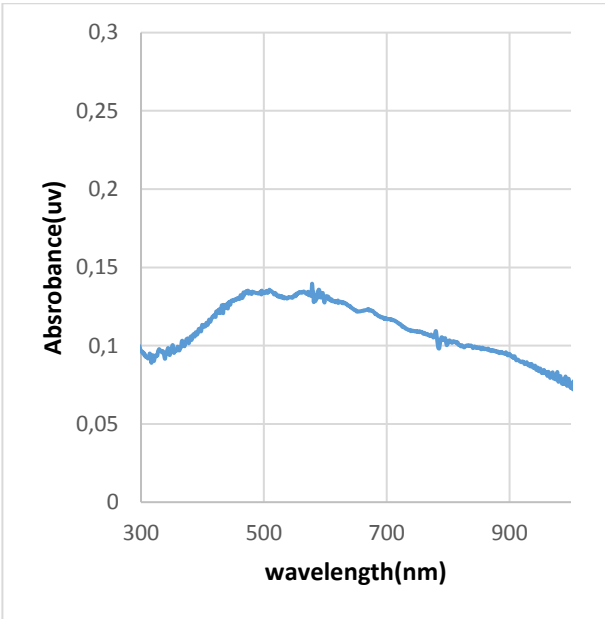


Figure.6: represents the absorption spectrum (UV-VIS) of the pure CdSe compound.

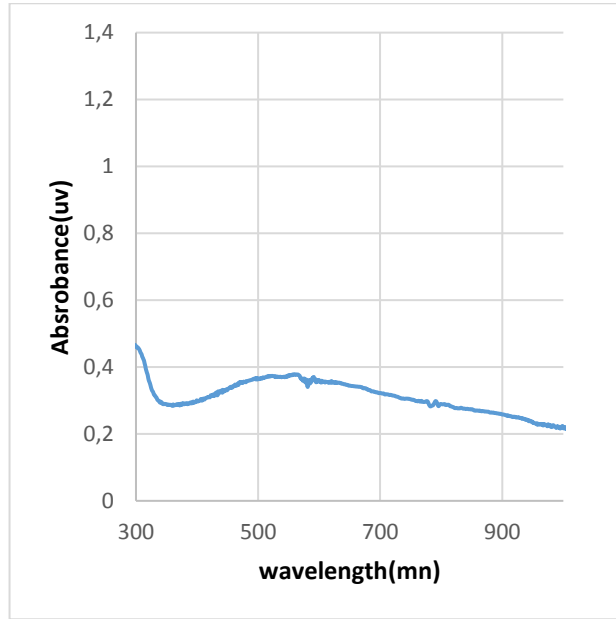


Figure.7: represents the absorption spectrum for the infected CdSe at 1% Mn.

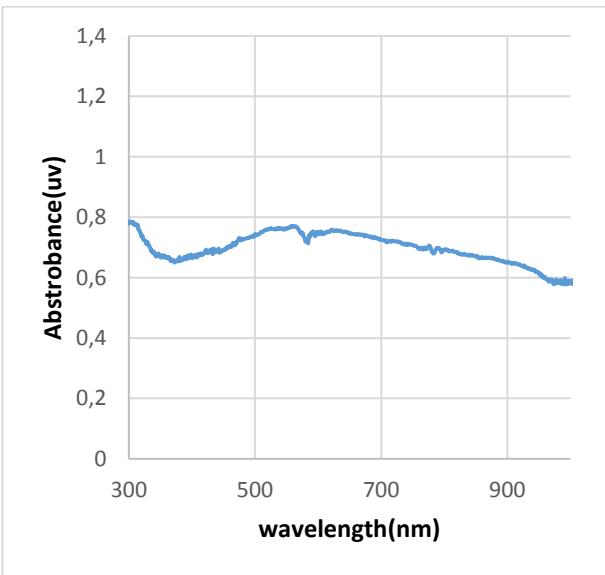


Figure.8: represents the absorption spectrum of CdSe with 3% statistically.

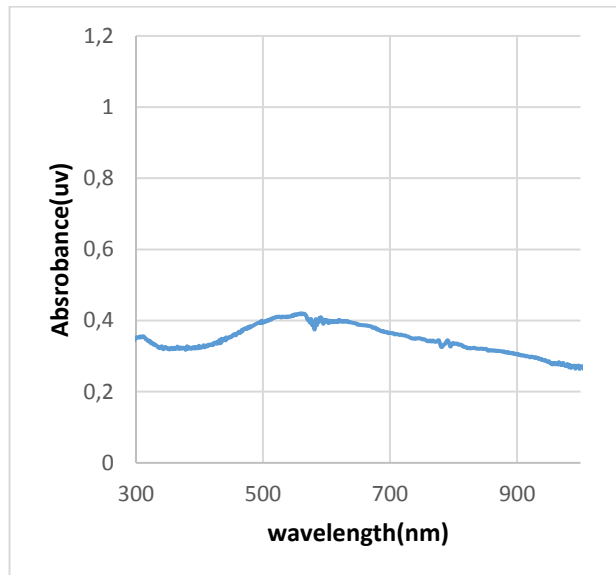


Figure.9: represents the absorption spectrum of CdSe with a static rate of 5%.

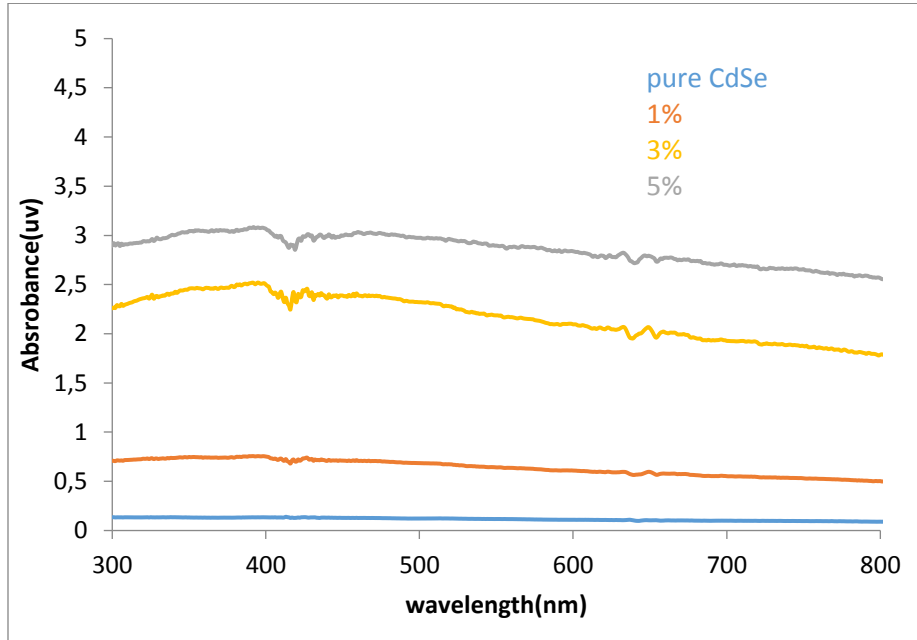


Figure.10: represents absorption spectra of pure CdSe and impure by manganese in ratios (1%, 3%, 5%).

It is observed from the figures (6-7-8-9) the presence of two absorption peaks, the first corresponding peak of length $\lambda = 480$ nm and the second peak corresponding to the wavelength $\lambda = 790$ nm belonging to CdSe of manganese Mn. It is also noticed that the absorption peak of CdSe is completely unclear at the wavelength $\lambda = 790$ nm, but as the proportion of doping increases, the absorption peak begins to gradually clear.

The Tauc relation can be used to calculate the energy gap value, where according to this relation the absorption coefficient for the material is given by the following relation (6): [4]

$$\alpha h\nu = A(h\nu - E_g)^n \quad (6)$$

Where E_g is the energy gap energy, $h\nu$ photon energy, A is constant, n is an indication of the nature of electronic transmission in the case of direct electronic transmission $n = \frac{1}{2}$ either in the case of indirect electronic transmission $n = 2$ or in the case of prohibited electronic transmission $n = 3/2$ and finally in the case of unforbidden electronic transmission $n = 3$.

Depending on the relationship (1), the variations of $(\alpha h\nu)^n$ with $(h\nu)$ are plotted by taking the tangent of the resulting curve and the tangent intersection point with the energy axis so we get the value of the energy gap as shown in the figures (12-13-14-15).

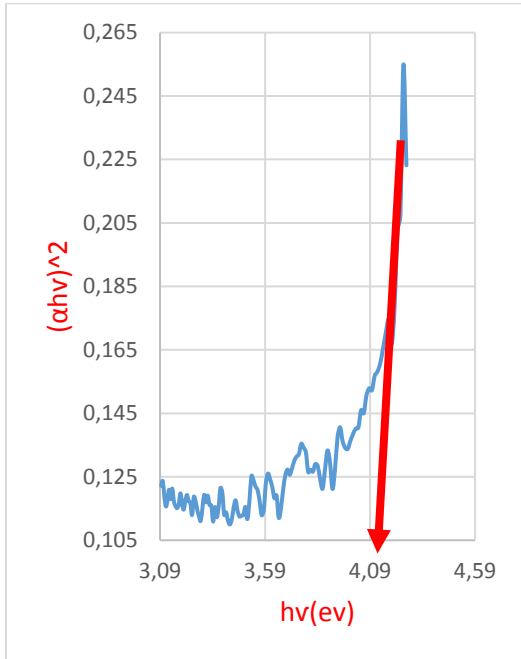


Figure.11: shows the width of the direct energy gap(4.09 ev) of the pure CdSe sample.

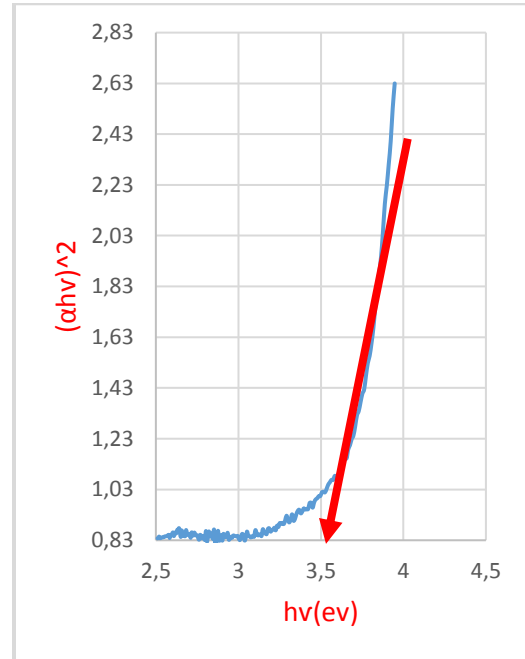


Figure.12: shows the width of the direct energy gap (3.5 ev) of the CdSe sample with a impurity ratio of 1%.

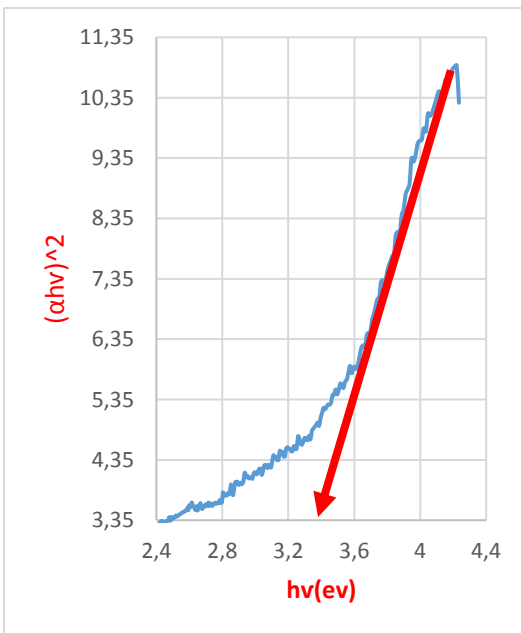


Figure. 13 shows the width of the direct energy gap(3.2ev) of the CdSe sample atimpurity ratio 3%.

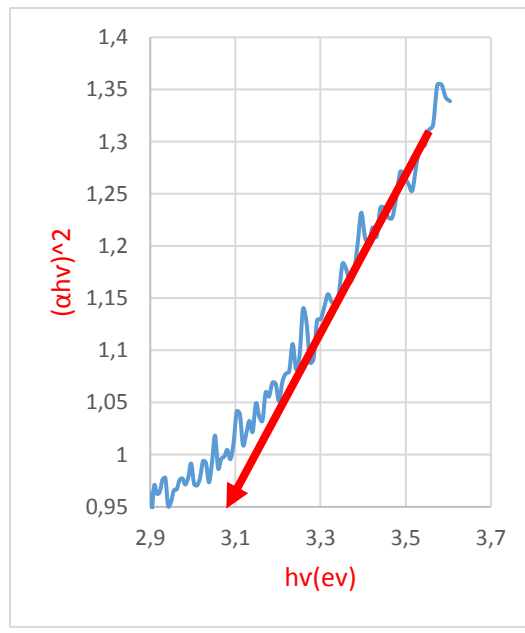


Figure. 14 shows the width of the direct energy gap(3 ev) of the CdSe sample with a impurity ratio of 5%.

Table.2: shows the values of the energy gap and its changes with changing percentage of impurity.

Impurity ratio by Manganese Mn	width of direct energy gap (ev)
Without impurity	4.09
1%	3.53
3%	3.25
5%	3

It is noted from Table (2) that when increasing the percentage of manganese infection for samples, the energy gap value will decrease.

This is explained by the increase in the percentage of doping resulting in localized levels within the energy gap above the valence bundle and below the conductivity bundle.

These levels are designed to receive electrons and thus reduce the energy gap [5].

3.2.3. Optical measurements: fluorescence spectroscopy:

Using the FS-2 Scinco-Fluorescence Spectrometer, the fluorescence spectra of the samples prepared within the wavelength range (200-900) nm at the excitation wavelength (λ), as shown in the following figures (16-17-18-19-20):

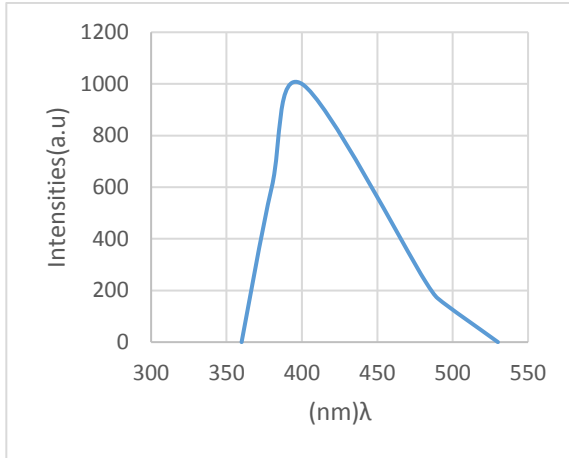


Figure.15: represents the fluorescence spectrum of the sample, representing pure CdSe.

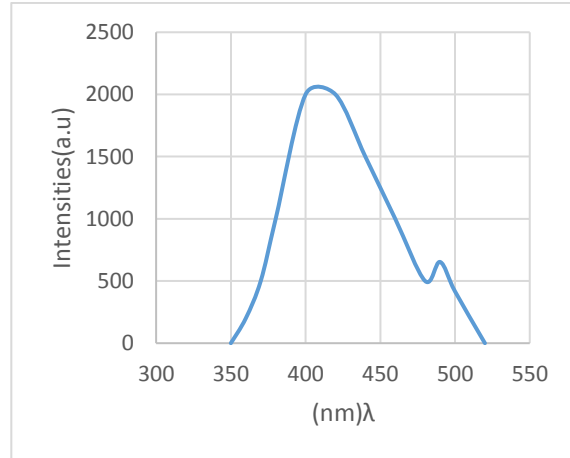


Figure. 16; represents the fluorescence spectrum of the CdSe sample with a impurity ratio of 1%.

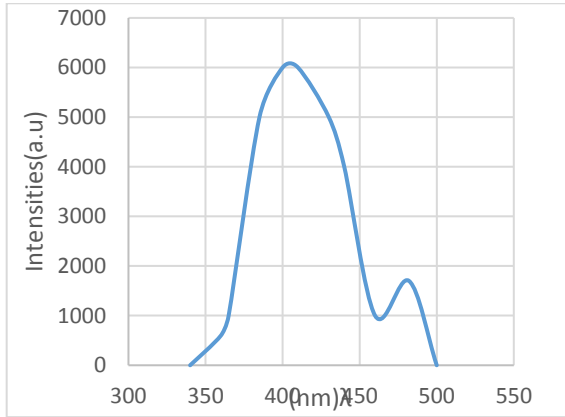


Figure. 17: The fluorescence spectrum of the CdSe sample with a impurity ratio 3%.

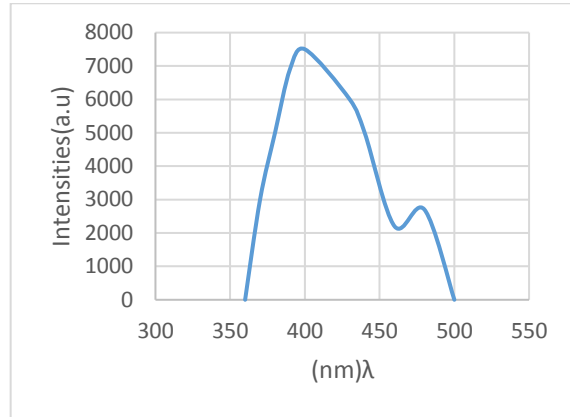


Figure. 18: represents the fluorescence spectrum of the CdSe sample with a impurity ratio of 5%.

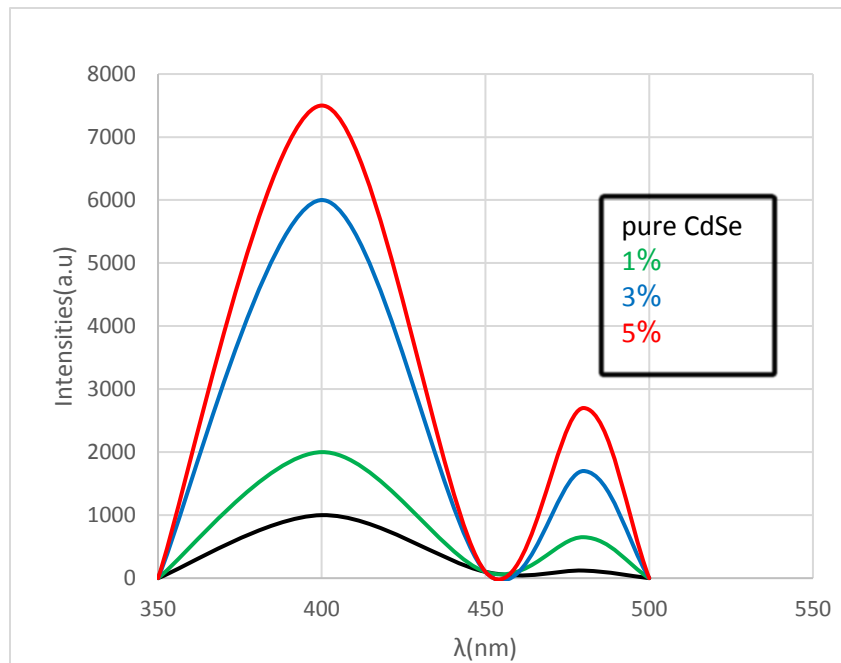


Figure.19: shows fluorescence spectra of pure and impure by manganese CdSe in different proportions (1%, 3%, 5%).

Notes from the shapes (16-17-18-15) fluorescence spectra for pure and impure by manganese CdSe films Mn PI spectra of all samples show two fluorescence peaks, the first at the 400nm wavelength of the CdSe and the second at the 480nm wavelength due to Mn.

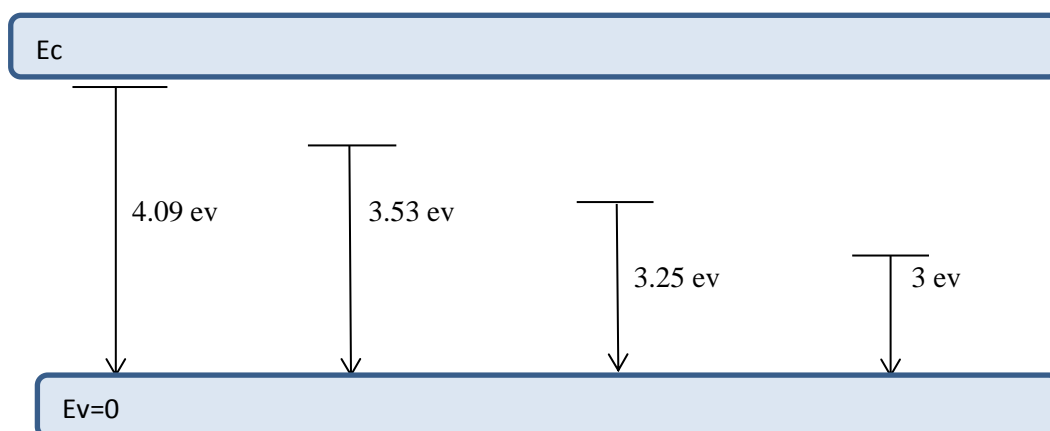
It is observed from Fig. 20 that the peak of pure CdSe at a weak intensity is approximately 1000, and for CdSe films with impure by manganese by 1%, the intensity was 2000, and at the 3% fertilization rate, the intensity was 6000, while at the percentage of the impurity 5%, the intensity is 7500 Thus, we find that pure CdSe films have approximately 1000 weak intensity at the same wavelength (peak).

We observe increased fluoridation with an increase in the proportion of Mn.

The figure shows that the density of the PI has improved when the sample was found to be impure by manganese without displacement of the peak, thus the peaks become denser after the impurity.

Table.3: shows the different fluorescence values for the CdSe sample according to the different ratios of impurity by Mn.

Intensity A	The proportion of impure by manganese Mn
1000	Pure CdSe
2000	1%
6000	3%
7500	5%



Scheme.1: shows different energy levels of pure CdSe and impure by manganese with different proportions (1% .3% .5%).

CONCLUSION

We provided an article about the quantitative points of selenide cadmium similar to manganese in the Sol-Gel way. Where we noticed that it's a good and inexpensive way, cheap and easy to apply to prepare thin films of impure by manganese CdSe. Through our study, the thin films showed high absorption within the wavelength range (300-500) nm and low absorbance outside this field. It was observed from the absorption spectrum that the value of the energy gap decreased, with an increase in the percentage of manganese infection (1%, 3%, 5%). It was also found from the fluorine spectrum that the severity of fluorine increases as the ratio of the alloyed increases in the rate of manganese infection, and by comparison between the fluorescence and absorption spectra, it was observed that there are stuxal transitions due to the absorption wavelength being smaller than the fluorescence wavelength.

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