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Short Essay

Blue Shift Behavior of CdSe Nano-particles Depending on the Concentration of Selenium

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Abstract

In this work, we examined the photoluminescence (PL) spectrum behaviour of freshly manufactured CdSe nano-flowers alongside their chemically or thermally modified nanoparticle equivalents. A solvothermal technique was used to create the CdSe nano-flowers, which had distinct petal structures and extremely crystalline, flower-like morphologies. Through carefully regulated post-synthesis procedures, the nanoparticles were then transformed into more spherical or irregularly shaped particles. Various CdSe nanostructures were created based on the selenium powder content. As the concentration of selenium powder increased and the size of the produced nanostructures decreased, a blue shift was observed. The band gap energy increased as the dimensions of the nanostructures decreased. It is evident from photoluminescence spectra that there was a prominent peak at higher wavelengths that could form a double in the spectrum.

Keywords: *X-ray diffraction; Photoluminescence; CdSe nanostructures; Solvothermal; UV-vis spectra.*

1. Introduction

Nanomaterials have garnered a lot of interest in recent decades due to their intriguing characteristics, which are very different from those of bulk materials [1–4]. Cadmium (Cd) and Selenium (Se) are essential precursors for the formation of cadmium selenide (CdSe) nanocomposites because of their unique chemical and physical properties. Cadmium selenide (CdSe) semiconductor nanocrystals are a model system for studying size- and composition–dependent optical properties in II–VI quantum dots. The II-VI family of nanotechnology semiconductors is well recognized for its sophisticated optical and electrical characteristics [5–9]. By adjusting the concentration of cadmium precursors, the morphology and size of CdSe nanoparticles can be controlled, which directly affects bandgap and emission properties. With a straight band gap of 1.24 eV at the surrounding temperature, cadmium selenide (CdSe), a member of the II-VI semiconductor classification, has a wide range of potential uses in solar panels, biological identification, and other fields [10–11]. It is also frequently employed in photovoltaic devices, electroluminescence, and catalysts [12–14]. Ramenery et al. was recorded the photoluminescence spectrum of cadmium selenium nanoparticle by using ethanol as a solvent and observed several peaks of nanocapsule due to variation of solvents [15]. Gilic et al. also reported

photoluminescence spectroscopy and surface morphology of cadmium selenium quantum dots using AFM measurement in a glass matrix [16].

The synthesis of CdSe nanostructured substance has made extensive use of several techniques such as solvothermal process, hydrothermal process, chemical vapour deposition (CVD), molecular beam epitaxy (MBE), metalorganic vapour chemical deposition (MOVCD), organometallic vapour phase epitaxy (OMVPE) etc [17-23]. It has previously been reported that 1-D ME (M=Cd; E=Se) nanocrystals can be synthesized utilizing ethylene diamine (EDA) as both a solvent & a template [24]. EDA served as simultaneously a solvent along with a pattern in research work. In this article, we describe a one-step, straightforward, easy, and environmentally benign solvo-thermal method for creating CdSe nano-flower. It is a distinctive hierarchical structure among many morphologies, with a large surface area, several crystalline facets, and the potential for improved light-matter correlations. To the ~~greatest~~ extent of our understanding, there are still relatively few reports on the development of a CdSe nanoflower-like arrangement. In this research, we concentrate on the architectural conversion of CdSe nano-flowers toward nanoparticles with a simple change in component content at low temperature. In the strong and intermediate-confinement regimes, the electronic bandgap widen as the particle radius decreases, producing a characteristic blue shift of the first excitonic absorption peak and the photoluminescence (PL) maximum. The blue shift observed in cadmium selenide (CdSe) nanocomposites mainly arises due to smaller CdSe nanocrystals within the composite absorb photons of shorter wavelengths.Thus, as particle size decreases, a clear ble shift in absorption and photoluminescence is observed. The creation of unique CdSe Nano-flowers & various subsequent conversion into nanomaterials are the main topics of this work, with special attention paid to the altering behaviour seen in their photoluminescence wavelengths. We hope to learn more about how optical characteristics change during developmental transitions by examining these spectral changes.

This knowledge is essential for customizing CdSe-based nanoparticles for certain optoelectronic uses.

2. Research Methodology

2.1. Materials for synthesis

The following materials were used as received commercially without further purification: cadmium acetate [Cd $(CH3COO)_2.2H_2O$], ethylene diamine (EDA) and Seleim powder purchased from Sigma Aldrich. Sodium Hydroxide pellets (NaOH), HCl (35% pure), ethanol was all purchased from Merck. Silica gel was purchased from Mereck.

2.2. Preparation of CdSe nanostructure

All the ingredients were suitable for analysis and didn't require any additional purification. For this procedure, 40 millilitres of EDA were added to a glass beaker containing 1.366 grams of cadmium acetate [$Cd(CH_3COO)_2.2H_2O$], and the entire mixture was swirled for 10 minutes at the ambient temperature. For 5 minutes at room temperature, 0.20 grams of selenium (Se) powder was added and vigorously mixed. The solution was then placed inside a stainless-steel autoclave lined with Teflon. After an hour of being kept at 160°C on average, the temperature of the incubator was reduced naturally to ambient temperature. After collecting and filtering the ensuing very dark brown precipitation, it was repeatedly cleaned with milli Q water and 100% ethanol. Ultimately, the item was allowed to air dry for 3 hours approximately 60°C to produce the outcome (CdSe1). Then, while maintaining the same other parameters, we altered solely the intrinsic selenium content to produce nanostructures with varying morphologies and dimensions. By increasing the percentage of selenium, we also prepared two other nanoflower that are CdSe2 and CdSe3. In this synthesis process 1.366 gm of cadmium acetate [$Cd(CH_3COO)_2.2H_2O$] was mixed with 0.20 gm of selenium (Se) powder to obtain the prepared product (CdSe1). For the preparation of CdSe2, 1.366 gm of cadmium acetate [$Cd(CH_3COO)_2.2H_2O$] was mixed with 0.40 gm of selenium (Se) powder. 1.366 gm of cadmium acetate [$Cd(CH_3COO)_2.2H_2O$] was mixed with 0.60 gm of selenium (Se) powder to obtain the prepared CdSe3 nanocomposites.

Only we have changed the amount of selenium to obtain the nanostructures of different morphology. For the preparation of CdSe1, the molar ratio of cadmium acetate and selenium powder is 1:0.5 whereas for the preparation of CdSe2and CdSe3 the ratio are 1:1 and 1:2, respectively. The process of reaction formation of nanoflower is given in below.

$$Cd^{2+} + 2IPA \leftrightarrow [Cd\,(IPA)_2]^{2+} \quad (1)$$

$$2\,Se + N_2H_4 + 4\,OH^- \rightarrow 2\,Se^{2-} + N_2\uparrow + 4\,H_2O \quad (2)$$

$$[Cd\,(IPA)_2]^{2+} + Se^{2-} \rightarrow CdSe\downarrow + IPA \quad (3)$$

$$Cd^{2+} + Se^{2-} \rightarrow CdSe\downarrow \quad (4)$$

3. Characterisation

Using scanning electron microscopy (SEM), the morphology of those objects was determined. The EVO, LS10, ZEISS, 2013 was used to capture the SEM images. Apex Instruments Co.'s computerized programmable sin coater was used to perform the SEM measurements on the substrate made of glass covered with the necessary materials. As-synthesized nanoflower were identified by an X'Pert PRO PAN analytical X-ray diffractometer (XRD) at 30 kV of applied voltage and 20 mA of

current to identify the resultant phase and crystal structure of the calcined powder. Miniflex 600 undergoes XRD examination. The electronic absorption wavelengths of the resulting substances were recorded at ambient temperature using a UV-vis scanned spectrophotometer. Photoluminescence spectra were carried out on a LS55, Fluorescence spectrometer, PerkinElmer using excitation source of 400 nm line of a He-Cd laser.

4. Result and Discussions

4.1 Morphology

Nanoflowers are a fascinating class of nanostructures with flower-like morphologies, usually synthesized from metals, metal oxides, semiconductors, or composites. As observed in figure 1(a-c), the shape of the CdSe nanoparticles is readily visible through both extreme and low-resolution SEM pictures. The Synthesized CdSe1nanocomposite illustrates the flower-like pattern. The nano-flower is roughly 10 µm in size. The result CdSe2 is revealed as a nanoparticle when the identical procedure is repeated with only the quantity of selenium powder altered. The size of the aggregated nanoparticles varies between 800 nm to 1 µm. We produced nanoparticles having an average size of 200 nm through increasing the elements selenium content. Figure 2(a-c) displays the EDX pattern for all three nanocomposites. The quantity of selenium and cadmium present in the corresponding CdSe nanoparticles is clearly seen in figure 2, which also shows that the proportion of selenium has risen from CdSe1 to CdSe3 during the steps we arrived at the processing. No other impurities were detected in the mixture. Synthesized nanoflowers crystalline structure was determined by XRD diffraction pattern. Figure 3 shows the XRD behaviour of three nanoparticles. All the peak patterns in diffraction that correspond to the zinc blende and wurtzite stages of CdSe are demonstrated to be connected to the produced CdSe nanostructured substances according to JCPDS file no 19-191.According to previously published observations [25], the XRD behaviours of CdSe nanorods clearly identify the distinctive zinc blende planes of (111),(220) and (311) positioned at 25.38°, 42.6° and 49.7° respectively. It's intriguing which the X-ray diffraction also shows that the CdSe nanoparticles as manufactured have a wurtzite plane [25]. Using the Debye–Scherrer equation

$$d=0.9*\lambda/\beta \cos\theta$$

where d denotes the breadth of the nanorods, λ represents the wavelength of the CuKα radiation (λ = 1.5418 Å), β is the full width at half maximum (FWHM) of the XRD peaks, and θ is the diffraction angle corresponding to the peaks, we estimated the average breadth of the nanorods. The calculated values for the as-synthesized CdSe1 nanoflower are 40.25 nm, for CdSe2 are 35.85 nm and 26.57 nm for CdSe3

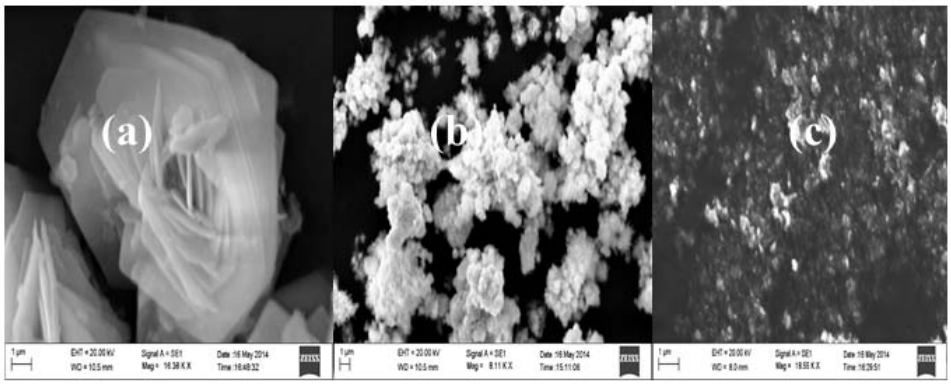

Figure 1: SEM for (a) CdSe1, (b) CdSe2 and (c) CdSe3

4.2. Optical Properties

4.2.1. UV-absorption spectroscopy

In semiconductor substances, the dimension and form of the particles determine their optical characteristics. Figure 4 displays the ambient temperature ultraviolet-visible spectrum of the CdSe compounds as they were created. The CdSe nanocomposites have an absorption edge of roughly 700 nm and an energy of roughly 2.5 ev. The properties of excitonic absorption lack sharpness. CdSe is predicted to exhibit an absorption peak at 716 nm. There is a slight shift towards smaller wavelengths in the UV-Vis spectra of the produced CdSe solutions. The blue shift is observed when the selenium concentration rises, which could be interpreted as a size-related characteristic of CdSe nanostructures. Their unique morphologies influence7 light absorption, scattering, and electronic properties**.**

The relationship shown below are used for assessing the Optical band gap for semiconductors [27-28]:

$$\alpha h\nu = A(h\nu - E_g)^n / h\nu \quad (1)$$

As previously reported [27], the assumed E_g values fall between 1.6 ev to 2.3 ev, where Ais a constantcorresponding with the effective massconnected with the bands and n is a constant, with n with value 1/2for direct band gap, 2 for indirect bang gap materials. The following relation is used to compute α, as shown below [28]:

$$\alpha = 1/t * \ln(1/(1-A)) \quad (2)$$

We obtain the band gap of all CdSe nanostructures products by extrapolating the linear portion of the plot $(\alpha h\nu)^2$ versus $(h\nu)$ as shown in fig. 5. Band gap is changing from 2.96 to 1.93 eV depending on different geometric configurations of CdSe nanoparticles. As the particle size decreases, the motion of electrons and hole becomes spatially confined. This confinement leads to quantization of energy instead

of continuous bands. Because of this, the lowest energy transition from the valance band to the conduction band requires more energy. This means the effective band gap increases as the size of the particle decreases.

4.2.2. Photoluminescence Spectroscopy

The photoluminescence spectra of the as prepared CdSe nano-flowers and nanoparticles, recorded at room temperature for the excitation wavelength 400 nm is shown in Fig. 6. In this study, the photoluminescence spectrum in the 400 to 700 nm spectral range was used to examine the emission properties of the previously prepared CdSe materials. All three of these composites exhibit a slight redshift and a minor peak at about 520 nm when we utilize the wavelength of stimulation of 400 nm to obtain the photoluminescence patterns. Additionally, for each of the three CdSe products, a distinct peak is seen at various locations. CdSe1 exhibits a prominent peak at 625 nm, CdSe2 at approximately 604 nm, and CdSe3it is 588 nm. The electric field variation, which is fundamentally related to the inter-particle association potential, is observed as 1.4 ev. Because of its strong surface interaction with the low-dimensional elements, CdSe3 has a greater ability to reduce the structure's length. As the dimension of the nanoparticles diminishes in this the peak becomes blue shifted. As we have previously discovered from band gap observations of such CdSe nanostructures, the change inenergy sufficiently significant to cause a notable phase shift.

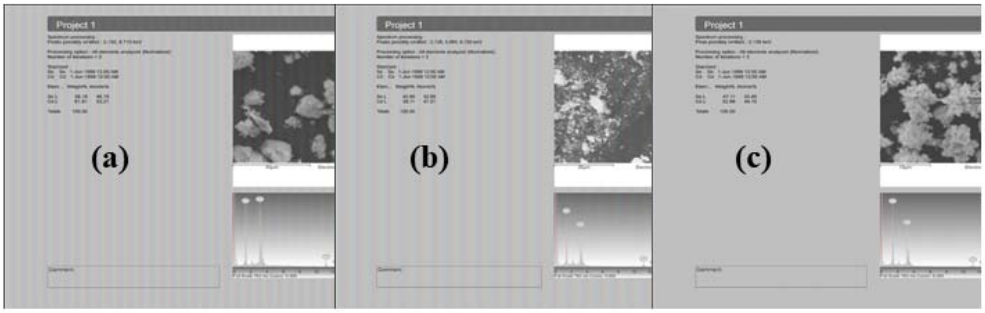

Figure 2: EDX for (a) CdSe1, (b) CdSe2 and (c) CdSe3

The broadness of the dominant peak observed in CdSe PL spectra is about comparable, but it has a slight rise at its upper shoulder. This is unmistakably suggesting that a doublet may emerge because it is appropriate for electrostatic interaction. In photoluminescence spectra the formation of doublet can occur due to several physical or electronic reasons depending on the material system. For cadmium selenium nanostructures semiconductor, exitons can form from heavy –hole and light –hole valance bands. These two types of exitons have slightly different energies, resulting in two distinct emissions peaks-hence a doublet in the PL spectrum. In

nanostructures, slight size differences between particles can shift the emission energy . If two dominant sizes are present, their emissions can appear as a doublet. Increasing selenium concentration during synthesis of CdSe nanoparticles enhances nucleation, yielding smaller particles and thus stronger quantum confinement, which manifests as a blue shift in absorption and emission spectra.

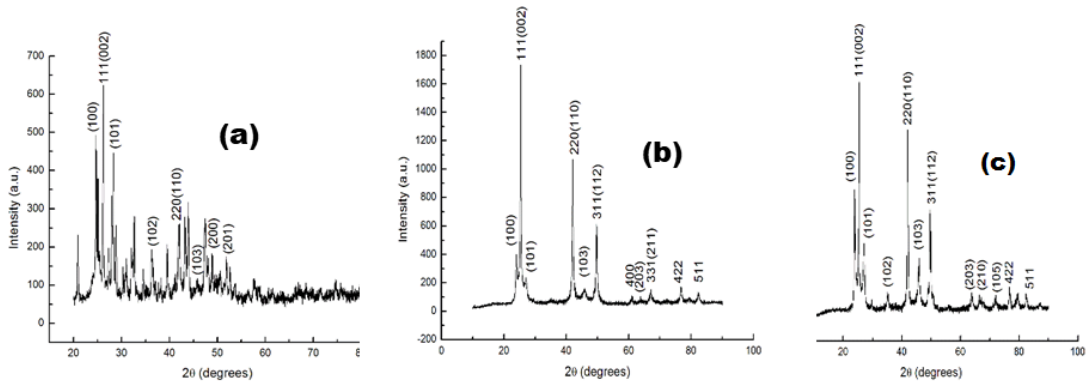

Figure 3: XRD for (a) CdSe1, (b) CdSe2 and (c) CdSe3

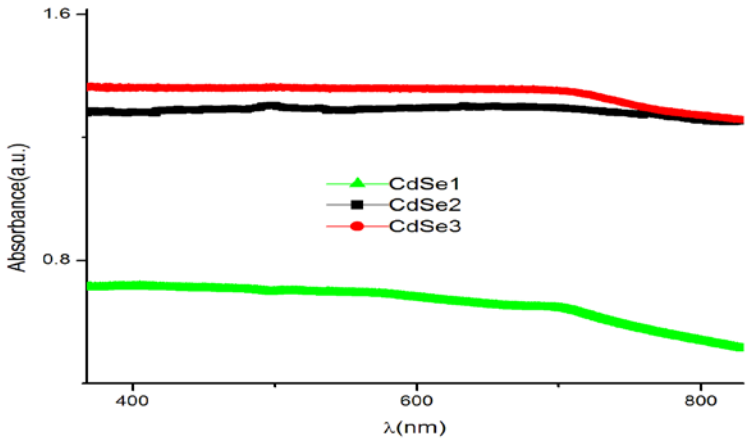

Figure 4: UV–vis absorbance spectra of CdSe1 CdSe2 and CdSe3 nanocomposites.

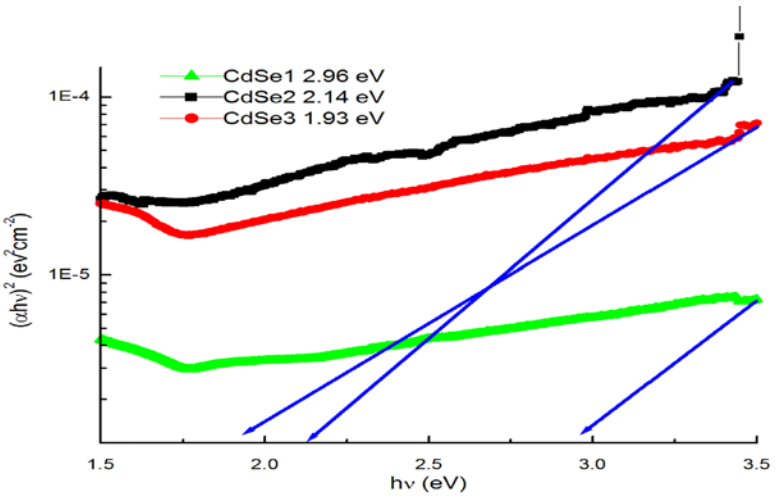

Figure 5: UV–vis absorbance spectra of CdSe1 CdSe2 and CdSe3 nanocomposites.

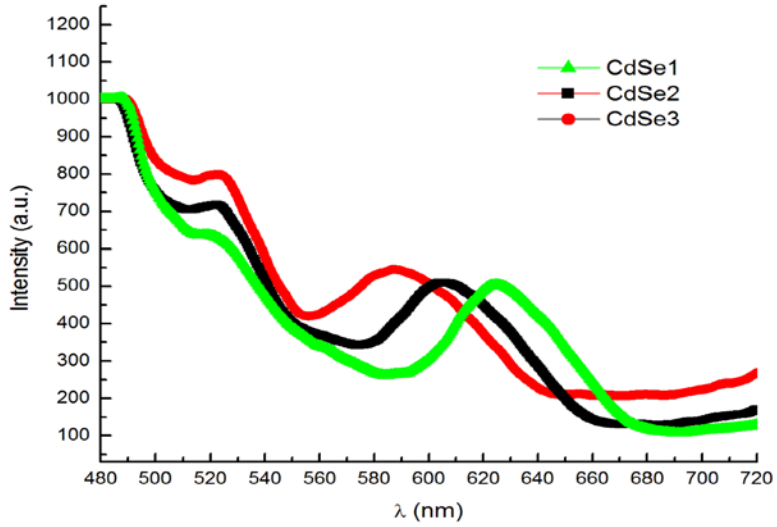

Figure 6: Photoluminescence spectra of CdSe1 CdSe2 and CdSe3 nanocomposites.

5. Conclusion

In conclusion, the study describe the production process of CdSe nanoflower and demonstrate how it may be converted into nanoparticles by merely altering the quantity of selenium powder while maintaining the same other reaction parameters. The photoluminescence (PL) maximise blue shifts during this synthesis

process because the nanostructures' sizes drastically decrease and their compositions suddenly alter. Additionally, by altering the size and configuration of the CdSe nanostructural material as they are created, we may adjust the bandgap power. Significant spectral variations associated with morphological and structural changes are revealed by analysing the photoluminescence patterns newly synthesized CdSe nanoflower and their converted nanoparticles. The blue shifts observed in the PL spectra are closely correlated with the particle size, surface states, and quantum confinement effects resulting from the transformation process.

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