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Room temperature synthesis, structural and optical properties of CdSe nanoparticles

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Abstract: Nanoparticles of CdSe nanoparticles have been synthesized in aqueous solution by reacting cadmium chloride ($CdCl_2.2.5H_2O$) and sodium hydrogen selenide (NaHSe) in presence of capping agent 3-mercaptopropionic acid (MPA). They are irradiated with a 2 MeV electron beam at a dose of 100, 200 and 300kGy. The effect of electron beam irradiation at different doses on the structural and optical properties of the prepared CdSe QDs is studied at different concentrations. Both the irradiated and unirradiated CdSe quantum dots have been characterized by XRD, TEM, EDX, UV-Vis spectroscopy, and photoluminescence spectro scopy. The XRD measurements of the functionalized CdSe quantum dots showed that these quantum dots have a cubic phase with zinc blend structure. The TEM measurements depicted that these quantum dots are mono-dispersed with spherical shape size about 5 nm. The EDX measurements indicated that the prepared quantum dots are highly pure and there are no impurities in the structures. The obtained CdSe NPs exhibit a relatively narrow PL band, as well as a high PL peak in the yellow spectral range. The irradiated CdSe@MPA QDs exhibit high photochemical stability and hold a good potential to be applied in optoelectronic devices.
Keywords: CdSe; 3-mercaptopropionic acid; TEM; Optical properties.

Introduction and Experimental:

Radiation-induced synthesis of metallic and semiconductor nanomaterials has been an extensively used method for its simplicity and effectiveness. In this process, the synthesis in the aqueous media mainly precedes through the reaction of the solvated electrons with the precursor ions. Semiconductor and metallic nanomaterials of different shapes and sizes have been synthesized earlier via radiation chemical routes in aqueous and non-aqueous media using different templates [1–4]. The templates usually determine the shapes and sizes of nanomaterials. Among other semiconductors, CdSe is an important one because of its potential applications in photovoltaic, LEDs and other optoelectronic devices. Several groups including us have reported the radiation-inducoed synthesis of CdSe nanoparticles in different condensed phases [5]. The yield of CdSe nanparticles depends on the absorbed dose and the concentration of the precursor ions.

In this paper, we report a simple one-step method for synthesizing CdSe NCs at room temperature by irradiation of a $CdCl_2$+ mercaptopropionic acid (MPA) aqueous solution with a 2MeV electron beam. In the synthetic process we adopted in this study, the morphology of the NCs that were formed varied dramatically

with the $CdCl_2$ concentration in the solution from a single phase composed of QDs to a mixed phase of QDs and nanorods (NRs).

The synthetic procedure to fabricate CdSe NC adopted in this paper is as follows. In a typical procedure, 0.1368 g of $CdCl_2.2.5H_2O$ (0.6 mmol) was dissolved in 50 mL deionized water in a 3-neck flask, followed by the addition of 3-MPA (0.1 mL/100 µl). The pH of the mixture was adjusted to a value of 10–11 by using 1.0 mol/L NaOH solution. The mixture was then purged with N_2 for 30 min. 20 mL of NaHSe solution (0.02 M) freshly prepared by the reaction of selenium (0.4 mmol/0.0316 g) with NaBH4(0.0302 g) was injected into the mixture solution. The molar ratio of Cd/MPA/Se was 1.5:2:1. The solution was further stirred for 60 min and a clear yellow CdSe solution was obtained. The electron beam apparatus used was the ELV8 (EB-tech, Daejon, Korea). The samples were taken in micro tubes and exposed to 8 MeV electrons at a distance of 30 cm from the beam exit port. Electron doses used were ranging from 100-300kGy. All the optical measurements were carried out within 48 h of electron beam irradiation. We illuminated the samples with a focused beam from a Philips 7072 halogen lamp to measure the absorption spectra in the wavelength range 300–800 nm. The radiation from a He–Cd laser (325 nm) was used as a pump beam for the PL measurements. An XRD pattern was collected using a Phillips X'pert MPD 3040 X-ray diffractometer with graphite monochromatized Cu Kα radiation. HRTEM study was conducted in a JEOL JEM 2100F operating at 200 kV.

Results and Discussion:

In a present work we have observed important modifications on the surface quality and optical properties of the CdSe radiated surfaces depending on the irradiation conditions. In order to understand the underlying physical phenomena, we have selected those conditions leading to the most important changes in the sample surface. Fig. 1 shows the XRD pattern of the CdSe nanoparticles.

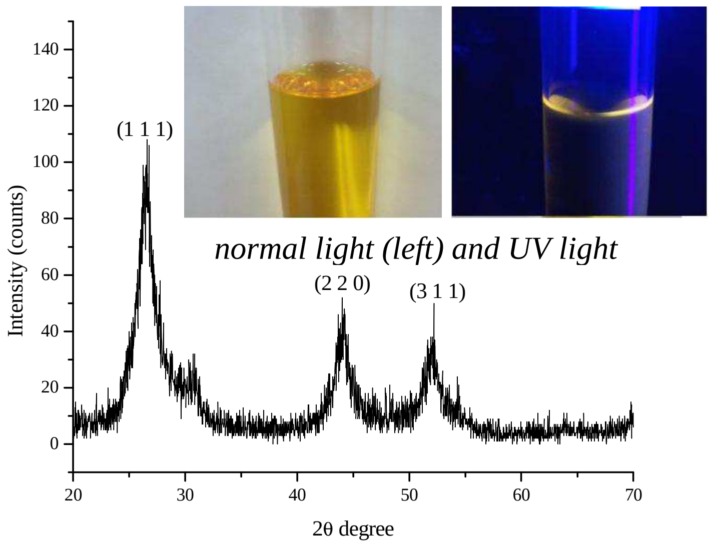

Fig.1. X-ray diffraction pattern of CdSe

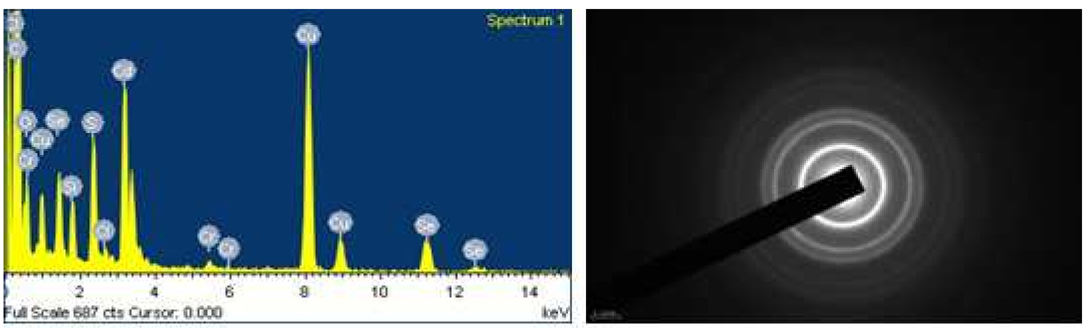

Fig.2. EDAX and SEAD spectrum of the irradiated CdSe nanoparticles at 300 k Gy.

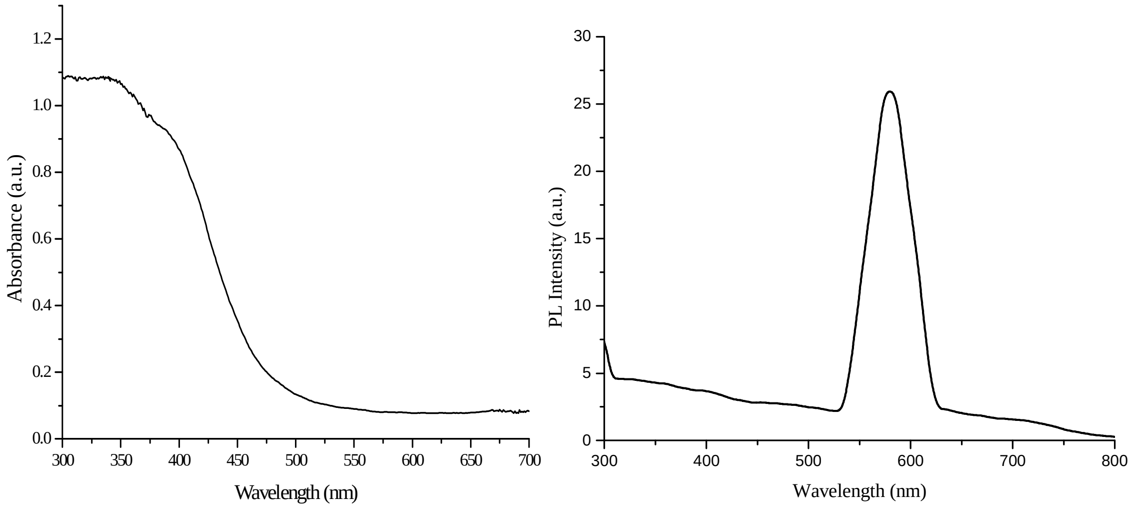

Fig.3. UV/Vis absorption and spectrum of the irradiated CdSe nanoparticles at 300 k *Gy*.

The diffraction peaks at 2θ are ca. 26.53, 43.86, and 51.77° can be readily assigned to (1 1 1), (2 2 0) and (3 1 1) planes, respectively. The broadening diffraction peaks of the XRD spectra indicate that the particles are in the quantum confinement regime. Using the full width at half maximum (FWHM) of the first main XRD peak and Debye–Scherrer's formula [6], the average particle size is estimated to be about 5 nm. The morphology and size of the CdS nanoparticles were observed adopting TEM. It was found that the nanoparticles were of uniform size, at about 5 nm. The EDAX revealed the presence of both Cd and Se in the nanoparticles synthesized (Fig. 2). The absorbance against wavelength curve (Fig. 3 left) reveals a nonlinear phenomenon and a decaying absorbance [7,8] with wavelength with edge at around 320 nm. The absorbance peak is blue shifted with respect to that of bulk (by 0.5 eV). In our work, the PL study of the prepared CdSe QD shows that CdSe QDs possess an emission peak at around 580 nm when excited with the optical source of around 520 nm as shown in Fig. 3 (right). The possible reason behind the luminescence of CdSe QD is the existence of surface-trapped electrons and holes created in CdSe specimen because of quantum confinement [9,10].

Conclusions:

In summary, we developed a novel route to synthesize CdSe NCs via electron beam irradiation of a $CdCl_2$.2.5+MPA aqueous solution with NaHSe as Se precursors. The ion beam bombardment used in this work makes use of low energy ions, thus, avoiding the formation of other defects, leading to a cleaning process and high quality surfaces. These results suggest that low energy bombardment process can be applied in the preparation of CdSe surfaces for improved CdSe-based devices.

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