



## Synthesis and optical studies of CdTe/CdSe core/shell nanostructure

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### Abstract

Highly luminescent GSH capped CdTe quantum dots (GSH-CdTe QDs) were prepared through a facile microwave (MW) aided wet chemical method. The GSH capped QDs were water soluble and bio-compatible. An effective shell-coating route was developed for the preparation of CdTe/CdSe core/shell (C/S) nanostructure by selecting green capping reagents and by adopting a low temperature shell deposition protocol. The as synthesized GSH-CdTe/CdSe C/S QDs were characterized by SEM and XRD studies. The Photoluminescence (PL) emission spectrum was employed to study the confinement of excitons within the CdTe/CdSe interface. Sharp visible photoluminescence emission peaks was observed in the visible region at 690 nm for CdTe/CdSe C/S QDs, attributed to the quantum confinement and effective capping of unsaturated bonds by GSH.

**Keywords:** Quantum dots; Capping; UV-vis; Core-shell; Photoluminescence (PL).

### 1. Introduction

Semiconducting nanocrystals such as QDs have attracted more attention due to their unique optical properties and many potential applications including nanolasers, biolabelings, and photovoltaics, etc. [1-2]. They possess unique optical properties such as narrow emission spectra, continuous absorption band, high stability against chemical and photo bleaching, and surface functionality. To date, QDs have various nanostructured configurations have been reported. Typically in C/S heterostructure QDs two different semiconductors are incorporated into single colloidal QDs [3]. There are type I and type II C/S QDs with different carrier localizations, depending on the band structure offsets between the semiconducting core and the shell [4]. Recently, the high-quality CdTe/CdSe hetero-structure QDs have been successfully synthesized by us, via microwave-assisted colloidal chemical routes [5-7]. Microwave-assisted synthesis has been proposed as one of the most effective method used for the synthesis of nanocrystals due to the advantages like reaction selectivity and high efficiency for obtaining the controllable products [8-10]. Further, the present study also investigates the possible tuning of the emission wavelengths of the obtained C/S nanocrystals into the visible spectrum.

### 2. Experimental

Present study describes a simple protocol for aqueous synthesis of CdTe/CdSe C/S, using CdCl<sub>2</sub>, K<sub>2</sub>TeO<sub>3</sub>, Na<sub>2</sub>SeO<sub>3</sub>, as Cd<sup>2+</sup>, Te<sup>2-</sup> and Se<sup>2-</sup> sources respectively, along with NaBH<sub>4</sub> as the reducing agent. The biological thiol and a tri-peptide GSH used here works both as a reducing and capping agent for the

aqueous synthesis of CdTe QDs, found in abundance in cells and are suitable for the stabilization of CdSe and CdTe QDs [11-13]. Moreover, all the operations could be performed in air, avoiding the need for inert atmosphere, due to the fact that K<sub>2</sub>TeO<sub>3</sub> is air stable [14-19].

#### 2.1. Synthesis of CdTe Core QDs

182 mg CdCl<sub>2</sub>.2.5H<sub>2</sub>O was diluted with 40 ml of Toluene, 240 mg GSH, 10 mg Sodium citrate, 2ml of K<sub>2</sub>TeO<sub>3</sub> and 20 mg of NaBH<sub>4</sub> were added into cadmium sol with constant stirring. Borax buffer solution was used to adjust the pH~10. The mixture was kept in ultra-sonicator for vigorous stirring. The as obtained mixture was kept in a MW oven for 1 min at 300W power. The mixture was cooled down to ~50°C. The as prepared CdTe solution was concentrated to ¼<sup>th</sup> of the original volume and was finally precipitated using 2-propanol and collected via centrifugation. CdTe QDs dispersion was prepared by re-dissolving this colloid precipitate in 3ml DD water.

The stock solution for CdSe shell growth was prepared by dissolving corresponding precursor solutions in borax buffer solution in appropriate amounts to ensure the growth of one mono layer of the shell.

A modified MW technique was adopted for the growth of CdTe/CdSe C/S nanocrystal, but at a much low temperature (70-80°C). The obtained CdTe dispersion was transferred drop wise into the CdSe stock solution and was kept in a MW oven for 5 min at 300W power. The mixture was cooled down to ~50°C, concentrated to ¼<sup>th</sup> of the original volume, was precipitated using 2-propanol and collected via centrifugation. The so

obtained CdTe/CdSe C/S QDs were re-dissolved in 3ml DD water to prepare C/S dispersion.

### 3. Result and Discussion

The core shell QDs are successfully synthesized using a green and cost effective MW assisted wet chemical method. MW assisted methods are fast and considered greener as compared to the conventional heating methods. Here too the whole process took just 5 to 10 minute under ambient conditions to synthesize C/S QDs with superior quality.

#### 3.1. SEM and XRD studies

Fig.1 (a) shows the SEM micrograph of the as prepared C/S QDs, obtained using SEM- JEOL JSM-5600. C/S QDs with a high yield and uniform size distribution can be observed in the micrographs. The MW assisted method ensure high yield due to availability of numerous nucleation sites produced simultaneously due to fast heating mechanism [20]. The water molecule vibration due to MW heating distributes the heat uniformly throughout the reaction bath, which may lead to a uniform particle size obtained in this case [21].

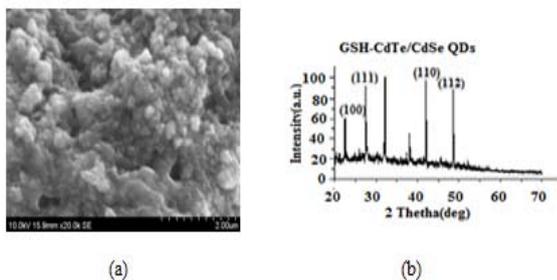


Fig.1: (a) SEM micrographs of CdTe/CdSe C/S QDs (b) XRD pattern of GSH-CdTe/CdSe C/S QDs

The XRD pattern of GSH-CdTe/CdSe C/S QDs is shown in Fig.1(b) obtained using XRD-Bruker/LynxEye1D-PSD. The XRD pattern of CdTe core consists of the characteristic peaks of cubic zinc blende CdTe. The diffraction peaks are broadened due to the finite particle size. When the CdSe shell is overgrown around the cubic CdTe template, the general pattern of the cubic lattice is maintained in the C/S structures, but the diffraction peaks shift to larger angles consistent with the smaller lattice constant for CdSe compared with CdTe. In addition, the diffraction peaks narrow further with the over coating of shell materials. This narrowing indicates that the crystalline domain is larger for the C/S structure, providing direct

evidence for epitaxial growth of the shell. The peaks obtained in the XRD studies matched with the standard data for CdTe (JCPDS card no.65-1046) and CdSe (JCPDS card no.00-019-0191). The XRD results confirm the formation of C/S structures. However since this study includes the samples with only one monolayer of CdSe for C/S structures, some peaks corresponding to the base materials also appear in the XRD pattern.

#### 3.2 PL studies

The PL spectra of the as obtained QDs is shown in Fig.2 obtained using PL- LS 45 Perkin Elmer Luminescence Spectrophotometer A very strong emission at ~ 685nm is observed for a monolayer of the shell structure in Fig.2(a). And also at 700 nm and 715 nm are observed for 2 ML and 3ML of Core/Shell QDs. Fig. 2(b) shows the peak shift with the 2 and 3 ML growth of CdSe shell over CdTe core, attributed to the bigger particle size of these QDs. We obtained PL spectra of CdTe/CdSe with Red Shift in peaks due to 2 and 3 ML of CdSe Shell. The PL emission of CdTe/CdSe C/S QDs should be attributed to an excitonic transition involving the relaxed electron (mainly localized in the conduction band of the CdSe shell) and hole states (mainly localized at the valence band of the CdTe core), which is illustrated in Fig.2.

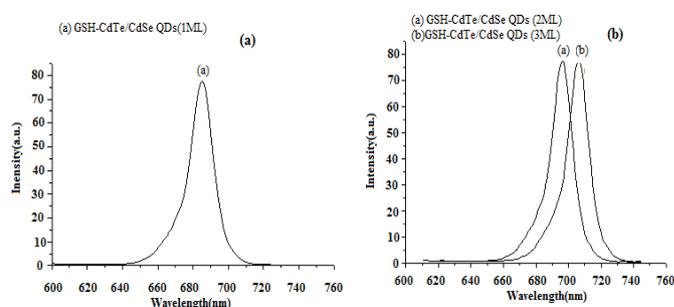


Fig. 2: (a) PL spectra of GSH-CdTe/ CdSe C/S structures. (b) Peak shift in the PL spectra with the two and three ML of CdSe shell layer.

It has been proven that surface passivation of nanocrystals with suitable an inorganic material with a high bandgap is the key to improving PL efficiency and the stability of nanocrystals [22]. When one ML of CdSe is grown around the CdTe cores, the optical properties of the resulting CdTe/CdSe C/S QDs behave more like a type-I structure. The radiative recombination is quenched because of the presence of some imperfections like traps on the crystal. These traps are Cd or Te atoms with dangling bonds, which can attract electron and holes, respectively, acting as



mid gap states. In the case of an electron, when declining from the conduction band it can be captured by a trap and then relax to the valence band without emitting.

#### 4. Conclusions

This study presents a quick and cost effective method of synthesis of highly luminescent QDs with C/S structures. The GSH capped biocompatible and stable QDs are obtained without compromising their optical properties. The optical properties of the QDs were tuned within a given visible range by varying the thickness of the shell layer.

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