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Capping Ligand Influence on the Structural, Optical and Luminescence Properties of CdTe Nanoparticles Prepared by a Simple Wet Chemical Process

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Abstract:

The nature of the capping ligands used and the strength of their interactions with the surface atoms of the nanoparticles (NPs) impact greatly on the material properties and the stability of the resulting NPs. The structural analysis revealed that all the as-prepared CdTe NPs samples had a zinc blende crystal structure of different phases. The glutathione and L-cysteine capped CdTe NPs had the same zinc blende phase (JCPDS no. 75-2086) while thioglycolic acid capped and co-capped CdTe NPs possessed another zinc blende phase (JCPDS no. 75-2083). The calculated crystallite sizes were in the range 2-26 nm for all the samples. The optical spectroscopy studies showed various properties when different capping ligands were used. The band gap energies for all the as-prepared CdTe NPs confirmed the results obtained from the X-ray diffraction. The band gap energies were in the range of 2.39-3.34 eV for all the as-prepared CdTe NPs.

1. Introduction

The unique nanomaterial properties have attracted the attention of numerous researchers into studying the optical and structural characterisation of the nanomaterials. These properties depend on the growth conditions leading to various synthetic approaches used to synthesize them. The

nanoparticles (NPs) are characterised by their superior properties which include resistance against photobleaching, long luminescence lifetimes, symmetric emission and narrow bands, high extinction coefficients, size-tunable emission spectra and quantum yields ^[1-3]. Specifically, the broad absorption bands of the NPs allow for a wide selection of possible excitation wavelengths from the visible to the near-infrared regions ^[4]. These features make NPs ideal choice for the versatile design of sensors and other numerous applications such as those used in clinical diagnostics ^[5-7] and photovoltaics ^[8, 9].

The superior characteristics of the NPs mentioned bring about many inherent advantages when compared to organic fluorophores. Major developments in cell biology, medical diagnostics and molecular biology have come as a result of the integration of nanotechnology and biotechnology in the science research ^[10, 11]. The surface coating material and the local environmental conditions, however, strongly affect the optical properties of the NPs under study.

The aqueous synthesis approach is used because of its numerous advantages for, instance, low-cost equipment required and production of water-soluble NPs obtained from the technique. Cadmium telluride (CdTe) is one of the semiconductors synthesized through the aqueous route using both organic and water-soluble stabilizer molecules. Rogach and co-workers synthesized water-soluble CdTe NPs using Thioglycerol (TGA) and mercaptoethanol as the stabilizers ^[12]. Various other groups have tried to use a variety of thiol-based stabilizers to cap the surface of the CdTe NPs ^[13, 14]. Weller et al. studied the impact of various thiol ligands such as the mercapto amines, mercapto acids and mercapto alcohols on the material properties of the as-prepared CdTe NPs in the aqueous phase ^[15].

From previous studies carried out on CdTe NPs, it has been realised that the nature of the capping layer surrounding the NPs (which prevents their coagulation) strongly affect their luminescent properties ^[16]. For example, CdSe NPs which were synthesized through the classic organometallic route after several “greener” changes done were found to be covered with organic ligands containing bulky (C8- C18) alkyl groups ^[17-23]. This is a disadvantage because NPs containing such hydrophobic capping ligands are not suitable for use in applications that require an effective charge transport or aqueous solubility properties. Otherwise, a surface ligand exchange reactions are performed to make them appropriate for the desired applications thus making the method tedious.

Moreover, most of the research conducted on II-VI semiconductor NPs prepared in aqueous phase displayed low quantum yields observed to be due to the surface traps and defects of NPs^[24]. These defects and traps could be attributed to the poor choice of the capping ligand nanocrystals^[25]. The thioglycolic acid (TGA), mercaptopropionic acid (MPA), L-cysteine (L-cyst) and glutathione (GSH) have been reported to be the appropriate ligand molecules to be used to grow CdTe NPs with good luminescent properties^[26, 27]. Effects of each ligand and combination of them on the material properties of the NPs under investigation need to be studied in detail in order to determine the best complexing agent required to cap or co-cap the surface of the NPs effectively. Furthermore, the ratio of the capping ligands to cadmium needs to be optimized as suggested by ref^[28-30]. Good choice of the stabilizer molecules to be used to cap the NPs results in the production of good quality NPs with enhanced crystal qualities like high quantum yields, narrow size distribution etc. For example, GSH does not only play a role in catalysis and metabolism but also acts as an antioxidant and an essential cofactor for antioxidant enzymes hence, therefore, GSH can be used to cap CdTe NPs for use in biological probes since they are more biocompatible compared to other thiol-capping ligands.

For NPs to be applied in medicine and biology, it is imperative to take into account the features that affect their optical and luminescent properties^[31]. Therefore, the capping ligands, being one of the factors to be considered, affect the stability of the NPs. This is because the nature and strength of the interaction between the capping ligands and the surface atoms of NPs determine their stability which affects their applications in various fields^[32-34]. Development of different passivation strategies has been on focus in the recent past on the ligand chemistry of the NPs^[35-37].

The simple wet chemical route (sol-gel) used to grow CdTe NPs was chosen due to the fact that it is economical, no use of sophisticated equipment, environmental friendly, easy to execute and more so it produces highly crystalline NPs which are water-soluble. The aim of this study is to study how well different capping ligands can passivate the surface of the CdTe NPs. TGA, GSH and L-Cyst were used in this study as a single capping agent or a combination of either of the two or all the three were employed to cap or co-cap the CdTe NPs. The structural and optical properties of the as-grown samples were investigated using various techniques in order to determine the best capping ligand or the best combination to co-cap the surface of the CdTe NPs.

The luminescence stability is greatly influenced by the type of capping ligand used especially if the NPs are to be used in bioimaging applications.

2. Results and discussion

2.1. XRD Analysis

X-ray diffractometer (XRD) was used to determine the crystal structure of the as-prepared CdTe NPs samples. CdTe NPs prepared using different capping ligands were analyzed and the XRD pattern is shown in Fig. 1. The CdTe NPs prepared using glutathione (GSH), L-cysteine (L-Cyst) and a combination of both GSH and L-Cyst (LG) matched very well with the zinc blende crystal structure which compared favourably with the standard JCPDS no. 75-2086. [111], [220] and [311] were the main observed diffraction planes with [200] plane observed for the samples prepared using L-Cyst and co-capping with GSH and L-Cyst (Fig. 1(i)). Broad diffraction peaks were observed for the samples capped with GSH and L-Cyst which are attributed to the infinitely small size of the particles obtained. On the other hand, the samples prepared using thioglycolic acid (TGA) and co-capping using TGA and any of the other capping ligand displayed a zinc blende crystal structure but of different phases from the GSH and L-cyst. This phase corresponded to the standard JCPDS card no. 75-2083 (Fig. 1(ii)). The extra diffraction peaks marked with asterisks (*) could be due to some unreacted precursors.

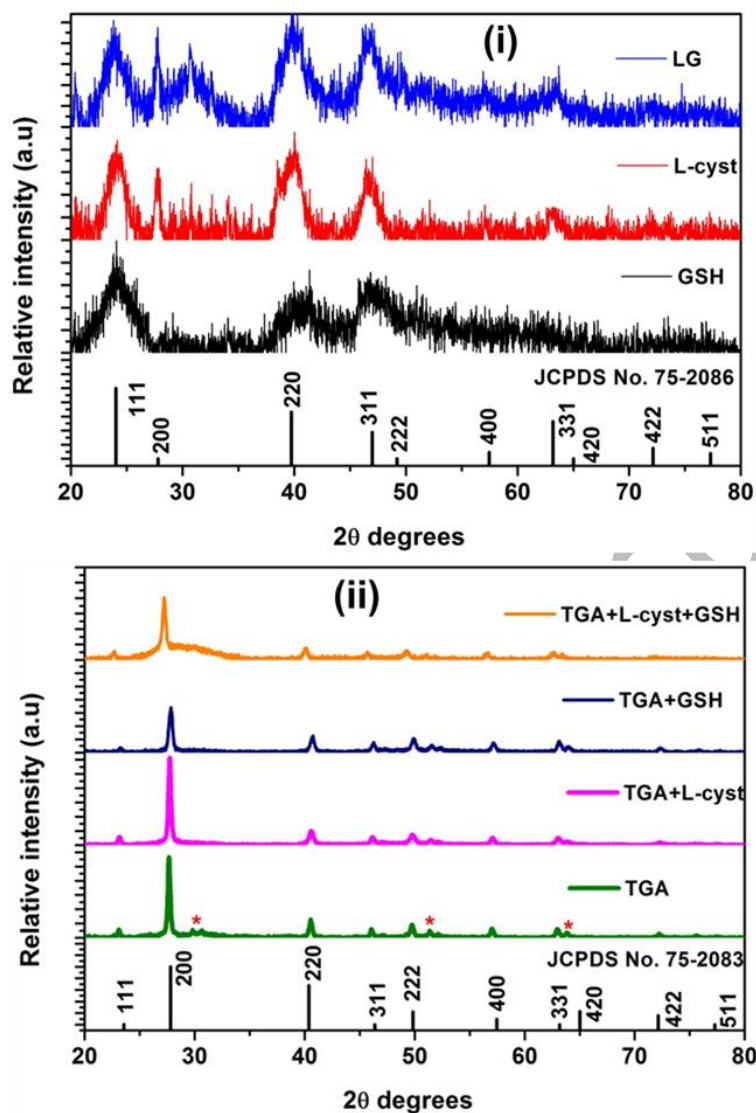


Figure 1: XRD patterns of CdTe NPs prepared using different capping ligands.

To confirm this further, the crystallite sizes were estimated using the common Debye-Scherrer equation^[38]; $S = \frac{K\lambda}{\beta \cos \theta}$ where S is the crystallite size, K is a constant equivalent to 0.9, λ is the wavelength of the X-ray radiation, β is full width at half maximum (FWHM) of the XRD peak and θ is the diffraction angle. Using the three prominent peaks, the crystallite sizes were estimated to be 2.5, 4.1 and 4.4 nm for GSH, L-Cyst and GSH+L-Cyst capped CdTe NPs respectively. Conversely, the CdTe NPs capped or co-capped with TGA had narrow diffraction peaks due to large crystallite sizes. The crystallite sizes were confirmed to be 26.7, 21.1, 20.8 and 20.9 nm for

TGA, TGA+L-Cyst, TGA+GSH and TGA+L-Cyst+ GSH capped and co-capped CdTe NPs, respectively. The smallest crystallite sizes were obtained when CdTe NPs were capped with GSH while TGA capped CdTe NPs appeared the largest in crystallite size. This was further confirmed by the scanning electron microscopy (SEM) measurement where TGA capped or co-capped CdTe NPs portrayed largest particle sizes compared to the GSH and L-Cyst capped or co-capped CdTe NPs. This shows that different capping ligands used in the precursor solution affect the growth mechanism and growth rate of the CdTe NPs being prepared.

2.2. SEM Analysis

Topographical and morphological analyses were conducted using scanning electron microscope. Fig. 2(a) shows representative SEM micrographs of CdTe NPs capped or co-capped with different capping ligands. Uniform and densely packed surface morphology were observed for all the as-prepared CdTe NPs samples. Small particle sizes were observed for GSH-capped CdTe NPs while the TGA-capped NPs displayed the largest particle sizes as shown in Fig. 2(a). All the as-prepared CdTe NPs exhibited spherical shapes with largest well-defined spheres observed for TGA-CdTe NPs. A mixture of small and large spheres were observed for CdTe NPs co-capped with GSH, TGA and L-Cyst. The observations made on the particle sizes in the XRD and SEM are slightly different in that the XRD gives the sizes in nanometer while the approximate values in SEM scale are in micrometer. This inconsistency could be due to the fact that during solvent evaporation, many small spherical particles might have associated with one another causing the resulting particles to be large and therefore the SEM images seen could be an ensemble of many small particles in the sample.

The composition analysis from Energy-dispersive X-ray spectroscopy (EDS) showed that the expected elements were present and impurities like oxygen were in trace level. Fig. 2(b) display representative EDS spectra of the as-grown CdTe NPs capped with different capping ligands. The elements like sodium and potassium are from the precursor materials. These materials did not affect the structural and optical properties of the CdTe NPs as could be observed in all the characterisation techniques used to analyse them. Sulphur observed in the EDS spectra shows the presence of the capping ligands in all the CdTe samples. The capping ligands used contain sulphur bonds that is why the sulphur element can be seen in the elemental composition.

GSH and L-Cyst were found to produce CdTe NPs with a fair weight percentages which are a mirror of the atomic composition.

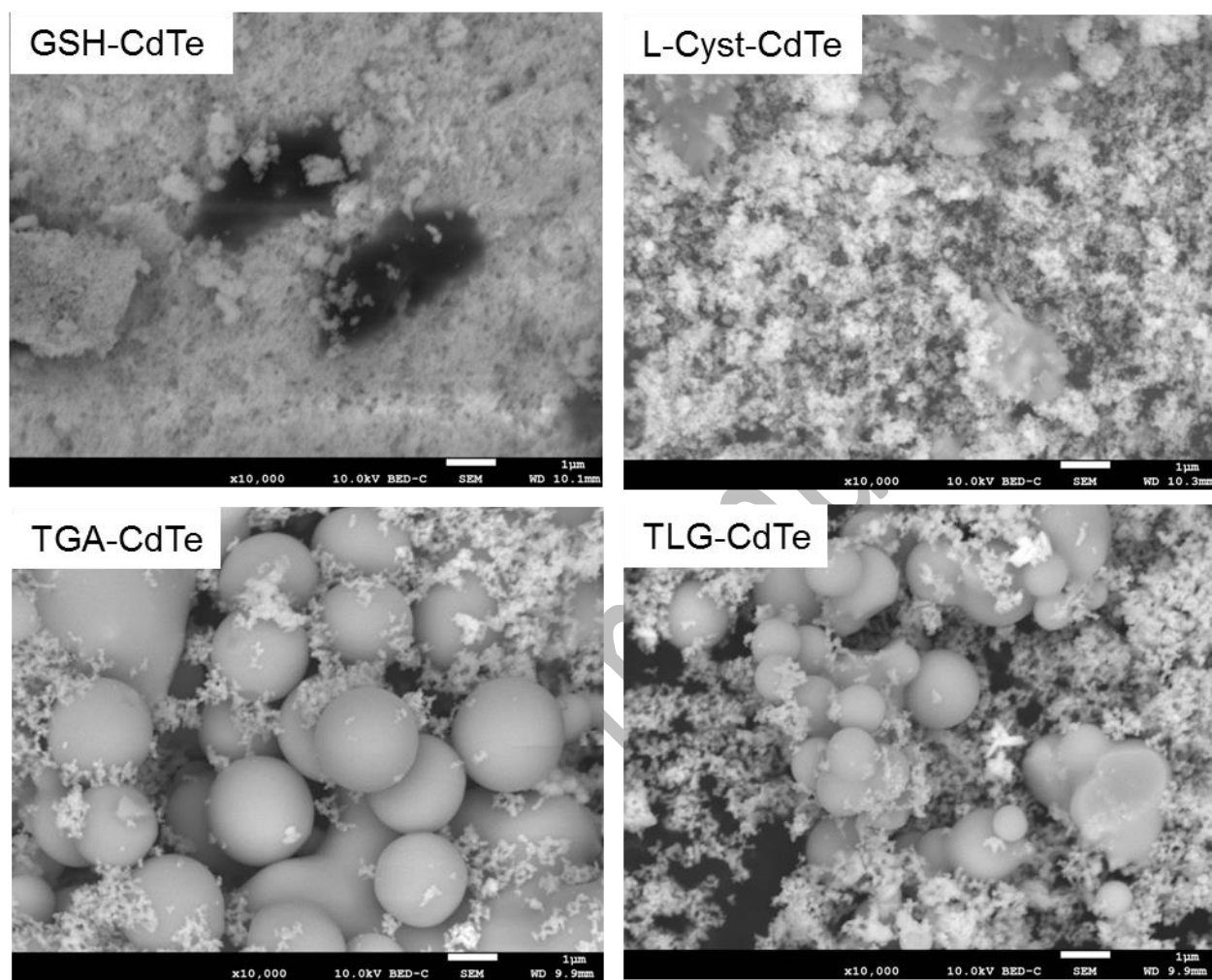


Figure 2(a): Representative SEM images of CdTe NPs capped with different capping ligands. TLG-CdTe NPs represent TGA+L-Cyst+GSH co-capped CdTe NPs.

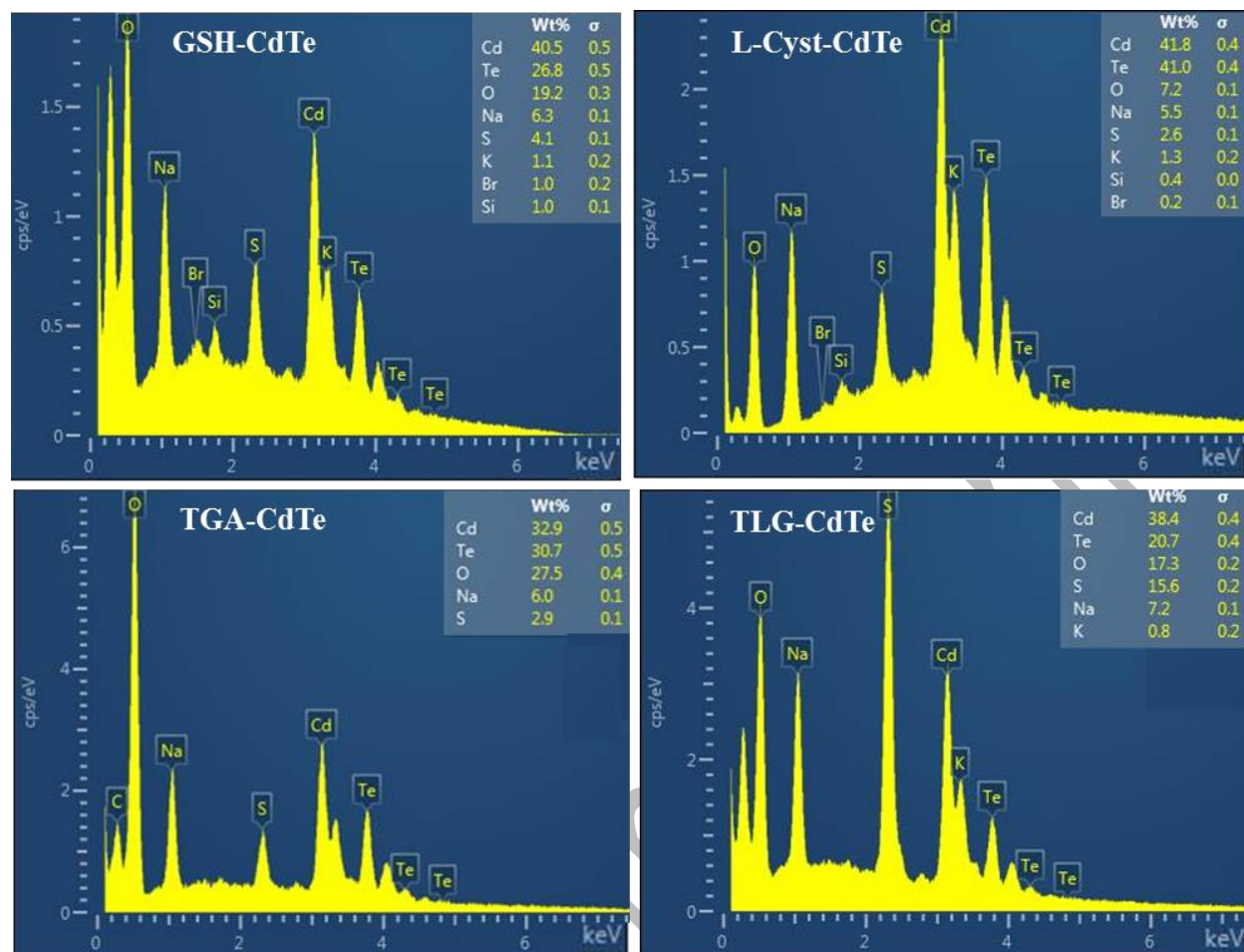


Figure 2(b): Representative EDS spectra of CdTe NPs capped with different capping ligands. TLG-CdTe NPs represent TGA+L-Cyst+GSH co-capped CdTe NPs.

2.3. Photoluminescence (PL) analysis

The coating of semiconductor NPs with capping ligands during preparation in aqueous media is of great importance especially when efforts are being put in trying to prevent the reduction of the PL relative intensity during the transfer from organic to aqueous phase and ligand exchange processes. The PL spectra of as-grown CdTe NPs taken at room temperature were measured using an optical spectrophotometer. Different excitation values give emission wavelengths of varied intensity ^[39]. The excitation wavelengths for all the CdTe NPs samples were set at 400 nm. This is the value that gave the most intense PL emission peak when compared to excitation wavelengths of 300, 350 and 450 nm for this study. Also, this is the value around which the CdTe NPs absorb light (as seen in the absorbance spectra Fig.5). The excitation value was kept constant for all samples to enable good comparison of the samples capped with different

complexing agents. The PL spectra for the CdTe NPs prepared using different capping ligands is presented in Fig. 3. The PL emission in semiconductor materials is said to originate from the recombination of charge carriers created by the process of light absorption. This recombination can take place in certain surface defect states. If for instance, the recombination occurs at the defect sites situated at the NPs' surface, there is a high probability that these defect sites will be affected by the nature of the capping ligand used. It is, therefore, imperative to study the effect of different capping ligands in similar growth conditions in order to gain insight on the various relaxation passages leading to the formation of the electron-hole pair when the as-obtained CdTe NPs are excited. It has also been reported that the non-radiative relaxation of trap states competes with the radiative recombination (band edge emission) due to the high surface area of the as-prepared NPs ^[40]. The capping ligands used in this study were the GSH, L-Cyst and TGA. Various combinations of these ligands were used to study the impact of their capping and co-capping on the luminescence properties of the as-prepared CdTe NPs. For the PL measurement to be conducted, aliquots of the each ligand-capped CdTe NPs were taken from the freshly prepared NPs and made ready for the measurement. It is very clear from the PL analysis that the nature and type of capping ligand used to grow CdTe NPs have a great impact on the PL characteristics of the resulting material. The GSH and L-Cyst-capped and co-capped CdTe NPs displayed a good symmetrical Gaussian-shaped PL spectra (Fig. 3(i)). L-Cyst-capped CdTe NPs had the longest emission wavelength (556 nm) while GSH-capped CdTe NPs emitted at 507 nm. The difference in the emission wavelengths could be due to their variation in the particle sizes as confirmed by the XRD and SEM analysis. These variations in the particle sizes are due to different growth mechanism caused by the different capping ligands. The emission at a longer wavelength for the L-Cyst-capped CdTe NPs could be due to agglomeration of the particles during the growth process. This agglomeration could be observed from the SEM image that the NPs were not completely well dispersed. Therefore, the excitation energy of one CdTe NP can be transmitted to another in a non-radiative manner due to the presence of different size distributions during the agglomeration process, which may result in the PL spectra to be red shifted as shown in the L-Cyst-capped CdTe NPs ^[41].

According to studies on the effect of the capping ratio ^[42], it was reported that the concentration of the capping ligands affect the fluorescence intensity. In this report, the concentrations of all the capping ligands were kept constant in order to study how each of them affect the PL

properties. The maximum PL intensity was obtained when the CdTe NPs was co-capped with GSH and L-Cyst. This phenomenon could be said to be due to well passivated CdTe NPs' surface.

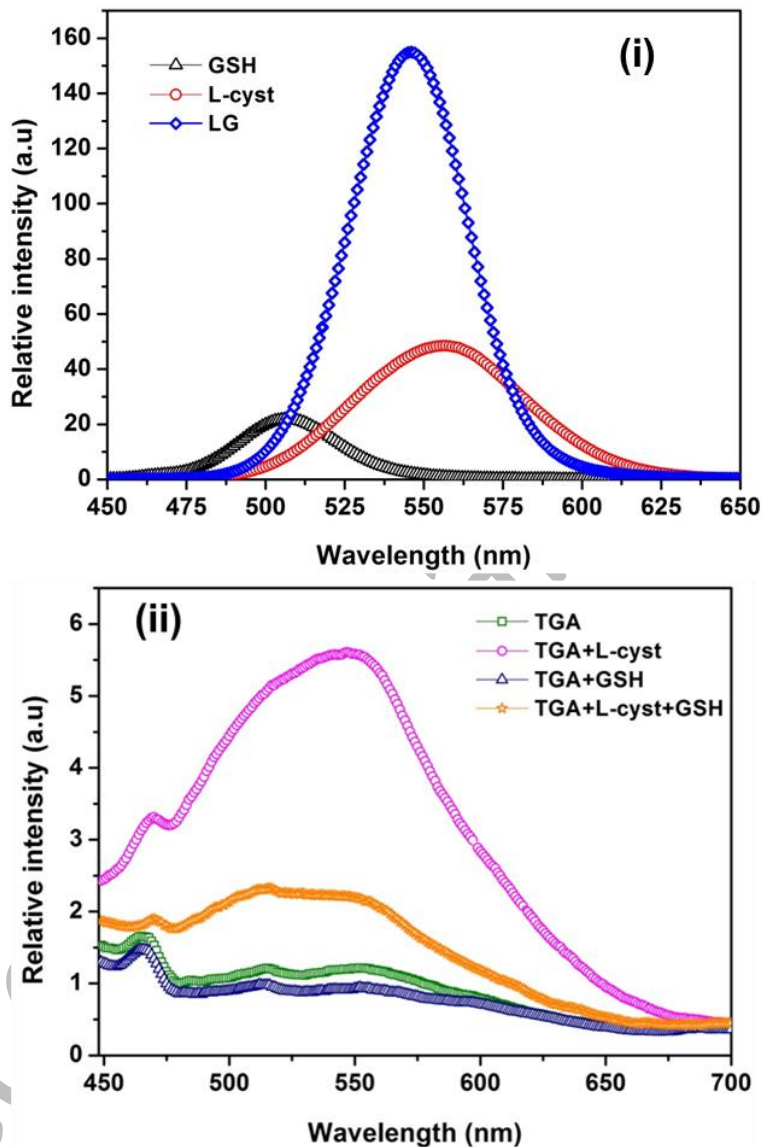


Figure 3: PL emission spectra of CdTe NPs synthesized using different capping ligands.

Also, the PL FWHM evaluated from the PL spectra indicated that the GSH-capped CdTe NPs had the smallest value while TGA-capped CdTe NPs possessed the largest PL FWHM. It has been reported in the literature that a narrow emission peak observed from the NPs could arise due to a direct band to band recombination of electrons and it is always referred to as band edge emission^[43]. The narrow FWHM of the NPs observed for GSH-capped CdTe can be said to be

due a uniform size and size distribution of the NPs prepared. On the other hand, the broad PL emission spectra observed from the TGA-capped CdTe NPs points to the inhomogeneous size distribution of the NPs. Also, the electron-hole recombination at the defect sites may cause the charge distribution to be reorganized thus leading to equilibrium bond length adjustment. These changes cause robust vibronic transitions which result in the production of PL spectra with broad emission bands ^[44].

Furthermore, for the TGA capped and co-capped CdTe NPs, the PL emission spectra displayed a broad less intense and asymmetric kind of spectra. The emission peaks are not well defined as in the case of the GSH and L-Cyst capped CdTe NPs. In trying to analyze the PL spectra of the TGA-capped CdTe NPs, emission peaks were observed at around 460 nm, 514 nm and 553 nm. The emission peak intensity was enhanced when the CdTe NPs was co-capped with TGA and L-Cyst. This indicates that L-Cyst is a good capping agent which can passivate the surface of the NPs well to produce good results. It was further confirmed that the capping and co-capping using both L-Cyst and GSH enhances the quality of the resulting NPs as confirmed by the enhanced emission peak intensity when these capping agents were used. The difference in the PL peak intensity with different capping ligands can also be ascribed to the variation in the emitting state densities ^[45]. The TGA-capped and co-capped NPs displayed a very small PL emission intensity when compared to the GSH and L-Cyst capped CdTe NPs. This observation could be due to non-radiative electron-hole recombination processes caused by stronger phonon coupling compared to the optical transitions which are commonly present in large particle sizes ^[46]. Moreover, depending on the molecular structure of the capping ligands, these ligands can form weak charge transfer complex that can either act as base or acid on the CdTe NPs thus impacting on the intensities of the PL emission ^[47].

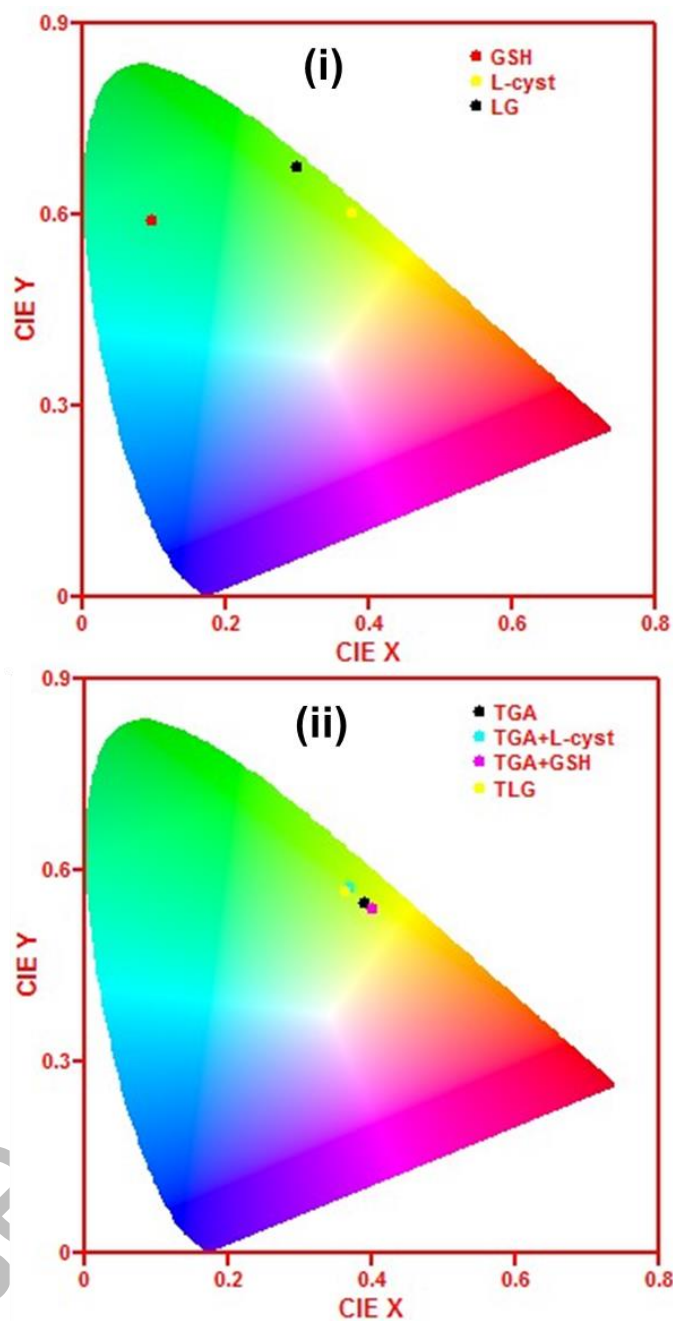


Figure 4: CIE chromaticity diagram of as-prepared CdTe NPs prepared using different capping ligands.

The Commission International de l'Eclairage (CIE) coordinate calculator was employed to determine the colour coordinates (x, y) using the values obtained from the PL emission spectra. These coordinates were used to locate the emission colour of various CdTe NPs samples. The CIE diagram shown in Fig. 4 describes the colour of the emission produced by the as-prepared

CdTe NPs. From the chromatic diagram, it can be deduced that the as-prepared CdTe NPs emit in the green-yellow region. From this CIE chromaticity study, it is realized that the nature and the type of capping ligand used in the preparation of the CdTe NPs greatly influence the emission colour of the NPs. Hence, therefore, great care must be taken into account when choosing the type of ligand to be used to prepare CdTe NPs for certain application.

2.4. Ultraviolet-visible (UV-vis) Analysis

UV-vis absorption spectroscopy was conducted in order to study the evolution of the CdTe NPs when different capping ligands are used during their preparation. Aliquots of the samples were taken for the PL and UV measurement. During the UV measurement, absorbance was measured and the obtained results plotted and analyzed. Fig. 5 shows the absorbance spectra of CdTe NPs prepared using different capping ligands. GSH and L-Cyst capped and co-capped CdTe NPs displayed well-resolved absorption maxima with definite absorption edges (Fig. 5(i)). The L-Cyst-capped CdTe NPs had its absorption band at a longer wavelength (around 550 nm) compared to the GSH and co-capping using both GSH and L-Cyst. This supports the results portrayed in the PL measurement by longest emission wavelength observed for L-Cyst-capped CdTe NPs. On the other hand, TGA-capped and co-capped CdTe NPs display sharp absorption edges ranging from around 400 - 600 nm (Fig. 5 (ii)). The sharp absorption edges observed in the GSH and L-Cyst capped CdTe NPs confirms the observation made in the EDS analysis. Sharper absorption edges indicate the presence of impurities in trace levels in the as-prepared CdTe NPs. When straight part of the absorbance graph is extrapolated to the wavelength axis, TGA-capped CdTe NPs possess the longest absorption edge, an indication of largest particle size obtained in this study. This further confirms the observation made from the XRD and SEM analysis. These findings agree well with the results obtained by Pesika et al. in their investigations^[48] who reported that the point of the absorption band edge can be used as an indication of the NP sizes. Absorption bands are, however, not observed for the TGA-capped and co-capped NPs. It was also noted that the TGA-capped CdTe NPs had high absorbance in the visible region compared to all other ligand-CdTe NPs conducted in this study.

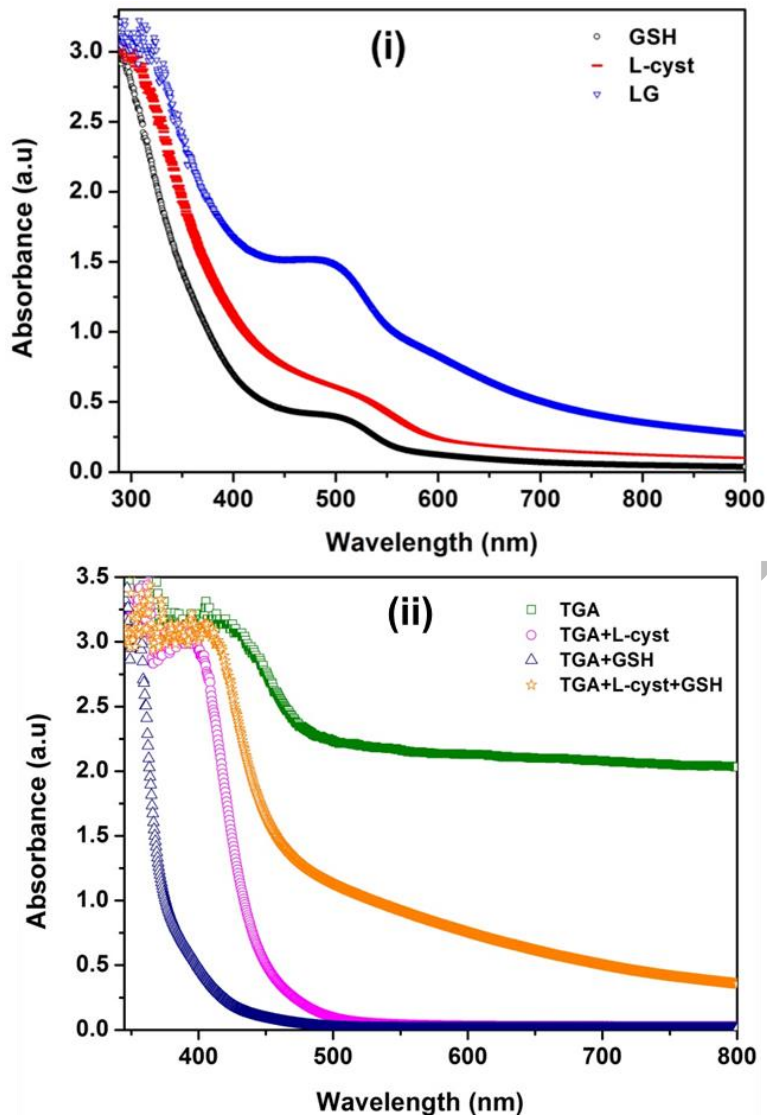


Figure 5: Evolution of absorbance spectra of CdTe NPs prepared using different capping ligands.

Furthermore, baseline shift of the absorption spectra of the as-prepared CdTe NPs to higher absorbance and longer wavelength can be attributed to being due to the formation of some large aggregates of the CdTe NPs^[49]. It was noted that the positions of the PL emission and absorption peak were at slightly different wavelengths especially for the GSH and L-Cyst- capped and co-capped CdTe NPs. This difference could be due to the short distances between the NPs owing to an increased dipole-dipole interaction between the NPs due to the electrostatic attraction between positively charged protein (L-cyst/GSH) and negatively charged CdTe NPs which causes a larger Stoke's loss^[50,51].

The band gap of a material defines its electronic condition. The band gaps of the as-grown CdTe NPs were approximated by means of the famous Tauc relation; $(\alpha hv) = C(hv - E_g)^n$ [52] where C is a constant, α is the absorption coefficient which has a direct relation with the measured absorbance and can be calculated by employing the Beer-Lambert's law, E_g is an estimate of the energy band gap of the as-prepared semiconductor NPs and n is a constant that relies on the transition type occurring in the material. The values of $n = 1/2$ and $n = 1$ are for direct and indirect allowed band gap transitions respectively. The average energy band gaps were extracted from the intercept of the linear portion of the $(\alpha hv)^2$ versus hv plots on the hv axis as shown in Fig. 6. The estimated band gap values obtained were: 3.34, 3.08, 2.63, 2.39, 2.86, 3.33 and 2.66 eV for GSH, L-Cyst, L-Cyst+GSH, TGA, TGA+L-Cyst, TGA+GSH and TGA+L-Cyst+GSH capped-CdTe NPs respectively. The largest and smallest band gaps were observed for GSH and TGA-capped CdTe NPs respectively. All the observed band gaps were larger than the bulk band gap (1.5) eV which could be due to small sizes (nanoscale) of the as-obtained CdTe NPs.

The NPs' sizes were further estimated using the obtained values of energy band gap by employing the effective mass approximation model (EMA) [53]; $E_g(NP) = E_g(bulk) + \frac{h^2}{8D^2\mu} - \frac{1.8e^2}{4\pi D\epsilon\epsilon_0}$ assuming that all the particles are spherical in shape as confirmed from the SEM images.

Where $\mu = \frac{M_e^*M_h^*}{M_e^*+M_h^*}$, M_e^* and M_h^* are effective electron and hole masses respectively. $E_g(NP)$ is the energy band gap of the as-prepared CdTe NP s while $E_g(bulk)$ is the reported bulk band gap of CdTe. h is the Planck's constant, D the particle radius, ϵ the dielectric constant, ϵ_0 is the permittivity of the free space and e corresponds to the electronic charge. The estimated values were: 3.08, 3.32, 3.92, 4.42, 3.54, 3.08 and 3.86 nm for GSH, L-Cyst, L-Cyst+GSH, TGA, TGA+L-Cyst, TGA+GSH and TGA+L-Cyst+GSH capped-CdTe NPs respectively.

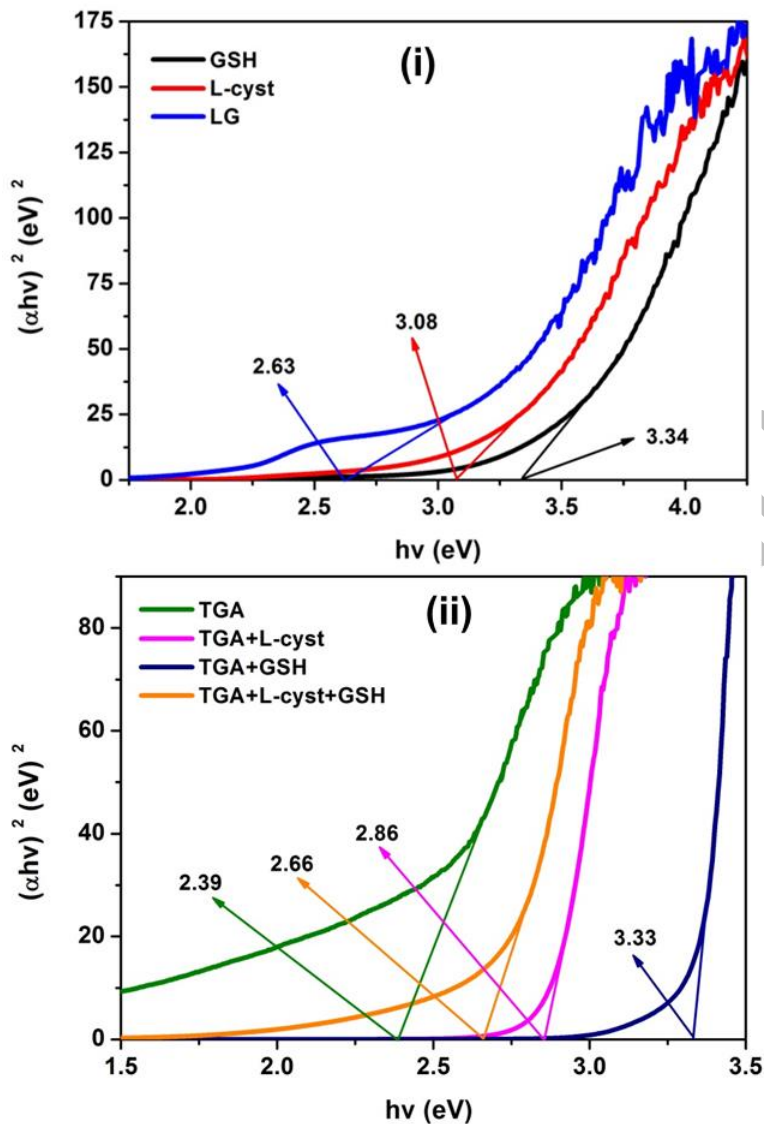


Figure 6: Graphs of energy band gaps of CdTe NPs prepared using various capping ligands.

These show similar trend and the values compare closely with XRD values for the GSH, L-Cyst and L-Cyst+GSH capped CdTe NPs but for the TGA capped counterparts there was a big difference in their values. These results show that the EMA model can approximate well for NPs under quantum confinement and not for large NPs like the TGA-capped CdTe NPs. When capping ligands are compared in terms of their different hydrocarbon chain lengths, the reported data show that the particle size and the hydrocarbon chain length in cationic surfactants have an inverse relation^[54]. A similar trend was also observed by Kumar et al.^[40] in their study on the

CdS NPs. This trend is confirmed here in our study since GSH has the longest while TGA has the shortest hydrocarbon chain lengths thus producing the smallest and largest particle sizes respectively.

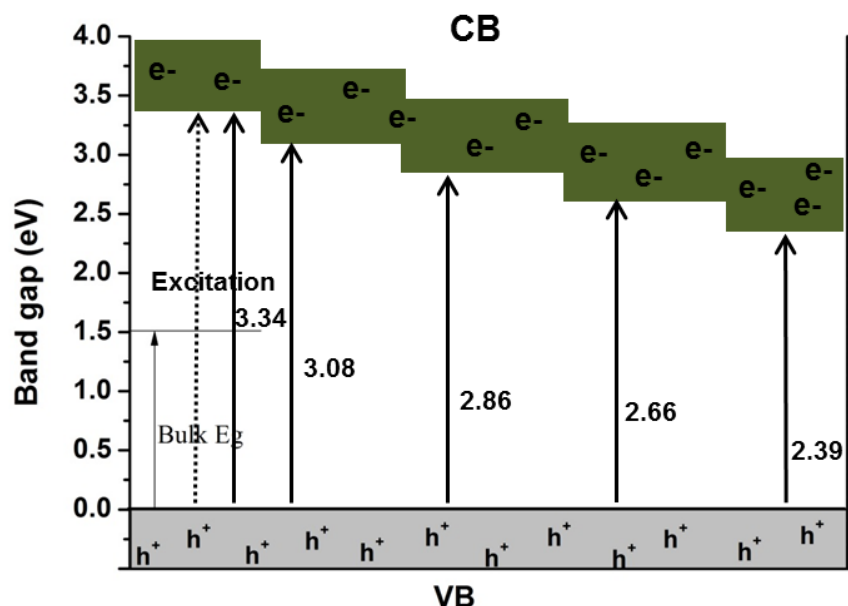


Figure 7: Graph showing representative energy diagram of CdTe NPs using different capping ligands.

Fig. 7 shows an energy diagram of the as-prepared CdTe NPs using different capping ligands. When excited, the electrons move to the conduction band (CB) from the valence band (VB) emitting light in the process. This summarizes the results obtained from the PL measurement. The PL results showed that there was only one emission peak which was red shifted as the NP size increased. The difference in the particle sizes was due to the different growth reaction process brought about by the use of different capping ligands. From the emission spectra it can be concluded that the larger NPs emitted light at longer wavelengths. This phenomenon was also observed in the UV-vis results where the band gap energy was inversely proportional to the size of the CdTe NPs obtained. The band gap energies shown in Fig. 7; 3.34, 3.08, 2.86, 2.66 and 2.39 eV correspond to the band gap energies of CdTe NPs prepared using GSH, L-Cyst, TGA+L-Cyst, TLG and TGA capping ligands respectively.

3. Conclusion

Detailed studies on the conjugation and evolution of the structural and optical properties of the as-prepared CdTe NPs have given an enhanced knowledge on the dependence of material properties on the nature and type of capping ligands used in the aqueous phase. The XRD results revealed that the type of the capping ligand used affects the structure formation of the CdTe NPs prepared in this wet chemical route. All the as-prepared CdTe NPs had a cubic crystal structure but different phases depending on the capping ligand used. The GSH and L-Cyst capped and co-capped CdTe NPs had one cubic phase while TGA-capped CdTe NPs had another cubic phase. The estimated crystallite sizes were under 30 nm for all the CdTe NPs prepared using different capping ligands. The SEM micrographs displayed spherical shaped NPs with varying sizes depending on the capping ligand used. GSH and TGA capped showed smallest and largest CdTe NPs respectively as confirmed by the XRD and SEM results. In the optical measurement, the UV-Vis absorbance and PL emission wavelengths and intensities were greatly influenced by the capping ligand used. In both cases, the PL and UV-vis analysis confirmed that the GSH and TGA-capped CdTe NPs had smallest and largest particle sizes respectively. The optical band gaps of the as-prepared CdTe NPs were all greater than the bulk band gap which could be due to quantum size effects. These results, therefore, give a better insight into the kind of capping ligand to be chosen in order to grow NPs to be used for biological applications.

Supporting information summary

The supporting information contains the experimental procedure of the reported study and the associated references.

Acknowledgement

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Keywords: Capping ligands; Co-capping; Glutathione; Luminescence; Material properties.

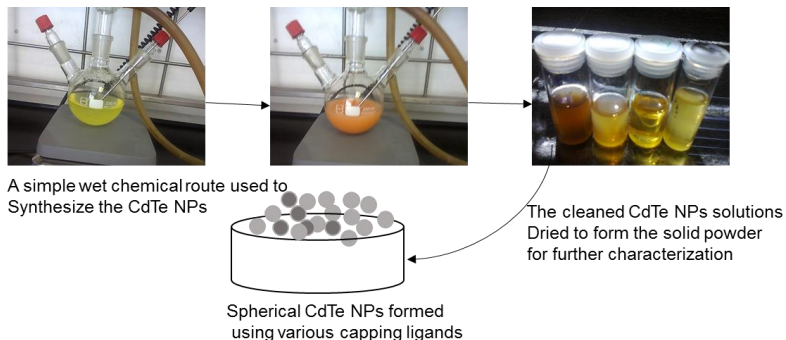
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The CdTe NPs were produced from the one pot and simple chemical route using various capping ligands (TGA, GSH and L-Cyst). The material properties of CdTe NPs were tailored by using different capping ligands and this is observed during synthesis as the colour of the NP solution changes with different capping ligands. Change of NP solution indicates the formation of CdTe NPs with various material properties.