

Supporting Information

Similar Topological Origin of Chiral Centers in Organic and Nanoscale Inorganic Structures: Effect of Stabilizer Chirality on Optical Isomerism and Growth of CdTe Nanocrystals

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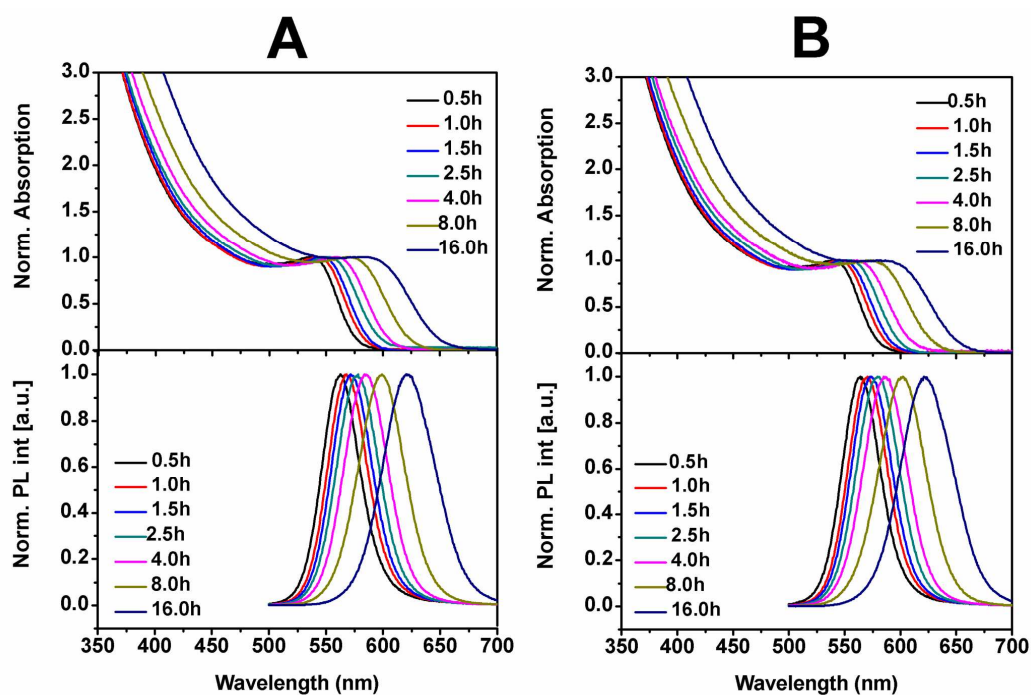


Figure S1. Typical temporal UV-vis spectra and PL spectra of D-cysteine stabilized CdTe NCs (A). Typical temporal UV-vis spectra and PL spectra of L-cysteine stabilized CdTe NCs (B).

Table S1. The experimental data of Figure 1.

Duration of synthesis	PL peak (nm)				Particle size (nm)			
	D- [*] Mean	Er [±] ^{**}	L- [*] Mean	Er [±] ^{**}	D- [*] Mean	Er [±] ^{**}	L- [*] Mean	Er [±] ^{**}
0.5h	564.2	1.2	566.3	0.9	3.06751	0.01015	3.10493	0.00203
1.0h	569.6	1.0	570.9	0.2	3.14642	0.00617	3.16948	0.00346
1.5h	574.4	1.3	576.1	0.9	3.19443	0.00268	3.22051	0.01001
2.5h	579.0	0.7	582.3	0.8	3.24844	0.00416	3.27765	0.00621
4.0h	586.1	0.8	590.0	0.5	3.30217	0.01078	3.33502	0.00866
8.0h	596.1	1.3	599.3	0.3	3.39527	0.00128	3.42690	0.00460
16.0h	616.3	0.8	620.3	0.4	3.49145	0.00226	3.52184	0.00114

Duration of synthesis	Particle concentration (mol/L)			
	D- [*] Mean	Er [±] ^{**}	L- [*] Mean	Er [±] ^{**}
0.5h	4.16099E-5	6.97084E-7	4.23742E-5	4.17830E-7
1.0h	3.86897E-5	5.12293E-8	3.93637E-5	8.52155E-7
1.5h	3.66443E-5	4.15954E-7	3.69019E-5	9.37019E-7
2.5h	3.30720E-5	8.53685E-7	3.28933E-5	6.88454E-7
4.0h	3.01687E-5	6.91022E-7	3.01454E-5	8.54090E-7
8.0h	2.55016E-5	4.88777E-7	2.57870E-5	4.25486E-7
16.0h	2.26091E-5	4.48397E-7	2.24026E-5	2.54647E-7

Duration of synthesis	Normalized particle concentration			
	D- [*] Mean	Er [±] ^{**}	L- [*] Mean	Er [±] ^{**}
0.5h	1	0	1	0
1.0h	0.92982	0.01511	0.92895	0.01701
1.5h	0.88066	0.01466	0.87086	0.01393
2.5h	0.79481	0.03310	0.77626	0.01214
4.0h	0.72504	0.02291	0.71141	0.01124
8.0h	0.61287	0.02001	0.60855	0.01321
16.0h	0.54336	0.01969	0.52868	0.00800

^{*}D-: D-cysteine stabilized CdTe NCs; L-: L-cysteine stabilized CdTe NCs

^{**}Er[±]: error bar

The size and concentration of NCs for CdTe were calculated based on the Peng's empirical equation in reference [S1].

$$D=(9.8127 \times 10^{-7}) \lambda^3 - (1.7147 \times 10^{-3}) \lambda^2 + (1.0064) \lambda - 194.84$$

$$A=\epsilon CL$$

$$\epsilon=10043(D)^{2.12}$$

In the above equations, D (nm) is the size of CdTe NCs, λ is the wavelength of the first excitonic absorption peak, A is the extinction coefficient, ϵ is the extinction coefficient per mole of particles, C is the molar concentration (mol/L) of the nanocrystals, L is the path length (cm) of the radiation beam used for recording the

absorption spectrum.

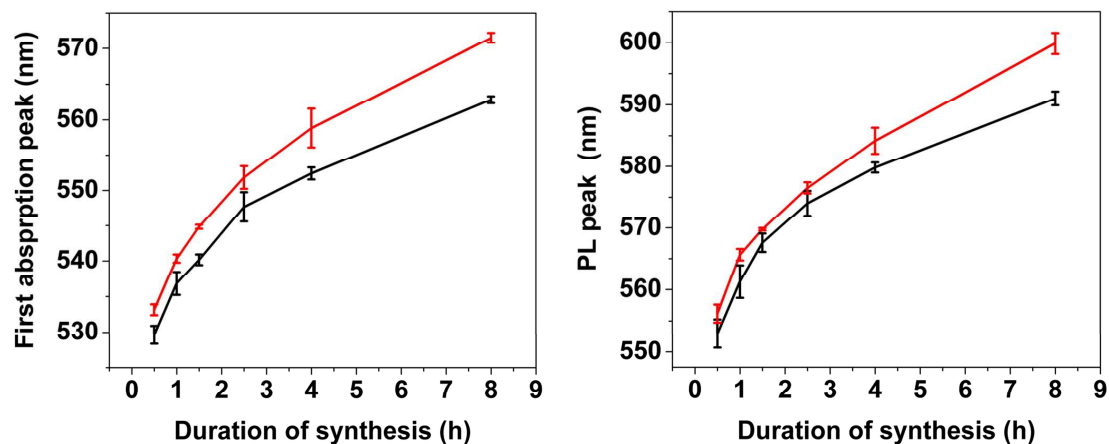
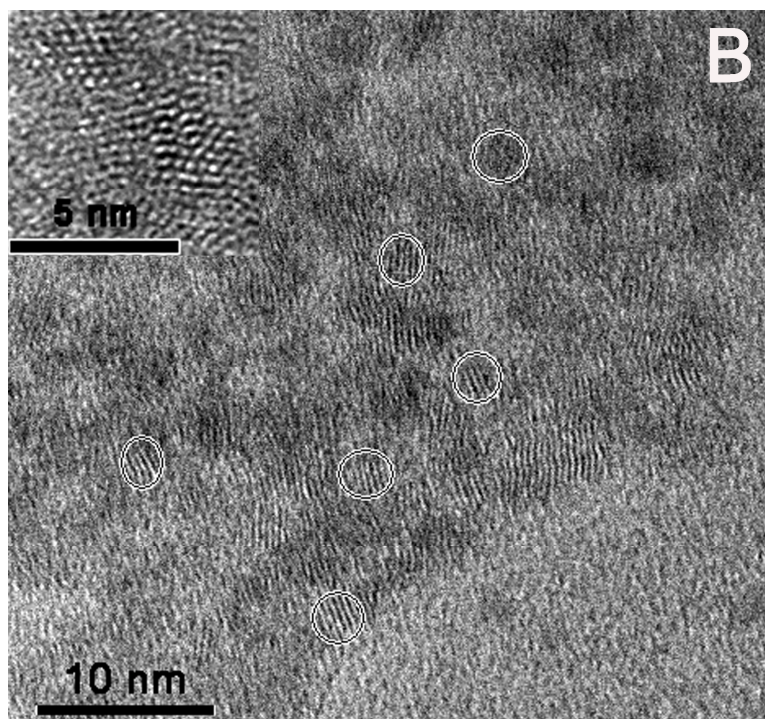
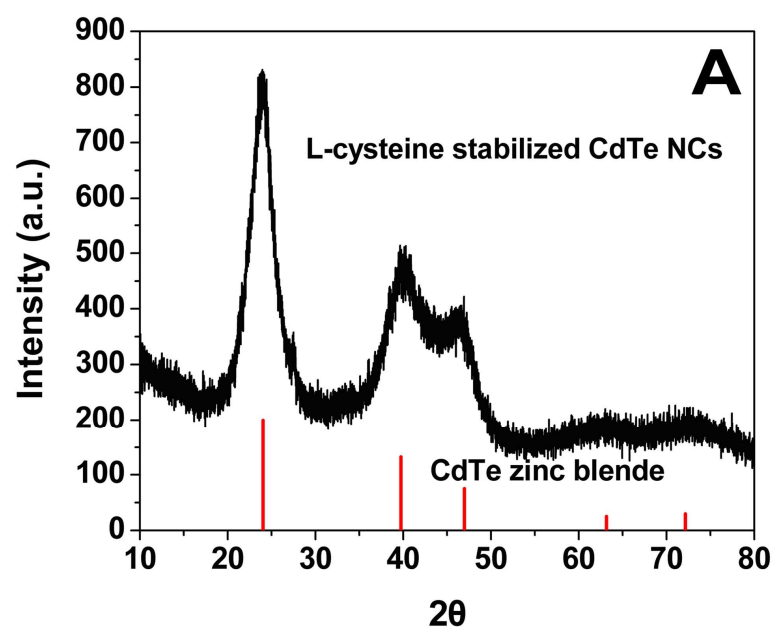


Figure S2. Temporal evolution of first absorption peak and PL peak of CdTe nanocrystals synthesized by D-cysteine hydrochloride monohydrate (98%, Sigma) (black) and L-cysteine hydrochloride monohydrate (99%, Alfa) (red). All data are average values obtained from at least three different experiments.

In order to preclude the possibility of unknown impurity, we also investigated the growth kinetics of CdTe NCs stabilized by (D, L) cysteine hydrochloride monohydrate purchased from different vendor companies (D-cysteine hydrochloride monohydrate from Sigma; D-cysteine hydrochloride monohydrate from Alfa). Notably, measurements on the positions of the first absorption peaks and PL peaks show similar result with the growth kinetics of CdTe NCs stabilized by (D, L)-cysteine.



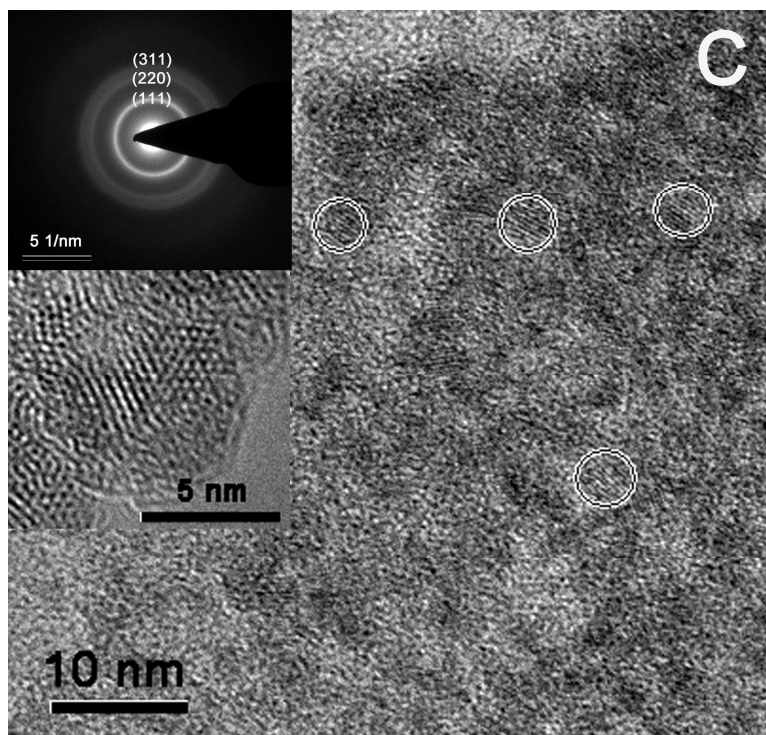
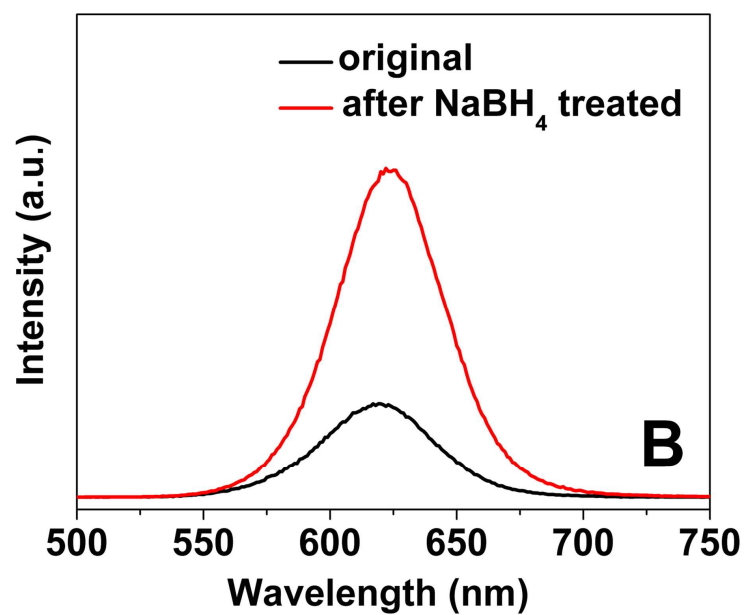
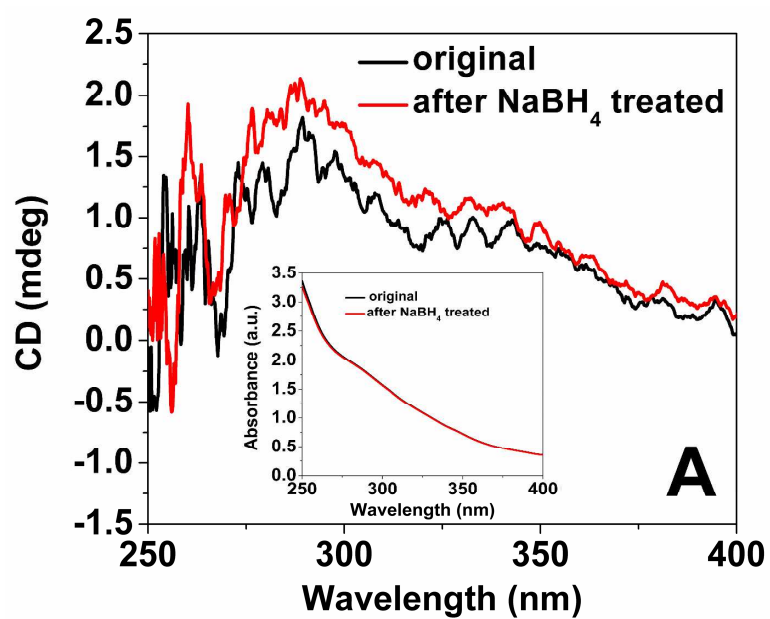


Figure S3. X-ray diffraction (A) and high resolution TEM (B) of L-cysteine stabilized CdTe; High resolution TEM and electron diffraction of D-cysteine stabilized CdTe (C).

As shown in the X-ray diffraction and high resolution TEM, the crystal structures of (D and L)-cysteine stabilized CdTe NCs are zinc blende, which results in the tetrahedral constitutive units according to the previous data of X-ray diffraction (S2, S3).



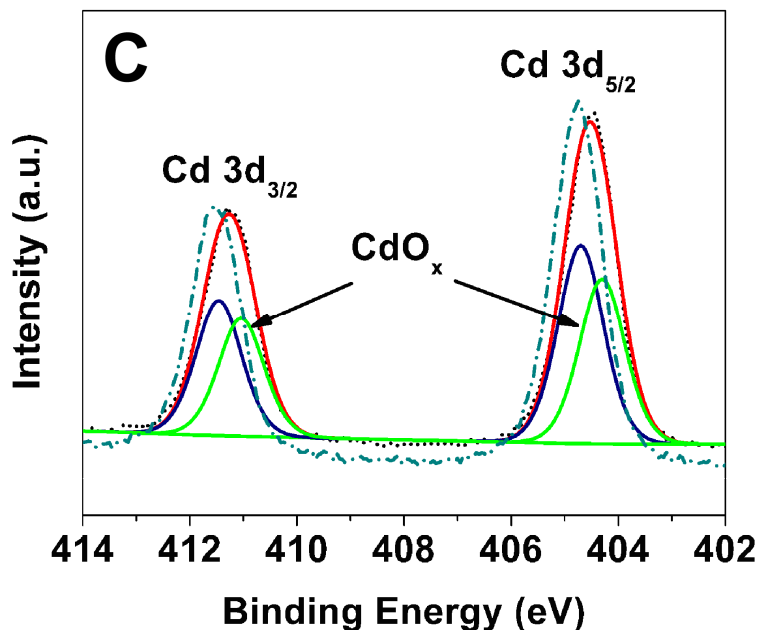


Figure S4. CD spectra of L-cysteine stabilized CdTe NCs (original NCs and NCs treated by NaBH₄) (A). PL spectra of L-cysteine stabilized CdTe NCs (original NCs and NCs treated by NaBH₄) (B). XPS spectra of L-cysteine stabilized CdTe NCs (C). The dotted cyan line represents original NCs, and the dotted black line represents NCs treated by NaBH₄. The blue and green solid lines are the deconvoluted curves, and the surface cadmium atom ratio, $\frac{\text{Cd}}{\text{Cd-O}}$, is calculated to be about 1.2.

Recent study has shown that NaBH₄ can reduce oxygen either from solvent or stabilizer molecules and lead to form new Cd-O bonds on the CdTe or CdSe core surfaces, which usually enhance the quantum efficiency without alternation of their absorbance or PL wavelength [S4]. In our experiment, 0.1% mass percent NaBH₄ was added into 2 mL L-cysteine stabilized CdTe NC solution, and after 5 minute treatment the NCs were centrifuged and precipitated by adding 2 mL 2-propanol in solution to remove NaBH₄ and excessive stabilizers.

As shown in Figure S4B and inset in Figure S4A, both the remarkable increase in PL intensity and unchanged in UV-Vis spectra show that the treatment of NaBH₄ just change the surface state of NCs without alternation of CdTe core sizes. Especially, as shown in the CD spectra of L-cysteine stabilized CdTe NCs (Figure S4A), it is evident

that the CD intensity increases after NaBH_4 treatment. Combined with the XPS results that the ratio of Cd-O is increased after NaBH_4 treatment (Figure S4C and Figure 5D), one can draw the conclusion that the increased CD signal is due to the increased percentage of Cd-O on NC surface [S4, S5]. The above experimental observation provides a direct evidence to demonstrate that Te-Cd-O is responsible for formation of the chiral centers, which is also consistent with our theoretical model (Figure 3).

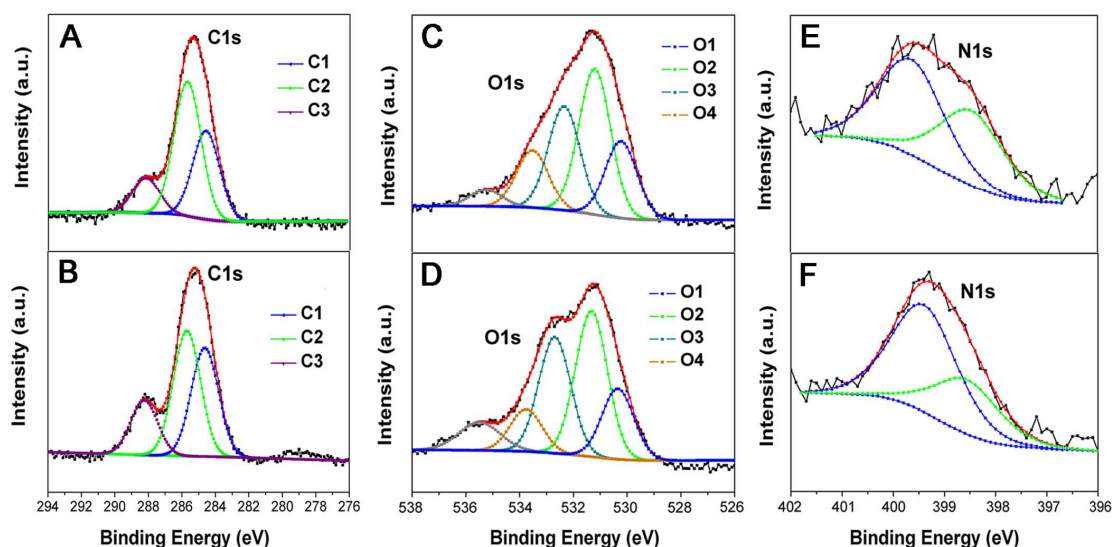


Figure S5. X-ray photoelectron spectra of D-cysteine stabilized CdTe NCs (A), (C), (E) and L-cysteine stabilized CdTe NCs (B), (D), (F). The spectra fitted with Pseudo—Voigt (GL) functions with a combined polynomial and Shirley background. (A), (B): C1($\text{—}\underline{\text{C}}\text{H}_2\text{—}$), C2($\underline{\text{C}}\text{—N}$), C3($\underline{\text{C}}\text{OO}^-$); (C), (D): O1(O—Cd), O2(C=O), O3(O—C—O) $^-$, O4(O=C—O—H $_2$ N).[S6, S7]

X-ray photoelectron spectroscopy (XPS) reveals the detailed binding energies of the cysteine attached on the surface of CdTe NCs. The best fitting functions of C 1s have also the same maxima at 284.6 eV (C1), 285.7 eV (C2), and 288.3 eV (C3) for (D, L)-cysteine stabilized CdTe NCs, which mean no pre-configuration for D-cysteine or L-cysteine absorbed on the CdTe surface.

In the O 1s core level regions, the signals are characterized by a broad and asymmetric peak. The marked shoulders on the high binding energy side (yellowish-gray curves) are from the auger signal of sodium. For D-cysteine stabilized CdTe NCs, the best fitting GL functions have maxima at 530.3 eV (O1), 531.2 eV (O2), 532.3 eV (O3) and 533.5 eV (O4), while the corresponding peaks at 530.3 eV (O1), 531.2 eV (O2), 532.7 eV (O3) and 533.8 eV (O4) for L-cysteine stabilized CdTe NCs. The slight difference of O1s peaks implies possible environmental variety for L-cysteine and D-cysteine on NC surfaces.

The N 1s spectra of D-cysteine stabilized CdTe NCs and L-cysteine stabilized CdTe NCs are very similar and have the same binding energy. It is also noted that there are two fitting N 1s peaks appearing, which means that the amino groups of cysteine molecules on the CdTe surface exist in two different environments. One of the signals can be ascribed to free amino group (399.4 eV) and the other (398.6 eV) is likely to correspond to the partial intermolecular hydrogen bond between carboxyl group and amino group of cysteine stabilizers on NC surfaces, which is further supported by the below NMR results.

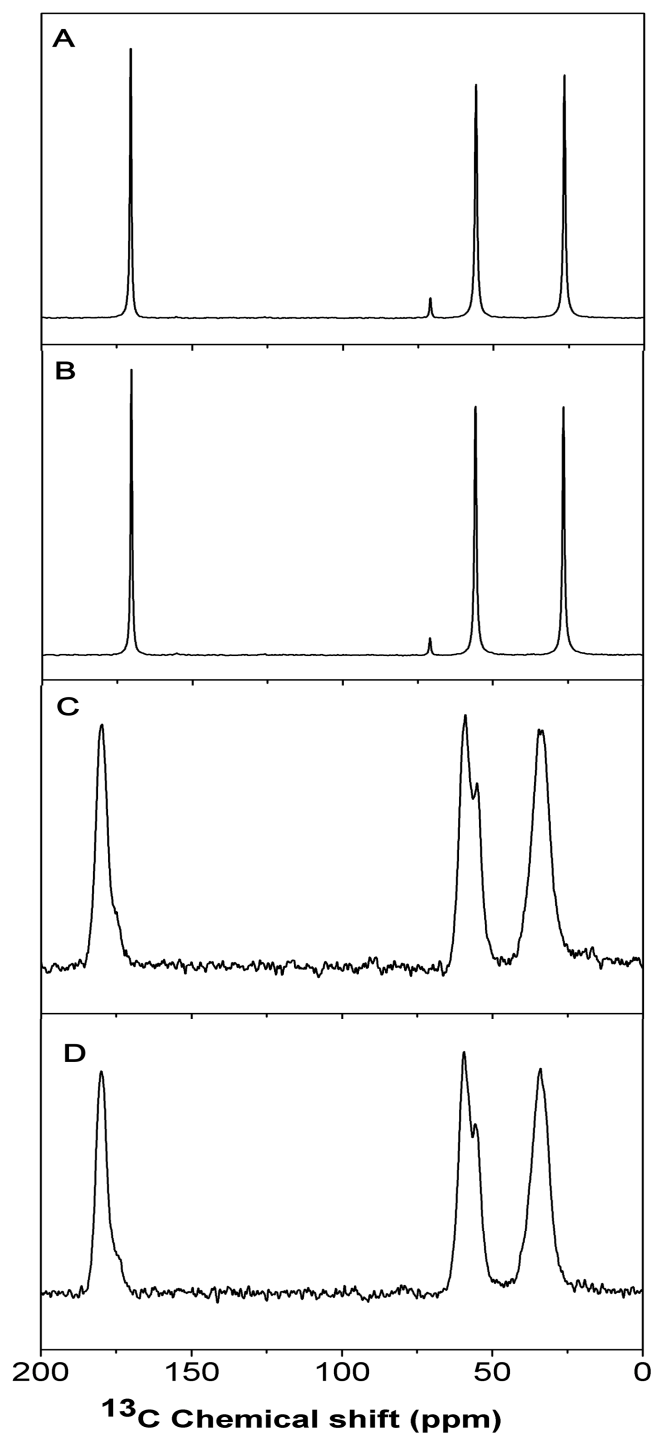


Figure S6. ^{13}C solid-state NMR of D-cysteine (A), L-cysteine (B), D-cysteine stabilized CdTe NCs(C), L-cysteine stabilized CdTe NCs (D).

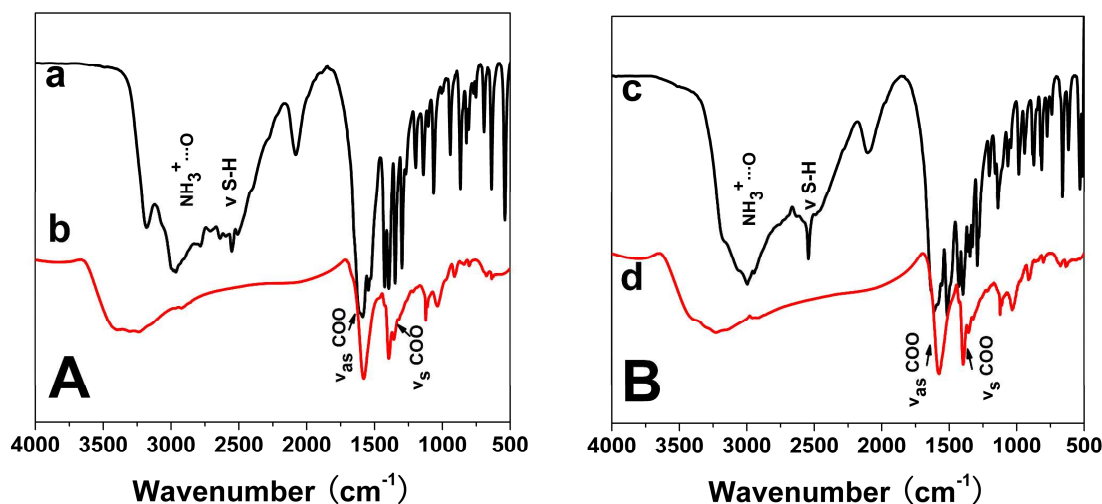


Figure S7. Infra spectra of D-cysteine (a), D-cysteine stabilized CdTe NCs (b), L-cysteine (c), L-cysteine stabilized CdTe NCs (d).

The spectra of cysteine stabilized CdTe NCs were analyzed in comparison to those of free cysteine molecules. The absorption band at $\sim 2540\text{ cm}^{-1}$, which attributes to the stretching vibration of S-H, is disappeared when the cysteine molecules are bound to the CdTe core. This indicates strong bonding between surface cadmium and thiol group of cysteine molecules.[S8] In high pH medium, the carboxyl groups of cysteine stabilizers are deprotonated and provides electrostatic repulsion to keep the NCs well dispersed in solution. Such phenomena can be found in the stretching vibration of carboxylate (peaks at $\sim 1380\text{ cm}^{-1}$ and $\sim 1570\text{ cm}^{-1}$ in curves b and d)[S9]. It is also observed that the broad absorption band exists between 2600 cm^{-1} and $\sim 3500\text{ cm}^{-1}$, which is likely to originate from the partial intermolecular hydrogen bond between carboxyl group and amino group of cysteine stabilizers on NC surfaces. All above analyses are consistent with both XPS and NMR results.

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