Supplementary information

Impact of native achiral ligands on the chirality of enantiopure cysteine stabilized CdSe nanocrystals

Additional results:

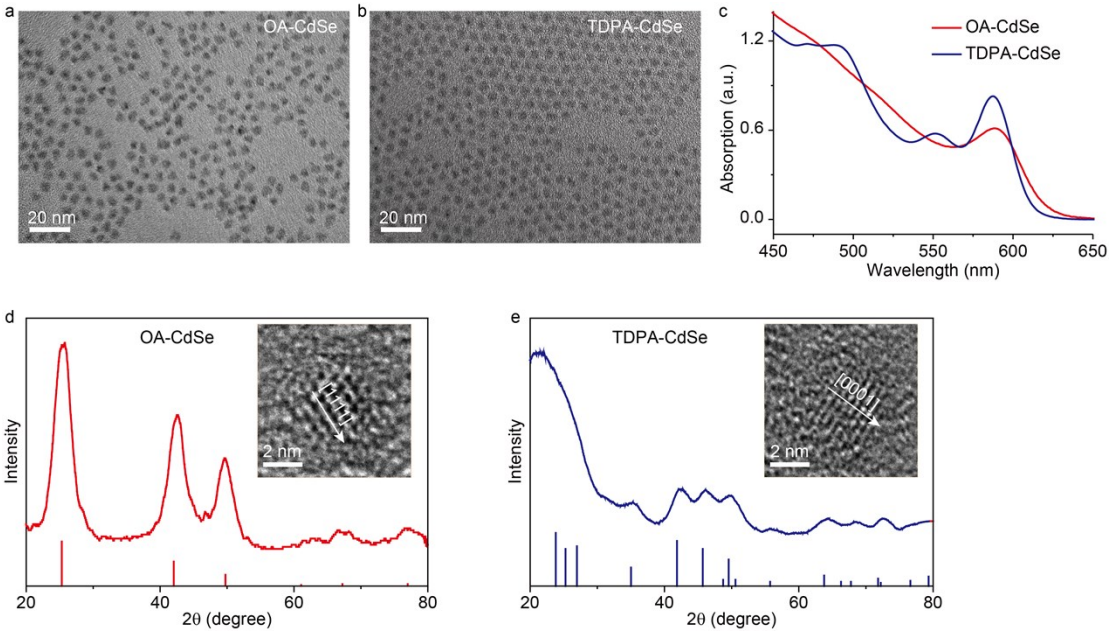


Fig.S1 TEM images of (a) OA-CdSe and (b) TDPA-CdSe QDs. (c) UV-vis absorption spectra of OA-CdSe and TDPA-CdSe QDs. XRD of (d) OA-CdSe and (e)TDPA-CdSe QDs. The insets are the image of magnified individual CdSe QDs.

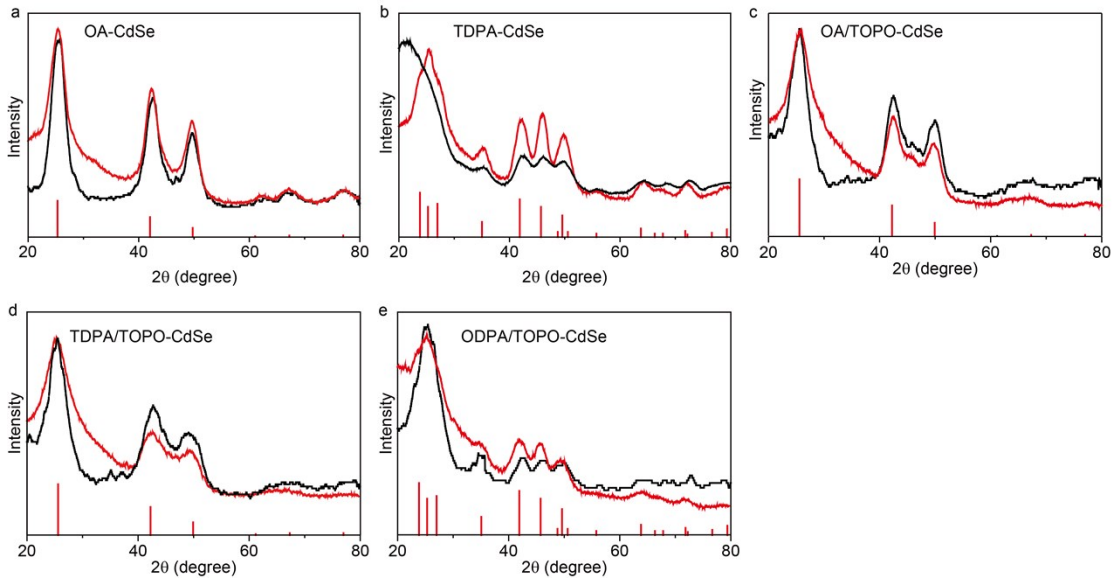


Fig. S2 Comparison of XRD patterns of (a) OA-CdSe, (b) TDPA-CdSe, (c) OA/TOPO-CdSe, (d) TDPA/TOPO-CdSe, and (e) ODPA/TOPO-CdSe QDs before (*black*) and after (*red*) ligand exchange by L-Cys. The vertical bars indicated Zinc blende (a, c, and d) and Wurtzite (b and e) structures.

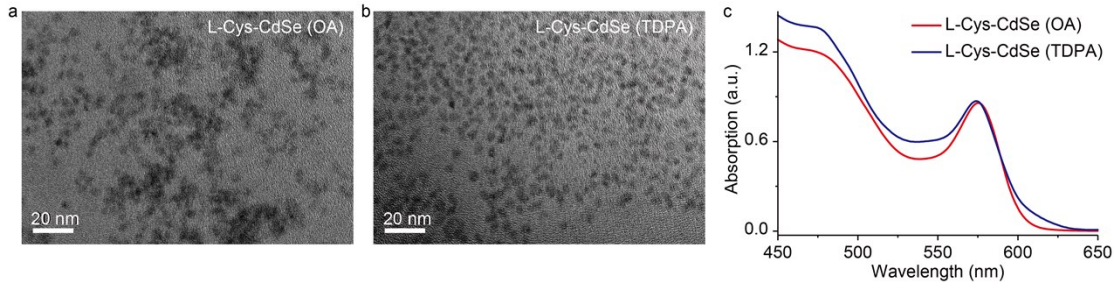


Fig. S3 TEM images of (a) L-Cys-CdSe (OA) and (b) L-Cys-CdSe (TDPA) QDs after ligand exchange; (c) UV-vis absorption spectra of L-Cys-CdSe (OA) and L-Cys-CdSe (TDPA).

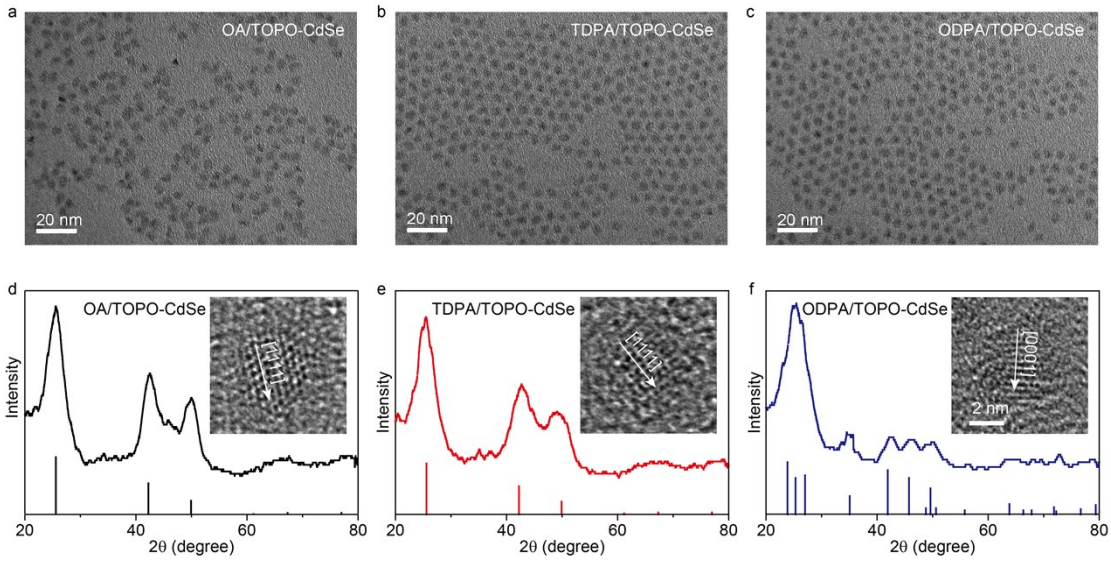


Fig. S4 TEM images of (a) OA/TOPO-CdSe, (b) TDPA/TOPO-CdSe, and (c) ODPA/TDPA-CdSe QDs. (d-f) Corresponding XRD spectra. The insets are the image of magnified individual CdSe QDs.

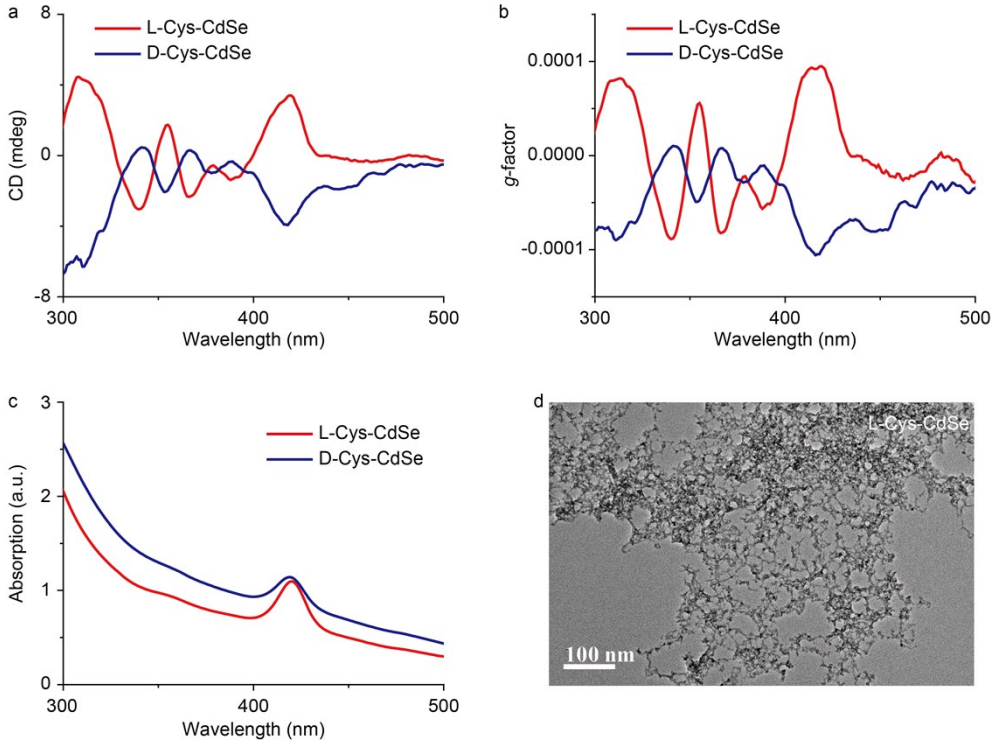


Fig. S5 The CD (a), *g*-factor (b), and UV-vis spectra of L/D-Cys CdSe QDs synthesized directly in aqueous solution. (d) Typical TEM image of the L-Cys stabilized CdSe QDs.

L/D-cysteine-CdSe QDs were synthesized according to the modified procedure reported by Masteri-Farahani et al[1]. In a typical synthesis, 0.04 mmol Se, 0.04 mmol $NaBH_4$, and 20 mL ethanol were mixed in a 100 mL three-mouth flask and stirred for 45 min at room temperature under N_2 flow. The mixture was then cooled down to 0 ℃ (ice bath). Simultaneously, 0.08 mmol $CdCl_2$ and 0.24 mmol L-cysteine were dissolved in 20 mL DI water. The solution pH was adjusted to 11 by adding dilute sodium hydroxide solution (0.01 M). The Cd solution was subsequently injected into the Se solution and the mixture was stirred for 30 min at 0 ℃. The temperature was then raised to 70 ℃ where the mixture was allowed to reflux for 4 hrs. The mixture was cooled down to room temperature and L/D-Cys-CdSe QDs rude products were precipitated with ethanol. The L/D-cysteine-CdSe QDs were purified by two cycles of precipitating with 8:1 (volume ratio) absolute ethanol/DI water. The final products were collected by centrifuging at 6,000 rpm for 5 min and dissolved in DI water.

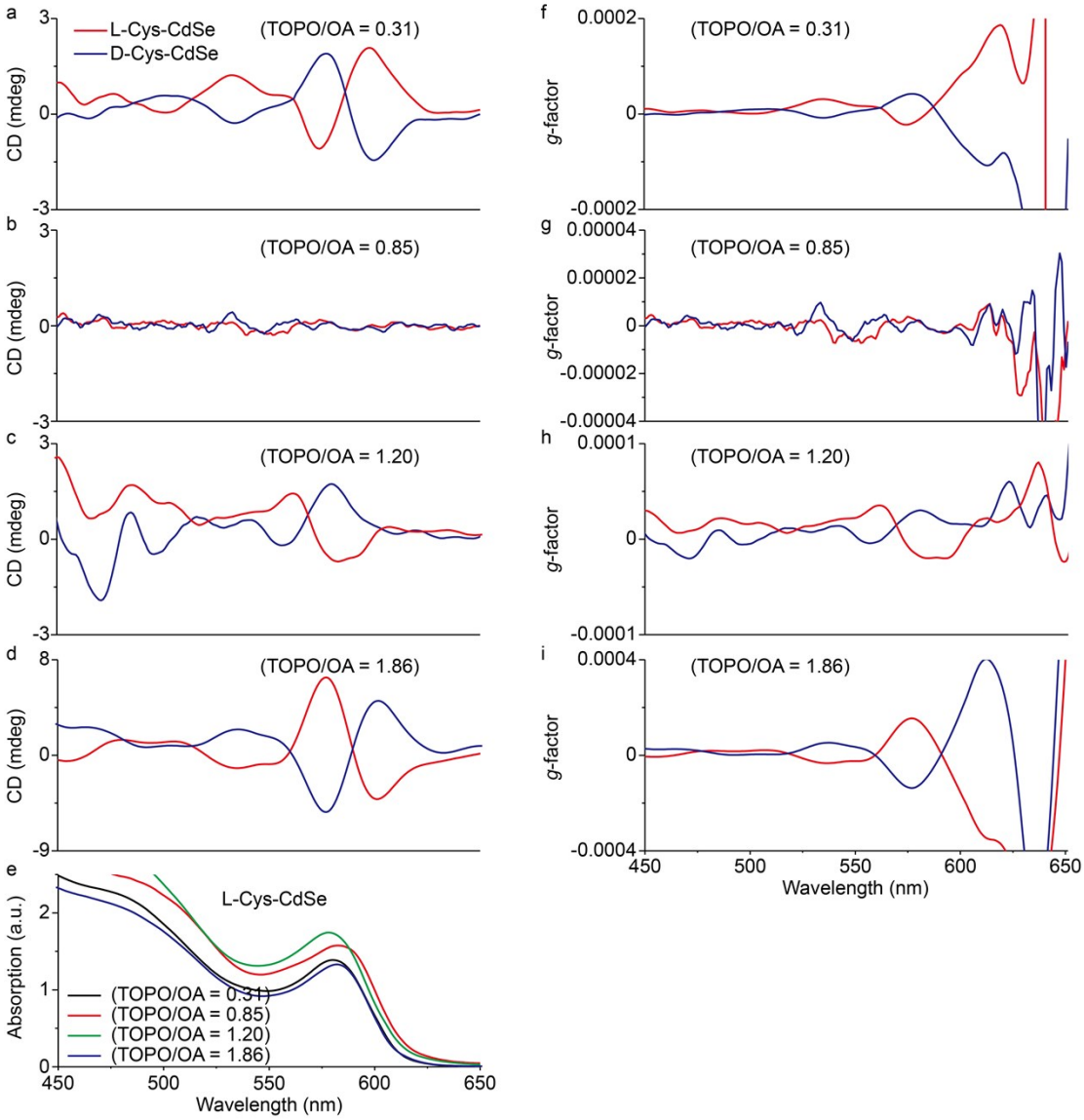


Fig. S6 The CD (a-d), *g*-factor (f-i), and UV-vis (e) spectra of L/D-Cys CdSe QDs prepared under different TOPO/OA feeding ratios in the synthesis of QDs.

When the TOPO ratio is low (TOPO/OA=0.31) in the synthesis of CdSe QDs, it showed the similar CD line shape as L-Cys-CdSe (OA). As the increase of TOPO ratio to 0.85, the CD signal was disappeared. When TOPO/OA ratio is higher than 0.85, (*e.g.* 2.25 in the main text), the inversed CD signal was observed. The changes of CD signal indicate that TOPO and OA have opposite effects on chiral CdSe QDs, which further verified the influence of native ligands on the chirality of CdSe QDs.

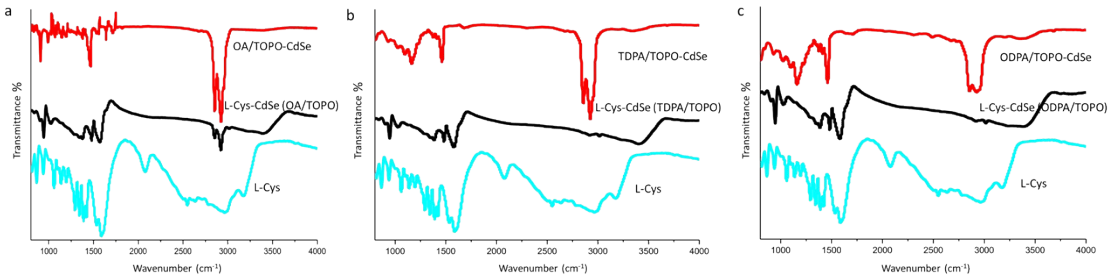


Fig. S7 FTIR spectra of chiral cysteine stabilized CdSe QDs where the native ligands were (a) OA/TOPO, (b) TDPA/TOPO and (c) ODPA/TOPO.

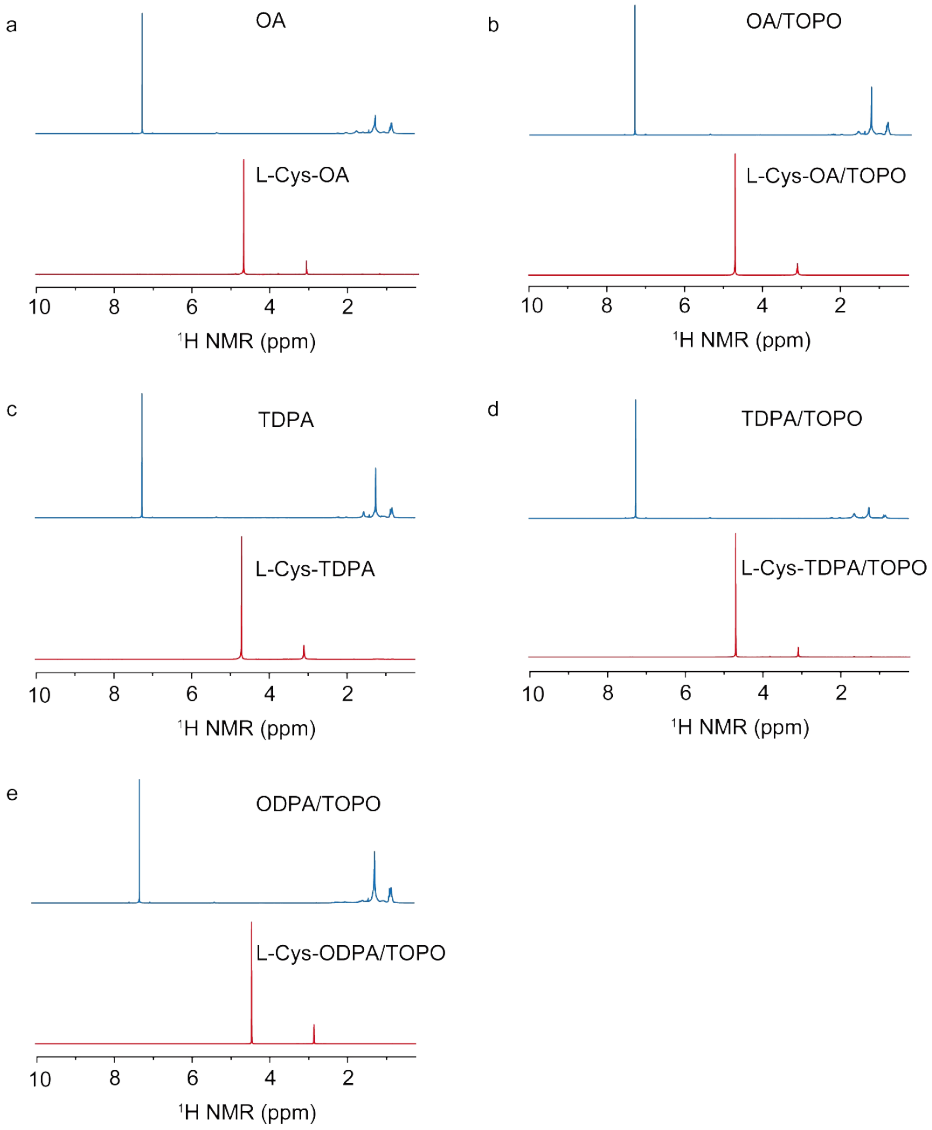


Fig. S8 ^{1}H NMR spectra of CdSe QDs before (*blue*) and after (*red*) ligand exchange with L-cysteine. The intense signals at 7.3 ppm (*blue*) and 4.7 ppm (*red*) were from the

solvent chloroform-d and D_2O before and after ligand exchange.

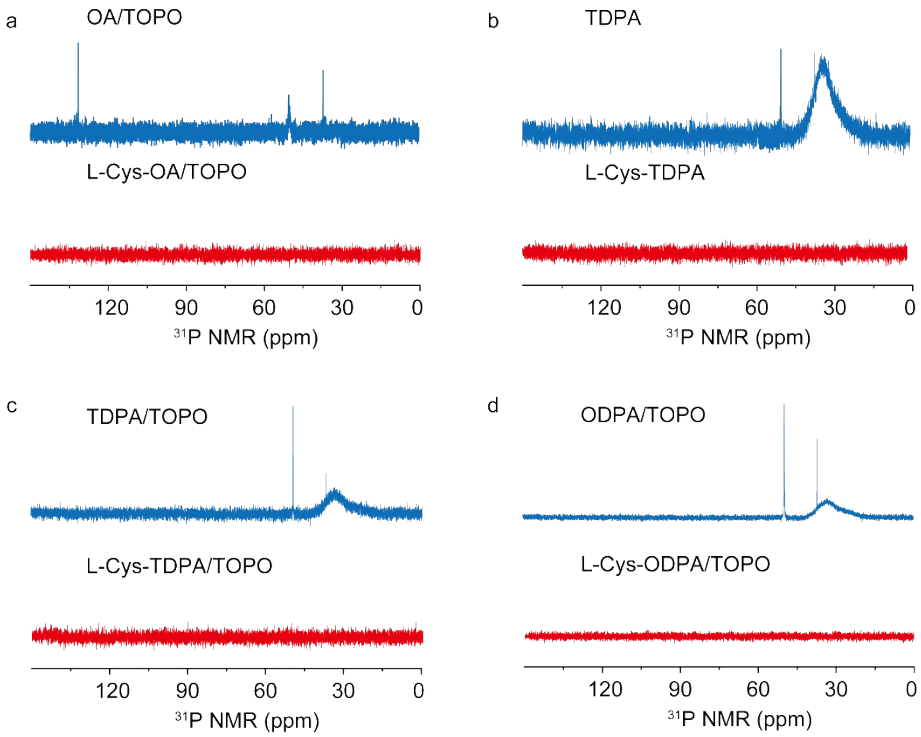


Fig. S9 ^{31}P NMR spectra of CdSe QDs before (*blue*) and after (*red*) ligand exchange with L-cysteine.

Table S1 Ligand surface coverage estimated from elemental analysis

Type of QDs	P% (before)	P% (after)	native ligands（%）	L-Cys（%）
L-Cys-CdSe (OA/TOPO)	0.911	0.048	5.27	94.73
L-Cys-CdSe (TDPA)	3.80	0.009	0.24	99.76
L-Cys-CdSe (TDPA/TOPO)	1.36	0.015	1.10	98.90
L-Cys-CdSe (ODPA/TOPO)	1.40	0.012	0.86	99.14

For L-Cys-CdSe (OA), the measured mass ratio of N and C was 30.66% (38.89% for pure Cys), indicating there was a small amount of remaining native OAs. We therefore estimated there was approximately 78.84% of Cys and the rest was OAs.

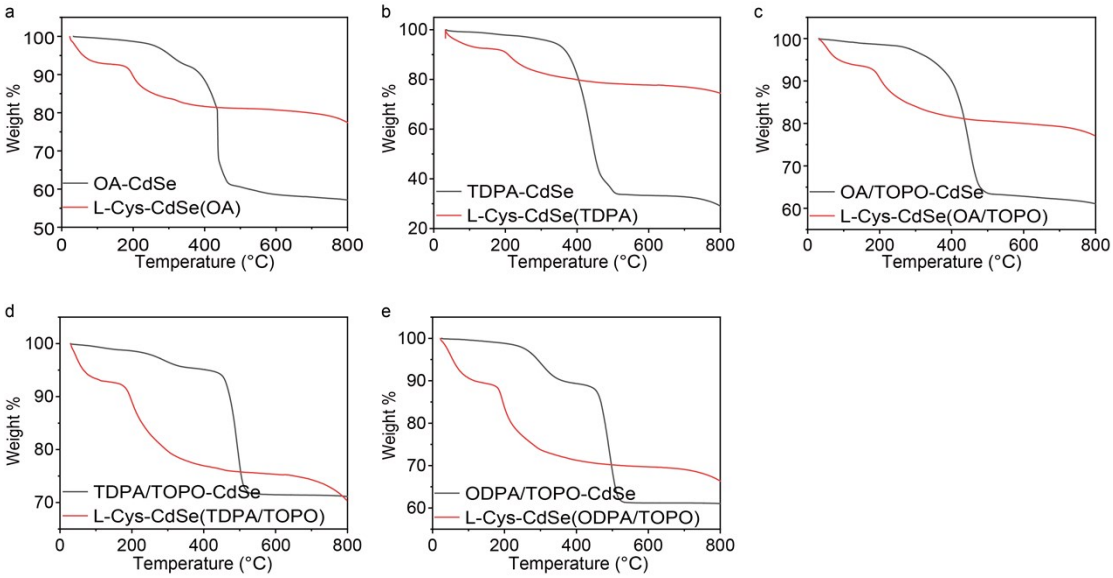
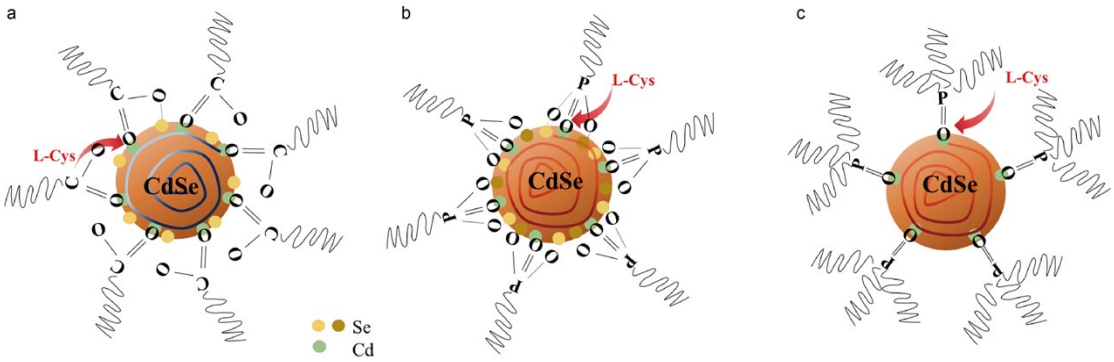


Fig. S10 TGA curves of (a) OA-CdSe, (b) TDPA-CdSe, (c) OA/TOPO-CdSe, (d) TDPA/TOPO-CdSe, and (e) ODPA/TOPO-CdSe QDs before (*black*) and after (*red*) ligand exchange with L-Cys.



Scheme S1 Schematic showing the attacking of L-Cys to the native ligand (a) OA, (b) TDPA, and (c) TOPO.

Table S2 Atomic compositions of CdSe QDs from ICP-AES

Type of QDs	Cd	Se	Cd/Se
L-Cys-CdSe (OA)	55.42%	31.77%	1.74
L-Cys-CdSe (TDPA)	57.48%	34.74%	1.65
L-Cys-CdSe (OA/TOPO)	54.81%	33.02%	1.66
L-Cys-CdSe (TDPA/TOPO)	54.18%	30.18%	1.80
L-Cys-CdSe (ODPA/TOPO)	55.23%	31.48%	1.75
OA-CdSe	42.38%	25.95%	1.63
TDPA-CdSe	28.11%	14.98%	1.88
OA/TOPO-CdSe	35.19%	22.38%	1.57
TDPA/TOPO-CdSe	43.85%	25.88%	1.69
ODPA/TOPO-CdSe	39.58%	21.72%	1.82

Reference

1 M. Masteri-Farahani, N. Mollatayefeh, *Colloids Surf. A*, 2019, **569**, 78–84.