Calculation the Ecb and Evb of CdTe QDs with different size: The particle size of π-conjugated ligand capped CdTe QDs is determined from the absorption maximum (Figure S3) by the following equation[1]

$$D = (9.8127\times10^{-7})\lambda^3 - (1.7147\times10^{-3})\lambda^2 + (1.0064)\lambda - 194.84 \quad (2)$$

Where D (nm) is the particle size of QDs and λ (nm) is the wavelength of first excitonic absorption peak of the corresponding QDs. When the emission wavelength of CdTe QDs is 550 nm, the first maximum absorption of CdTe QDs is located at 500 nm (Figure S3). The calculated result showed that the diameter of the prepared CdTe QDs is about 2.34 nm. The corresponding valence and conduction band-edge energies were calculated by the following equation [2].

$$E_{vb} = -4.74 - 0.80D^{-0.97} \quad (3)$$

$$E_{cb} = -3.29 + 4.19D^{-1.21} \quad (4)$$

The fluorescence spectra and quantum yields of QDs:

The fluorescence spectra and quantum yields (QYs) of TGA-QDs, 4-MBA-TGA-QDs and 2-MBTH-TGA-QDs were also measured and shown in Figure S1. Regardless of what kind of ligand is used, the emission wavelength of CdTe QDs can be tuned from 520 to 590 nm. All the fluorescence spectra band of CdTe QDs prepared with different ligands were relatively narrow and symmetric, and the full width at half maximum (FWHM) of the PL peaks were about 30-50 nm, which indicated that all as-prepared CdTe QDs were nearly mono-disperse and homogeneous [3]. The TEM images in Figure S3 also proved the as-prepared CdTe QDs are nearly mono-disperse and homogeneous. These results indicated that the addition of π-conjugated ligand did not affect the growing process of CdTe QDs. The emission intensity of TGA-QDs and 4-MBA-TGA-QDs were similar, while 2-MBTH-TGA-QDs had a little lower PL intensity and QYs than those of TGA-CdTe QDs. This may be due to the fact that large sterohindrance of 2-MBTH made the CdTe QDs have more surface defects than TGA-CdTe QDs and the defects quenched the fluorescence of CdTe QDs.

Figure S2 showed clearly that when the reaction time was the same, the emission wavelength and FWHM of CdTe QDs changed little whether 4-MBA, 2-MBTH or TGA was used as capping ligands. For example, when the reaction time was 2 hrs, no matter which ligand was used, the emission wavelength of the obtained CdTe QDs was about 550 nm and the FWHM was about 30 nm. These results further confirmed that using π-conjugated compounds as capping ligands of CdTe QDs did not disturb the growing process of CdTe QDs and high quality CdTe QDs can be prepared.

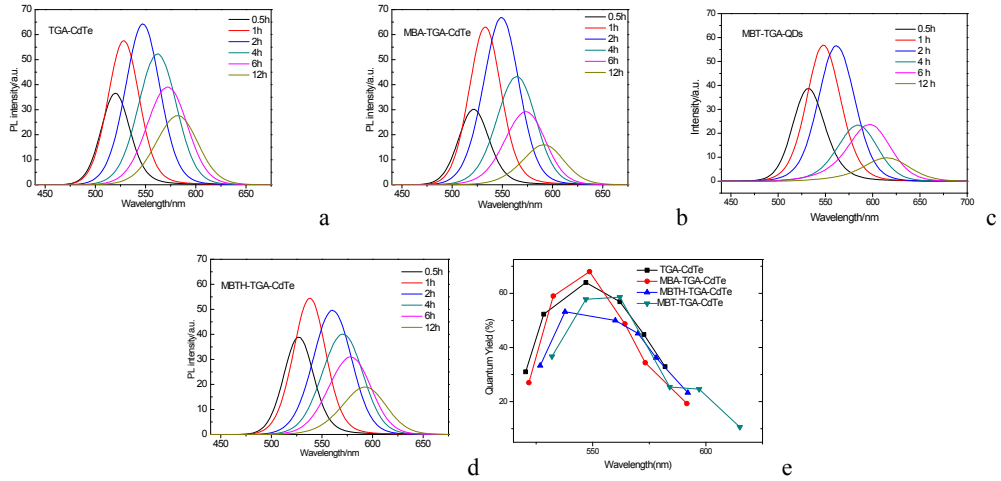
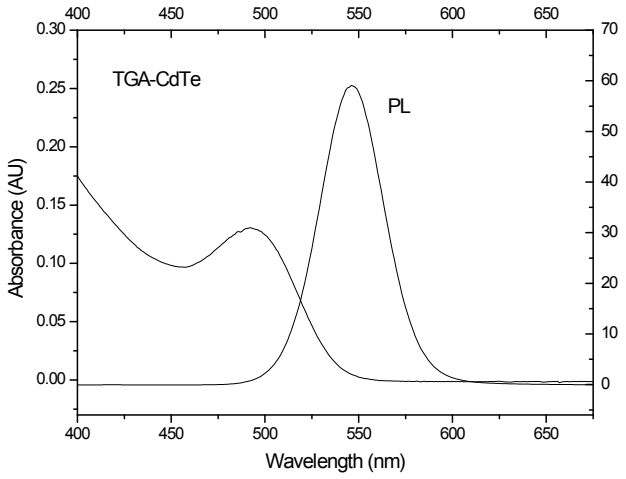
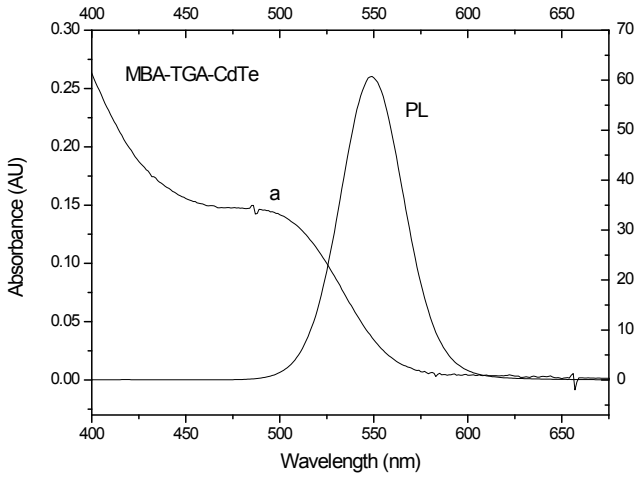


Figure S1. a-d, Fluorescence spectra of different ligands stabilized CdTe QDs at different reaction times. (a)TGA-CdTe (b)MBA-TGA-CdTe (c)MBT-TGA-CdTe (d)MBTH-TGA-CdTe (e) PLQYs of different ligands stabilized CdTe QDs at different reaction times (the concentration of QDs was same and the measurement conditions remain the same, λ ex=365nm)





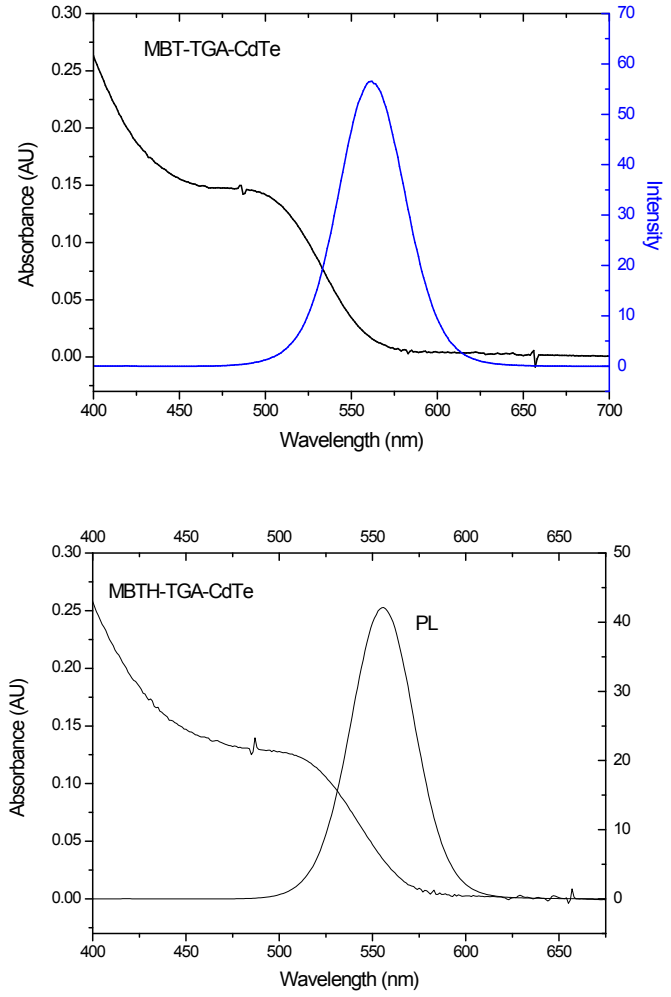


Figure S2. Absorption and emission spectrum of CdTe QDs (the reaction time was 2h, the concentration of QDs was same and the measurement conditions remain the same, λex=365nm)

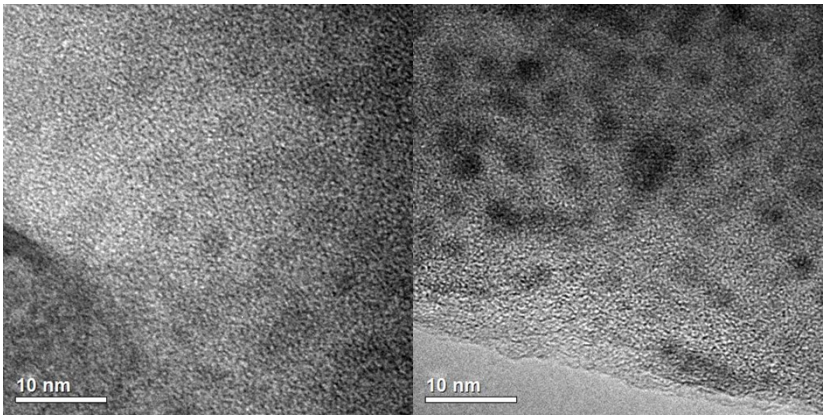


Figure S3. TEM image of TGA-CdTe (left) and MBA-TGA-CdTe QDs (right)

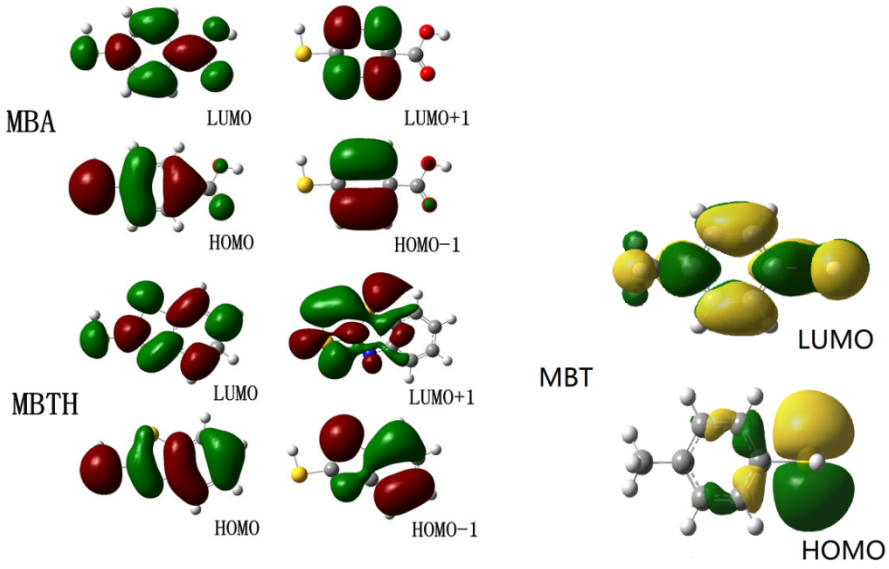


Figure S4. Representation of Frontier Molecular orbitals of MBA and MBTH. Calculated at B3LYP/6-31G (d) level with Gaussian 09W.

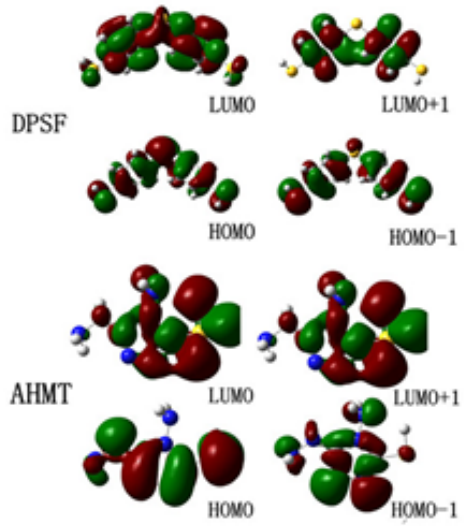


Figure S5. Representation of Frontier Molecular orbitals of DPSF and AHMT. Calculated at B3LYP/6-31G (d) level with Gaussian 09W.

Reference

[1] Qing Yang, Xi-minZhou, Yi-shuoZhu, Xing-guoChen J. Lumin. Volume 135, March 2013, 335–338

[2] Jacek Jasieniak, Marco Califano, and Scott E. Watkins. Acs nano. 5 (2011) 5888-5902

[3] C.R. Tang, Z.h. Su, B.G. Lin, H.W. Huang, Y.L. Zeng, S. Li, H. Huang, Y.J. Wang, C.X. Li, G.L. Shen, R.Q. Yu, Anal. Chim. Acta 678 (2010) 203.