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Supplementary data

XRD and HRTEM-SAED Studies of CdSe Quantum Dots

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Method: The crystalline structure of the quantum dots was studied using x-ray diffraction (XRD) (Philips PW3040 with filtered Cu Kα radiation (λ = 1.54056 Å) and JOEL JEM-1230 high resolution transmission electron microscope (HRTEM) at 200 keV.

Results and Discussion: The morphologies of CdSe quantum dots with different ligands are studied by the high-resolution transmission electron microscopy (HRTEM). The results indicate the crystalline phase of the TOPO capped CdSe quantum dots (Figure S1(b)) is not as clear as the other three (Figure S1(c), 1(f), 1(g)), because the bulky alkyl TOPO surfactants surrounded on the CdSe quantum dots. The selected area electron diffraction (SAED) studies show the crystalline quality is not as good as one would like. The results may be due to the size of quantum dot (~3nm) is too small to obtain clear diffraction patterns. Compared with the other three ligands capped CdSe quantum dots samples, there is no speckle in the TOPO capped CdSe quantum dots sample, because the bulky alkyl TOPO ligand makes the sample become an amorphous structure. However, the fast Fourier transform (FFT) of single crystal in the inset of the HRTEM images (Figure S1(b), S1(c), S1(f), S1 (g)) shows the crystalline is in high quality. The X-ray diffraction pattern (XRD) of CdSe quantum dots with different ligands are shown in Figure S2. The results are similar to that of SAED. The width of the diffraction peaks is considerably broadened as expected from quantum dots. The XRD patterns indicate the quantum dots exhibit hexagonal wurtzite phase[1]. The intensity of XRD peaks of TOPO capped CdSe quantum dots (Figure S2, line (a)) is weaker than those of other three ligands capped CdSe quantum dots (Figure S2, line (b), (c), (d)). The results are similar to that of HRTEM-SAED study that is due to the amorphous phase from bulky alkyl

TOPO surfactants on the surface of the CdSe quantum dots. We also find the peak positions of the XRD patterns remain the same after ligand exchange. Both HRTEM-SAED and XRD results show the crystalline structure of CdSe quantum dot not only remains but also improves by the ligand exchange of TOPO with thiol molecules.

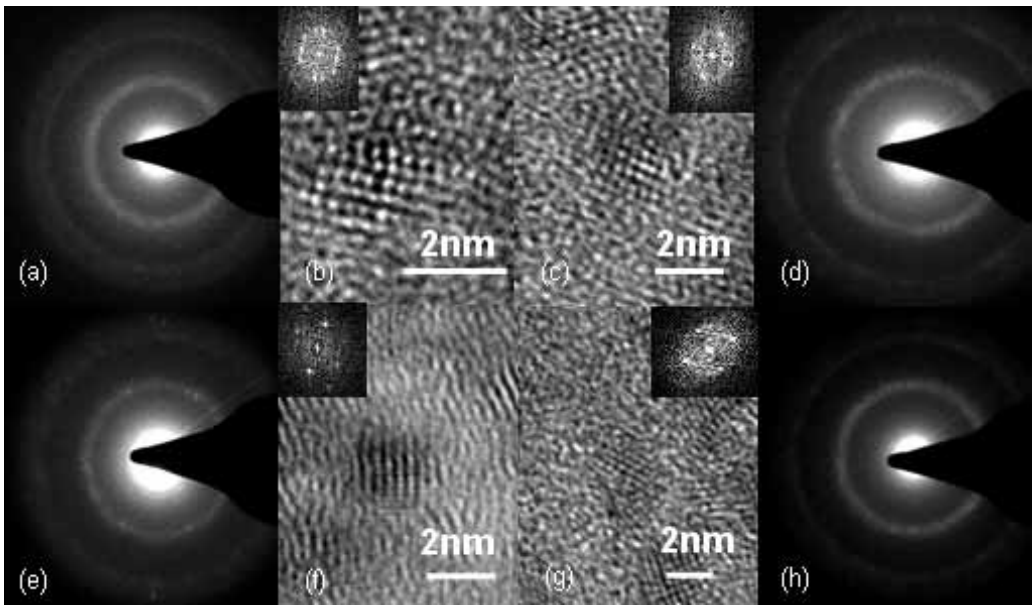

Fig. S1 HRTEM-SAED Images of CdSe quantum dots with different ligands: TOPO capped CdSe quantum dot s (a) SAED, (b) HRTEM; α-toluenethiol capped CdSe quantum dots (c) HRTEM, (d) SAED; thiophenol capped CdSe quantum dots (e) SAED, (f) HRTEM ; p-hydroxy thiophenol capped CdSe quantum dots (g) HRTEM, (h) SAED.

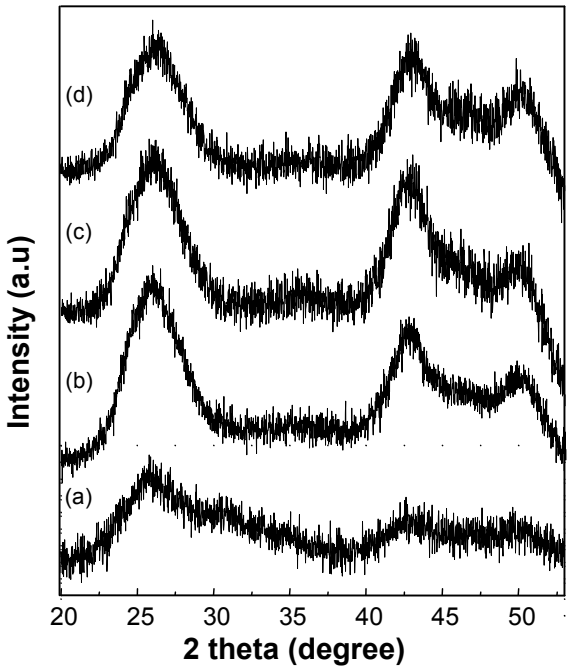

Fig. S2 Wide-angle powder X-ray diffractograms of (a) TOPO capped CdSe quantum dots, (b) α-toluenethiol capped CdSe quantum dots, (c) thiophenol capped CdSe quantum dots, (d) p-hydroxy thiophenol capped CdSe quantum dots.

Reference

1 D. V. Talapin, A. L. Rogach, A. Kornowski, M. Haase, and H. Weller, *Nano Lett.*, 2001, **1**, 207-211.