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# **Electronic Supplementary Information**

# Preparation of water-soluble, PEGylated, mixed-dispersant quantum dots, with preserved

# photoluminescence quantum yield

Christoph Zaba, Oliver Bixner, Florian Part, Christian Zafiu, Cherng-Wen Darren Tan and Eva-Kathrin Sinner\*

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#### **Experimental Details**

#### Reagents

All reagents were purchased from Sigma-Aldrich, USA, and used as received without further purification.

Cadmium chloride ( $\geq$  99.0 %), cadmium oxide ( $\geq$  99.99 %), tellurium powder (99.997 %), selenium powder (-100mesh, 99.99 % trace metal basis), sodium borohydride ( $\geq$  98.0 %), *N*-acetyl-L-cysteine ( $\geq$  99 %), synthetic ( $\pm$ )-α-lipoic acid ( $\geq$  99 % by titration), poly(ethylene glycol) methyl ether (M<sub>n</sub> 750), *N*,*N'*-dicyclohexylcarbodiimide (99 %), ReagentPlus<sup>®</sup> 4-(dimethylamino)pyridine ( $\geq$  99 %), trioctylphosphine (TOP) (technical grade, 90 %), trioctylphosphine oxide (TOPO) (technical grade, 90 %), hexadecylamine (HAD) (technical grade, 90 %), *n*-dodecylphosphonic acid, nonanoic acid (96 %), diethyl zinc solution (15 wt. % in toluene), hexamethyldisilathiane (synthesis grade), sodium sulfide (Aldrich), zinc chloride (99.999 %, trace metal basis), 1-dodecanethiol (DDT) ( $\geq$  98 % Aldrich), sodium sulfate (ACS reagent  $\geq$  99 %), sodium chloride (BioXtra  $\geq$  99.5 %), dichloromethane (anhydrous  $\geq$  99.8 %, contains 50 – 150 ppm amylene as stabilizer), methanol (CHROMA SOLV, for HPLC,  $\geq$  99.9 %), ethanol (CHROMA SOLV, absolute, for HPLC  $\geq$  99.8 %), ethylene glycol (anhydrous, 99.8 %), N-methyl-2-pyrrolidone (anhydrous, 99.5 %), 2-propanol (LC-MS CHROMASOLV), hexane (anhydrous 95 %), ethyl acetate (CHROMA SOLV Plus, for HPLC, 99.9 %), 1-butanol (ACS reagent,  $\geq$  99.4 %), ultra-pure water (Millipore Milli-Q-Integral 10, R=18.2 MΩcm).

All reactions, especially melt ligand exchange, were performed under inert gas conditions to prevent oxidation.

#### **Measurement conditions**

**TEM and analysis:** TEM images were recorded on a FEI Tecnai G2 20 transmission electron microscope operating at 160 kV. Samples were prepared by dropping toluene dispersions onto 300-mesh carbon-coated copper grids and subsequently evaporating the solvent in air. Size distributions were evaluated using ImageJ.<sup>[1]</sup>

**TGA measurements:** Thermograms were recorded on a Mettler-Toledo TGA/DSC 1 STAR System in the temperature range 25 - 650 °C with a ramp of 10 K/min in synthetic air. 70 µl aluminum oxide crucibles were filled with 0.5 – 2 mg sample and the rest mass was evaluated by horizontal step setting.

<sup>1</sup>**H-NMR measurement:** <sup>1</sup>H-solution spectra were collected on a Bruker DPX operating at 300 MHz using TMS as an internal standard.

**ATR-FTIR measurements:** Mid-IR powder spectra of the lyophilized samples were collected using a Bruker Tensor 37 FTIR spectrometer with a Bruker Platinum Diamond single reflection ATR equipment at a resolution of 4 cm<sup>-1</sup> by averaging 32 scans.

**UV-Vis spectroscopy:** UV-Vis absorption spectra were collected at a scan speed of 400 nm/min on a Hitachi UV-2900 spectrophotometer.

**EDX measurement:** EDX measurements were carried using a FEI Inspect S50 scanning electron microscope (SEM) equipped with an AMETEK/EDAX device. Electron penetration depth is limited, and precatuions were taken to only analyze the sample's topmost layer. For this purpose a thick and homogeneous layer of sample of around 1 mm height was loaded onto the sample holder to largely avoid signal contributions from the support. As such, the measurements should primarily reflect the sample composition.

**Fluorescence spectroscopy**: Fluorescence spectra were recorded with a PerkinElmer LS 55 luminescence spectrometer at room temperature. The absorbance of each sample was adjusted to OD values below 0.1 to avoid homo-aggregation and self-quenching effects. The emission spectra were collected in the range between 500 – 750 nm at a scan speed of 400 nm/min and an excitation and emission slit-width of 4 nm. The photoluminescence quantum yields (PLQY) were determined according to a protocol of Würth *et al.* and, for comparison, also according to similar methods described in literature.<sup>[2-5]</sup> Würth recommended choosing an excitation wavelength at plateau-like regions of the sample's absorption spectra. For this reason, we chose fluorescein in 0.1 M NaOH as a reference material at an excitation wavelength of 470 nm. To illustrate the importance of careful reference selection we compared our measurements to those using Rhodamine 6G in EtOH at an excitation wavelength of 400 nm as a reference, as was used in several published studies.<sup>[3-6]</sup> Brouwer reviewed that Rhodamine 6G should be used when excited at wavelengths between 470 – 510 nm, instead of the low wavelengths typically reported.<sup>[7]</sup> This is of concern since exciting Rhodamine G, or any reference material, at wavelengths too low for adequate excitation would introduce significant errors in PLQY determination. To illustrate this problem, we measured PLQY using both fluorescein ( $\lambda_{ex}$  = 470 nm according to the recommendations of Würth *et al.*) as well as Rhodamine 6G ( $\lambda_{ex}$  = 400 nm according to other published protocols).<sup>[2-5]</sup> The resultant disparity in PLQY, of low values obtained with fluorescein and high values obtained with Rhodamine G, is show in Table S2.



**Figure S1.** Normalized absorption (full lines) and emission spectra (dashed lines) of aqueous-synthesized DHLA-PEG<sub>750</sub>-OMe-capped CdTe/CdS/ZnS core-shell-shell QDs (green), DHLA-PEG<sub>750</sub>-OMe-capped high-temperature synthesized CdSe/ZnS reference (red) and the fluorescein standard (blue). Samples were excited in ultrapure water at a wavelength of 470 nm.

### SI 1 Synthesis and spectral characteristics of ligand

#### SI 1.1 DHLA-PEG<sub>750</sub>-OMe



DHLA-PEG<sub>750</sub>-OMe was synthesized as reported in the literature with slight modifications.<sup>[8, 9]</sup> 2.48 g (±)- $\alpha$ -lipoic acid (12.00 x 10<sup>-3</sup> mol), 9 g poly(ethylene glycol) mono methyl ether (12.00 x 10<sup>-3</sup> mol), 147 mg 4-(dimethylamino)pyridine (1.20 x 10<sup>-3</sup> mol) and 60 mL dichloromethane were placed in a round-bottom flask and degassed with a stream of nitrogen (N<sub>2</sub>) for 30 minutes. After cooling the mixture to 0 °C in an ice-bath, a solution of 2.72 g dicyclohexylcarbodiimide (13.20 x 10<sup>-3</sup> mol) in 20 mL dichloromethane was added dropwise. The reaction mixture was stirred at 0 °C for 60 minutes. After removing the ice-bath the reaction mixture was allowed to warm to room temperature and stirred for 20 h. The crude reaction mixture was filtered through a paper-filter to remove the contaminating precipitate. The filtrate was diluted with dichloromethane to a volume of 100 mL and extracted three times with brine (100 mL each). The combined organic extracts were dried over sodium sulfate, filtered and evaporated to dryness under reduced pressure at room temperature to give lipoic acid (LA)-PEG<sub>750</sub>-OMe as a yellow oil in 95 % yield (TLC EtOAc/MeOH = 9/1 (v/v); R<sub>f</sub> = 0.35).

8.45 g LA-PEG<sub>750</sub>-OMe (9.00 x  $10^{-3}$  mol) was dissolved in 20 mL ethanol 20 mL and cooled to 0 °C in an ice-bath. 375 mg sodium borohydride (10.00 x  $10^{-3}$  mol) was slowly added to 80 mL ice-cold water, then added drop-wise to the pre-cooled alcoholic solution. After complete addition the ice-bath was removed and the reaction mixture was stirred for 4 h at room temperature under inert atmosphere. Ethanol was removed *in vacuo* at room temperature and the aqueous phase was extracted three times with dichloromethane (80 mL each). The combined organic phases were dried over sodium sulfate and filtered. After evaporation of the solvent, DHLA-PEG<sub>750</sub>-OMe was obtained as a clear colorless oil, at a yield of 96 %.

<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300MHz, ppm): 4.25 (t, 2H, -COOCH<sub>2</sub>-), 3.66 (m, ~66H, -CH<sub>2</sub>OCH<sub>2</sub>-), 3.40 (s, 3H, -OCH<sub>3</sub>), 2.93 (m, 1H, -CH-), 2.73 (m, 2H, -CH<sub>2</sub>S-), 2.37 (t, 2H, -CH<sub>2</sub>COO-), 1.90 (m, 2H, -CH<sub>2</sub>OMe), 1.45 – 1.85 (m, 8H, -CH<sub>2</sub>-), 1.37 (t, 1H, -SH), 1.32 (d, 1H, -SH)

ATR-FTIR (liquid, cm<sup>-1</sup>): 2865 (CH<sub>2</sub>, s), 2554 (SH, vw) 1732 (COOR, s), 1454 (g-CH<sub>2</sub>, m), 1349 (g-CH<sub>2</sub>, m), 1296 (CH<sub>2</sub>, m), 1248 (CH<sub>2</sub>, m), 1096 (C-O, C-C, vs), 1039 (C-O, C-C, m), 947 (g-CH<sub>2</sub>, m), 849 (g-CH<sub>2</sub>, m)

**TLC**: EtOAc/MeOH = 9/1 (v/v); R<sub>f</sub> = 0.35

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Figure S2: <sup>1</sup>H-NMR of DHLA-PEG<sub>750</sub>-OMe in CDCl<sub>3</sub>.



Figure S3: ATR-FTIR profile of liquid DHLA-PEG<sub>750</sub>-OMe.

### SI 2 Synthesis and characterization of NAC-CdTe/CdS/ZnS-QD

*N*-acetyl-L-cysteine–coated core-shell-shell cadmium telluride/cadmium sulfide/zinc sulfide (NAC-capped CdTe/CdS/ZnS) QDs were synthesised according to a modified procedure of Xiao *et al.* (2012).<sup>[10]</sup>

#### SI 2.1 Synthesis of NAC-capped CdTe-cores

Sodium hydrogen telluride (NaHTe) was prepared by reacting tellurium powder (Te) with sodium borohydride (NaBH<sub>4</sub>) in N<sub>2</sub>-purged ultra-pure water. The employed molar ratio of NaBH<sub>4</sub> to Te was 2 : 1. A stock solution was prepared by mixing 50.0 mg NaBH<sub>4</sub> ( $1.30 \times 10^{-3}$  mol) and 83.0 mg Te ( $6.50 \times 10^{-4}$  mol) in a 50 mL-Schlenk flask. Under inert gas atmosphere 10 mL ice-cold N<sub>2</sub>-saturated ultra-pure water was added. The mixture was stirred under a constant N<sub>2</sub> stream in an ice-bath for 60 minutes and then allowed to warm up to room temperature until the reaction was completed (5 – 6 hours). The freshly prepared purple NaHTe stock solution was kept under N<sub>2</sub>-atmospheare at 4 °C until further use.

18.3 mg CdCl<sub>2</sub> (1.00 x  $10^{-4}$  mol) and 40.8 mg NAC (2.50 x  $10^{-4}$  mol) were dissolved in 40 mL N<sub>2</sub>-saturated ultra-pure water. The pH of the precursor solution was adjusted to 8.3 by addition of 1.0 M NaOH and it was subsequently purged with N<sub>2</sub> for 30 minutes at room temperature.

0.77 mL NaHTe stock-solution (5.00 x  $10^{-5}$  mol) was quickly injected into the precursor solution at room temperature under inert-atmosphere and vigorous stirring. The reaction mixture was heated to 100 °C and refluxed for 60 minutes to obtain green-emitting CdTe cores ( $\lambda_{em} \sim 525$  nm). The reaction was quenched in an ice-water-bath. The crude mixture was lyophilized, resuspended in 1 – 2 mL ultra-pure water and syringe-filtered through a 0.2 µm polyethersulfone (PES) membrane (Millex, Merck-Millipore). The resultant quantum dots were precipitated in 45 mL cold 2-propanol, collected by centrifugation at 3,200 x g, for 10 min, at 4 °C, then dried under high vacuum for 1h.

### SI 2.2 Synthesis of NAC-capped CdTe/CdS core-shell QDs

The precipitated NAC-capped CdTe-cores were re-dispersed in 40 mL N<sub>2</sub>-saturated ultra-pure water containing 183.3 mg CdCl<sub>2</sub> (1.00 x 10<sup>-3</sup> mol), 15.6 mg Na<sub>2</sub>S (2.00 x 10<sup>-4</sup> mol) and 811.0 mg NAC (5.00 x 10<sup>-3</sup> mol). The solution was purged with N<sub>2</sub> for 30 minutes at room temperature and heated to 100°C for 45 min to obtain yellow-emitting CdTe/CdS core-shell QDs ( $\lambda_{em} \sim 564$  nm). The reaction was then quenched in an ice-water-bath, lyophilized, resuspended in 1 – 2 mL ultra-pure water and syringe-filtered through a 0.2 µm PES-membrane (Millex, Merck-Millipore). The core-shell QDs were precipitated in 45 mL cold 2-propanol, collected by centrifugation at 3,200 x g, for 10 min, at 4 °C, then dried under high vacuum for 1h.

#### SI 2.3 Synthesis of NAC-capped CdTe/CdS/ZnS core-shell-shell QDs

The precipitated NAC-capped CdTe/CdS QDs were re-dispersed in 40 mL N<sub>2</sub>-saturated ultra-pure water containing 136.3 mg ZnCl<sub>2</sub> (1.00 x  $10^{-4}$  mol), 15.6 mg Na<sub>2</sub>S (2.00 x  $10^{-4}$  mol) and 811.0 mg NAC (5.00 x  $10^{-3}$  mol). The solution was purged with N<sub>2</sub>

for 30 minutes at room temperature and heated to 60°C for 30 min to obtain orange-emitting CdTe/CdS/ZnS core-shellshell QDs ( $\lambda_{em} \sim 588$  nm). The reaction was quenched in an ice-water-bath, lyophilized, resuspended in 1 – 2 mL ultra-pure water and syringe-filtered through a 0.2 µm PES-membrane (Millex, Merck-Millipore). The core-shell-shell QDs were precipitated in 45 mL cold 2-propanol, collected by centrifugation at 3,200 x g, for 10 min, at 4 °C, then dried under high vacuum overnight. The QDs were stored at 4 °C under nitrogen until further use.



SI 2.4 EDX, UV/Vis and fluorescence spectroscopy

Figure S4: Energy dispersive x-ray (EDX) spectrum of NAC-capped CdTe/CdS/ZnS QDs and calculated sample composition.



**Figure S5**: UV/Vis absorption (full lines) and photoluminescence (dashed lines) spectra of green-emitting NAC-capped CdTe core QDs ( $\lambda_{em}$  = 525 nm, green), orange-emitting NAC-capped CdTe/CdS QDs ( $\lambda_{em}$  = 564 nm, orange) and orange-red-emitting NAC-capped CdTe/CdS/ZnS QDs ( $\lambda_{em}$  = 588 nm, red). (Colors are described as green, yellow and orange in text).

## SI 3 Ligand exchange and characterization of DHLA-PEG<sub>750</sub>-OMe-capped CdTe/CdS/ZnS QDs

All ligand exchange reactions were performed using the same batch of DHLA-PEG<sub>750</sub>-OMe stock solution and NAC-capped CdTe/CdS/ZnS QDs, in order to avoid batch-specific variation.

## SI 3.1 Direct ligand exchange

a) 1:1 molar ratio of NAC to DHLA-PEG<sub>750</sub>-OMe direct ligand exchange



The QD size was approximately 3.2 nm according to the micrographs. The sample had to be drop-cast using MeOH due to incomplete ligand exchange and a high percentage of residual NAC-capped QDs. DHLA-PEG<sub>750</sub>-OMe-capped QDs were observed as well-separated individual nanocrystals and poorly-exchanged NAC-capped QDs were observed to aggregate as darker areas of poor contrast (a). A more detailed micrograph, at higher magnification, of these regions is show in (b).

# SI 3.2 Melt ligand exchange



**Figure S7**: TEM micrographs of DHLA-PEG<sub>750</sub>-OMe-capped CdTe/CdS/ZnS QDs after 12h of melt ligand exchange. The QDs were of size similar to those prepared using direct ligand exchange. DHLA-PEG<sub>750</sub>-OMe-capped QDs were observed as well-separated individual nanocrystals (a). A more detailed micrograph, at higher magnification, is shown in (b).

The following lists the solvents used for the various melt ligand exchange reactions:

## a) Aqueous melt

200µl of ultra-pure water was used as solvent

# b) Methanolic melt

 $200 \mu l$  of MeOH was used as solvent

# c) Ethylene glycol melt

200µl of EG was used as solvent

## d) N-methyl-2-pyrrolidone melt

 $200 \mu l$  of NMP was used as solvent

## SI 3.3 EDX, TGA, ATR-FTIR, UV/Vis and fluorescence spectroscopy



Figure S8: Representative EDX spectrum of DHLA-PEG<sub>750</sub>-OMe-capped CdTe/CdS/ZnS QDs exhibiting a C/O-ratio of 2.3/1,

which closely matches the composition of PEG-repeat units.

Exchange method	–∆m <sub>tot</sub> [%w/w]	–∆m <sub>NAC</sub> [%w/w]	–∆m <sub>PEG</sub> [%w/w]	–∆m <sub>NAC,corr</sub> [%w/w]	–∆m <sub>PEG,corr</sub> [%w/w]	ρ <sup>graft</sup> tot [nm <sup>-2</sup> ]	σ <sup>graft</sup> <sub>corr</sub> [nm <sup>-2</sup> ]
None (NAC-capped)	30	18	12 <sup>a</sup>	30	0	4.3	4.3
1:10 direct ligand	70	23	47	38	32	4.7 <sup>b</sup>	0.9
aqueous melt	66	16	50	27	39	3.9	1.3
MeOH melt	64	15	49	25	39	3.6	1.3
EG melt	66	9	57	15	51	3.9	2.1
NMP melt	55	9	46	15	40	2.4	1.3
reference <sup>c</sup>	47	4	43	/	/	2.2	2.2

Table S1: TGA values obtained for var	ious QD preparations
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<sup>a</sup>Refers to NAC residue.

<sup>b</sup>A value higher than that of the starting material suggests slight impurities of residual free DHLA-PEG<sub>750</sub>-OMe in this

preparation.

<sup>c</sup>Melt ligand exchange of TOP/TOPO-capped CdSe/ZnS QDs.

 $-\Delta m_{\text{NAC}}$  was obtained from horizontal step setting in the interval 150 – 280°C.

 $-\Delta m_{PEG}$  was calculated by subtraction of  $-\Delta m_{NAC}$  from  $-\Delta m_{tot}$  which corresponds to the remaining mass loss in the interval

280 – 550°C.

Corrected values for the lost mass fractions of the melt preparations ( $-\Delta m_{NAC,corr}$ ) were obtained by accounting for the persistent NAC content above 280 °C (NAC residue) in addition to the primary mass loss [150 – 280 °C] (e.g. for the aqueous melt  $-\Delta m_{NAC,corr}$ = $-\Delta m_{NAC}$ –12/18 x  $\Delta m_{NAC}$ = – 26.7%).  $-\Delta m_{PEG,corr}$  corresponds to the difference  $-\Delta m_{tot}$ – $\Delta m_{NAC,corr}$ .

Equation S1: Grafting densities were calculated according to Benoit et al.:[11]

$$\rho^{graft} = \frac{\frac{(\%\frac{W}{W})_{shell}}{(\%\frac{W}{W})_{core}} * \rho_{core} * V_{core} * N_A}{S_{core} * M_{lig}}$$

 $M_{ligand}$  for NAC was assumed to be that of NAC<sup>-</sup>Na<sup>+</sup> (see FTIR and EDX spectra).

Corrected grafting densities ( $\rho_{corr}^{graft}$ ) refer to DHLA-PEG750-OMe ligands only, therefore  $-\Delta m_{PEG,corr} = -\Delta m_{tot,shell}$ .



**Figure S9**: Scaled ATR-FTIR spectra of NAC- (**red**) and DHLA-PEG<sub>750</sub>-OMe- (**blue**) capped CdTe/CdS/ZnS QDs before (**dark**) and after (**light**) TGA. The spectra show minimal residual ligand absorption.

Exchange method	λ <sub>abs</sub> [nm]	λ <sub>em</sub> [nm]	Δ Stokes [nm]	Δ FWHM [nm]	Φ [%]
None (NAC-capped)	554	588	34	53	5 - 14
1:10 direct ligand exchange	554	602	54	56	4 - 10
aqueous melt	548	602	54	57	5 – 13
MeOH melt	554	590	36	57	5 – 14
EG melt	548	602	54	57	5 – 12
NMP melt	548	589	41	29	2 – 4
reference melt	586	592	6	29	3 – 8
None (TOP/TOPO-capped)	586	592	6	29	11 – 27

Table S2: Spectral data of QDs prepared using various methods

#### SI 4 High temperature-synthesized TOP/TOPO capped-CdSe/ZnS QDs and ligand exchange

## SI 4.1 TOP/TOPO capped-CdSe/ZnS QDs

TOP/TOPO-capped CdSe cores were prepared according to Reiss *et al.* while the ZnS shell was formed according to Dabbousi *et al.* to give the core-shell architecture for our reference QDs.<sup>[6, 12]</sup>

In brief, 51.4 mg CdO (4.00 x 10<sup>-4</sup> mol), 2.85 mL HDA and 1.15 mL TOPO were placed in a three-neck round-bottom flask and heated under N<sub>2</sub>-atmosphere to 270 °C. After addition of 230  $\mu$ L dodecylphosphonic acid (8.00 x 10<sup>-4</sup> mol) the temperature of the, now-colorless, solution was lowered to 250 °C. Next, 2.5 mL of 0.2 M Se in TOP was rapidly injected into the precursor solution and nanocrystal growth was stopped after approximately 20 minutes to give yellow/orange-emitting TOP/TOPO-capped CdSe cores ( $\lambda_{em}$  = 589 nm). Once the mixture had cooled to about 100 °C, 1.0 mL of nonanoic acid was added to prevent solidification of the mixture. The crude reaction mixture was transferred at 50 °C into 10 mL methanol. The QDs were collected by centrifugation at 3,400 x g, for 15 min, at 20 °C. The pellet was washed three times with MeOH and finally re-dispersed in chloroform and photometrically adjusted to a concentration of 1.1 mM.

Next, 2 mL of the QD-core stock solution was transferred into a melt of 5 g TOPO ( $12.93 \times 10^{-3}$  mol) and 1.5 mL TOP ( $3.36 \times 10^{-3}$  mol) which was pre-heated under vacuum to 190 °C for 2 – 3 hours and subsequently cooled to 60 °C prior to addition of the QDs. Chloroform was removed under reduced pressure and the temperature was raised to 160 °C.

Then, 0.76 g diethylzinc ( $6.20 \times 10^{-3}$  mol) and 0.22 g hexamethyldisilathiane ( $1.20 \times 10^{-3}$  mol) were mixed separately in 5 g TOP ( $13.49 \times 10^{-3}$  mol) under inert gas to give the shelling solution. Aliquots of 0.5 mL of the shelling solution were added to the CdSe-cores at 160 °C to form a passivating layer of ZnS. After each addition, the sample fluorescence properties were

measured. The photoluminescence quantum yield maximum was obtained after addition of three to four aliquots of shelling solution. The resultant core-shell QDs were cooled to 90 °C and stirring was continued for 2 – 3 hours. While cooling to room temperature 5 mL of 1-butanol was added to prevent solidification. The QDs were recovered by precipitation as described above and repeatedly wash with MeOH. They were finally re-dispersed at a concentration of 15 mg/mL in chloroform.



**Figure S10**: TEM micrograph of TOP/TOPO-capped CdSe/ZnS QDs after high temperature-synthesis and the corresponding size histogram.



Figure S11: EDX-spectrum of TOP/TOPO-capped CdSe/ZnS QDs.

### SI 4.2 Melt ligand exchange

Preparation of DHLA-PEG<sub>750</sub>-OMe-capped CdSe/ZnS QDs *via* methanolic melt ligand exchange was carried out using a modified procedure of Uyeda *et al.*<sup>[9]</sup>

First, 15 mg of TOP/TOPO-capped QDs (see SI 4.1) were suspended in 200  $\mu$ L MeOH. Next, 200  $\mu$ g DHLA-PEG750-OMe (2.00 x 10<sup>-4</sup> mol) was added and the reaction mixture was heated to 65 °C under inert gas with stirring for 12 hours. After cooling to room temperature the solvent was removed under reduced pressure using a rotary evaporator. The crude reaction mixture was resuspended in 3 – 6 mL of ethanol. Then, 3 – 7 mL of hexane was added slowly until a monophasic turbid solution was formed. The resultant DHLA-PEG750-OMe-capped, water-soluble QDs were collected by centrifugation at 3,200 x *g*, for 15 min, at 20 °C. The clear supernatant was discarded and the pellet was resuspended in 2 mL of ultra-pure water, filtered through a 0.2  $\mu$ m PES syringe-filter and freeze-dried.



Figure S12: TEM micrograph of DHLA-PEG<sub>750</sub>-OMe-capped CdSe/ZnS QDs. The size of the QDs was approximately 4.2 nm as

determined from the micrographs (a). A more detailed micrograph, at higher magnification, is show in (b).

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