

Supplemental Materials

High-Conjugation-Efficiency Aqueous CdSe Quantum Dots

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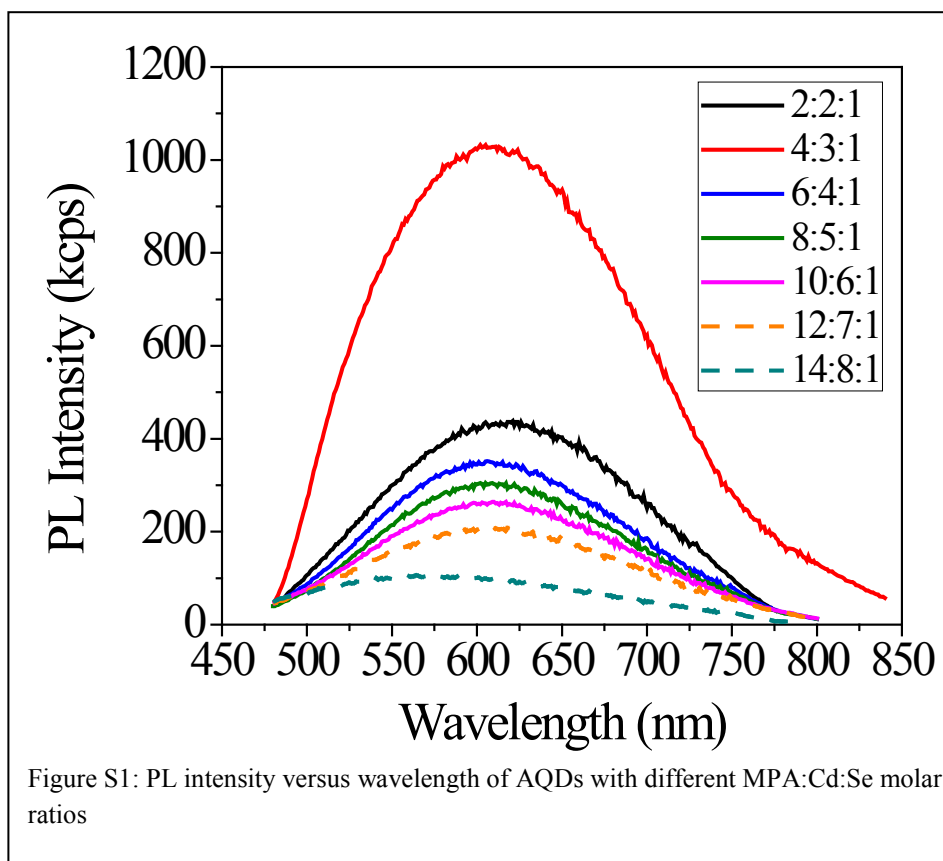
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Materials and Methods

1. CdSe AQDs synthesis at different MPA:Cd:Se ratios

A cadmium precursor solution (0.08 M) was first prepared by dissolving 1.19 g of Cd(NO₃)₂ powder (Alfa Aesar, Ward Hill, USA) in 50 mL of deionizer (DI) water. The selenium precursor solution (0.08 M) was prepared by dissolving 0.315 g of a selenium powder (Sigma-Aldrich, MA) and 8.2 g of sodium sulfite (Na₂SO₃) (Sigma-Aldrich, MA) in 50 mL DI water at 80°C under constant stirring for 2 hours until the selenium was completely dissolved. These precursor solutions were stored for later use.

To make such AQDs, an appropriate amount of 3- mercaptopropionic acid (MPA) (Sigma-Aldrich, St Louis, MO, USA) was added to 40 ml of DI water and stirred for 10 minutes, followed by adjusting the pH to 11 using tetrapropylammonium hydroxide (TMAH) (Alfar Aesar, Ward Hill, USA). Next, 1 ml of the 0.08M Cd(NO₃)₂ precursor was added and stirred for 10 minutes. 1 ml of the selenium precursor was then added to the MPA-Cd mixture, followed by quickly adjusting the pH to 12, stirred for 10 minutes to precipitate the CdSe AQDs. To further enhance the photoluminescence (PL) intensity, an appropriate amount of excess Cd precursor was added to the above CdSe AQDs suspension followed by quickly re-adjusting the pH to 12. The thus-obtained CdSe AQD suspension was clear with a dark yellow tint. The final concentration of the MPA-capped CdSe AQDs was 1.6 mM in terms of the Se atom with a nominal molar ratio MPA:Cd:Se = 2:2:1, 4:3:1, 6:4:1, 8:5:1, 10:6:1, 12:7:1 and 14:8:1. The PL of the MPA-capped CdSe AQDs were measured using a QM4/2005 spectrofluorometer (Photon Technology International, Birmingham, MA, USA) and a USB2000 UV-vis spectrometer (Ocean Optics, NJ, USA) respectively. It was found that CdSe AQDs with MPA:Cd:Se = 4:3:1 provided the best PL intensity as shown in Fig. S1. For storage, the suspension was kept at pH = 12 at 4°C. This may be understood as follows. Under basic conditions each excess Cd was chelated with two MPA's.¹ These MPA-chelated excess Cd's would mostly sit on top of the Se's on the AQD surface, forming a MPA-chelated Cd "shell" on the AQDs surface. The fact that the CdSe AQDs had a size of 4 nm size and that the nominal molar ratio, MPA:Cd:Se of 4:3:1 support the notion that there was a MPA-chelated Cd "shell" on the CdSe AQDs. In addition, given that the emission of the AQDs was due to surface trap states, the notion that the AQDs had a MPA-chelated Cd "shell" was also consistent with the fact that the emission of the AQDs increased with an increasing amount of extra Cd and MPA (with a 1:2 Cd:MPA molar ratio). Note packing an extra amount of MPA on the AQD surface through the chelation of extra MPA to extra Cd precursor was only possible in an aqueous environment.



2. *Standard curve for the number of Streptavidin, AQDs and OQDs determined by gel-electrophoresis analysis*

To generate the standard curves for SA, AQD and OQD, we loaded each channel with 15 μL of a SA solution or a QD suspension of different concentrations. We had a total of 3 separate gels for SA, AQD, and OQD each. The concentration range was 0.2-2 μM . Each molar concentration was converted to the number of SA or QD by multiplying the molar concentration of SA or QD by the volume (15 μl) and by the Avogadro's number (6.02×10^{23}) as follows.

$$\# SA = [SA] \mu\text{M} \times 15 \mu\text{l} \times 6.02 \times 10^{23} \text{ molecule/mole}$$

$$\# QD = [QD] \mu\text{M} \times 15 \mu\text{l} \times 6.02 \times 10^{23} \text{ molecule/mole}$$

The total intensity of each band was obtained by integrating the number of pixels per unit area over the entire area of the band for each SA and each QD concentration using AlphaView software. The obtained standard curves of integrated intensity versus concentration were plotted in Figs. S2(a), S2(b), and S2(c) for AQDs, OQDs, and SA,

respectively. Also shown on the top x-axis are the corresponding total numbers of AQDs, OQDs, and SA in a volume of 15 μl .

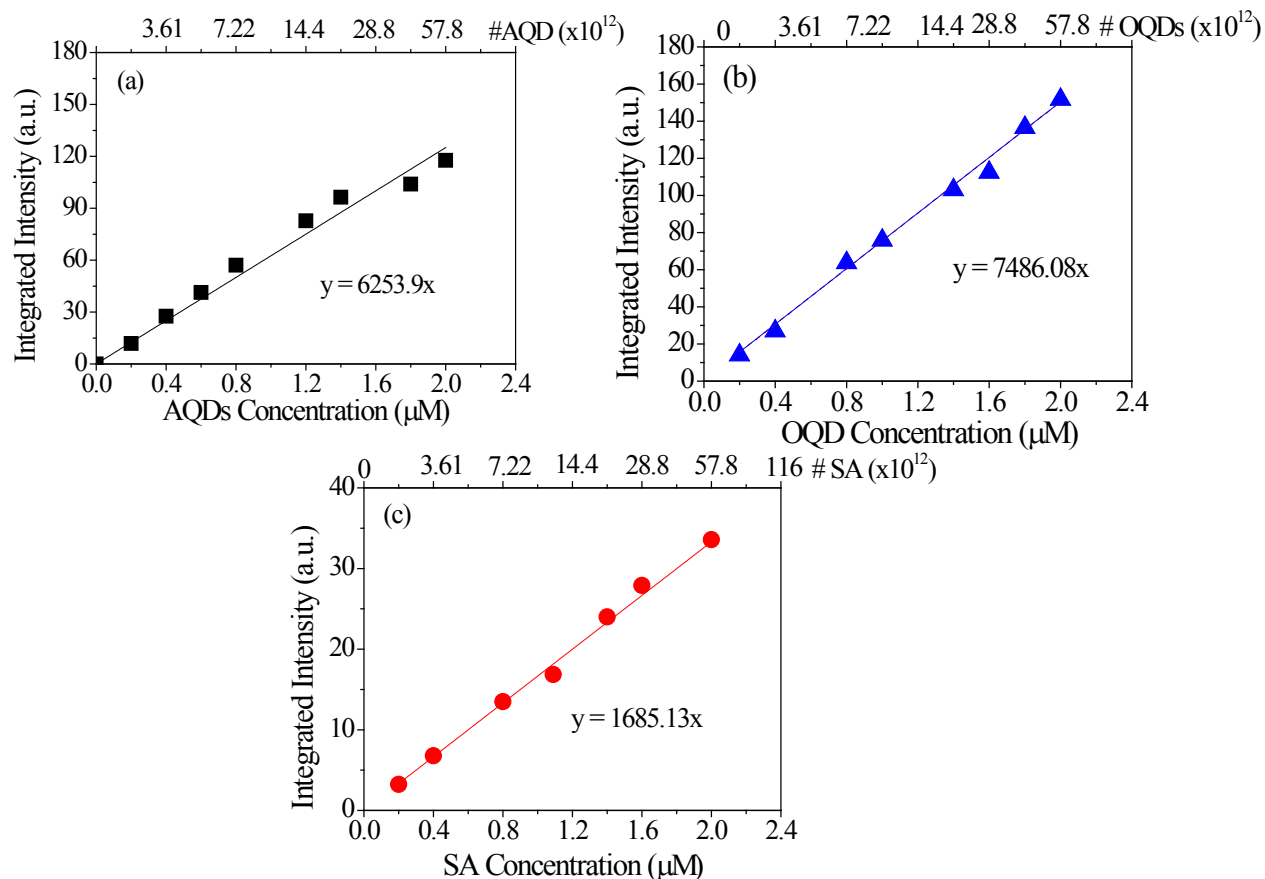


Figure S2. Standard curve of integrated intensity vs. concentration of (a) AQDs, (b) OQDs, (c) SA. The number of AQDs, OQDs, and SA deduced in the 15ml of each concentration was labeled on the top x-axis of (a), (b), and (c), respectively.

Based on these standard curves the total number of SA, AQDs, or OQDs in each band in Fig. S2 was deduced. The total number of bound SA per QD in each band was obtained by dividing the total number of SA by the total number of QDs in the same band.