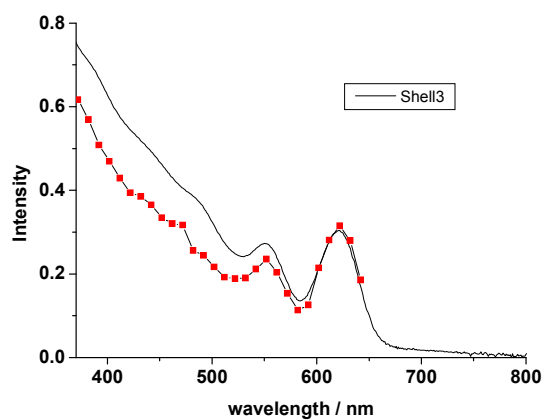
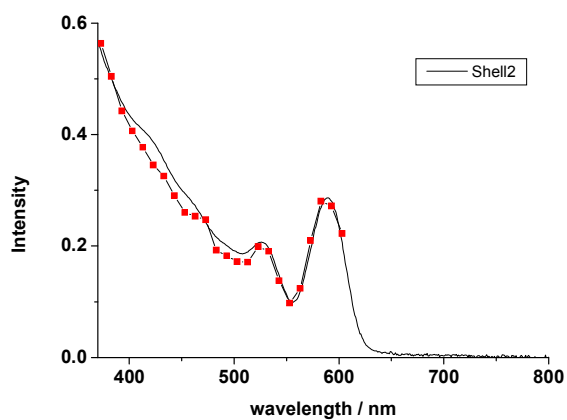
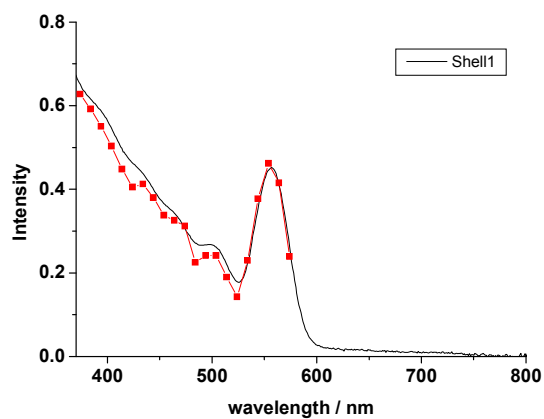
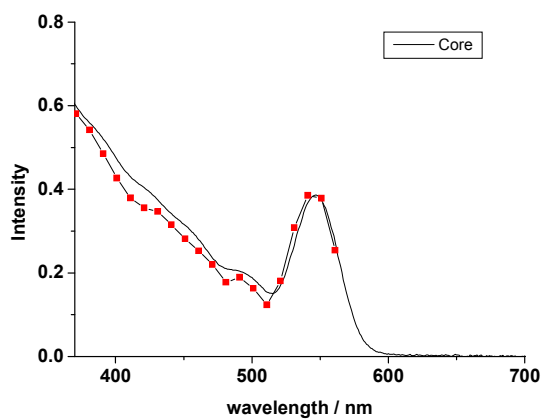


Supporting Information for “Extinction Coefficients, Oscillator Strengths and Radiative Lifetimes of CdSe, CdTe and CdTe/CdSe Nanocrystals”

Ke Gong, Youhong Zeng and David F. Kelley

PLE spectra.



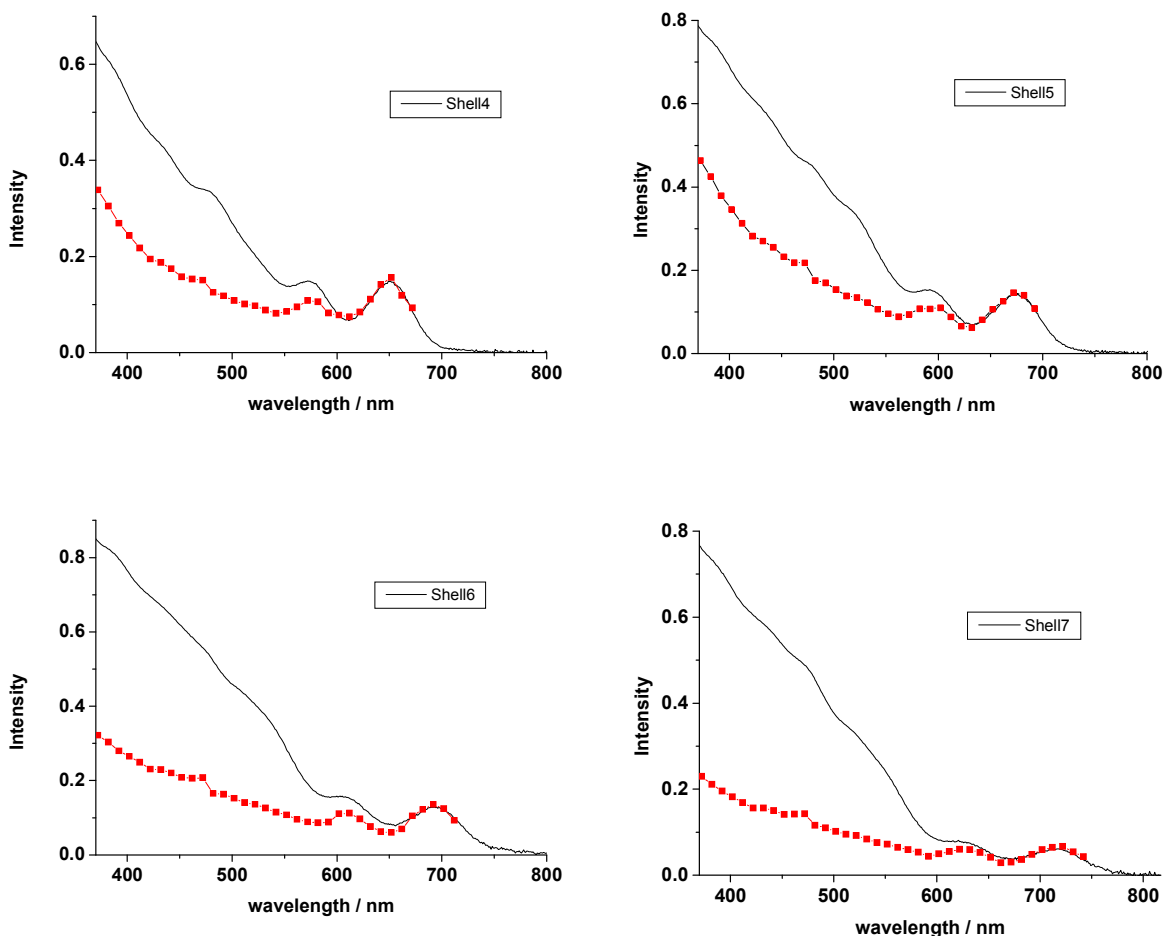


Figure SI-1. Comparison of absorption ($10^{-\text{absorbance}}$) and excitation spectra of CdTe core and subsequent CdSe shell growth.

Particle syntheses.

Standard synthesis:

0.4 mmol of CdO was mixed with 1.6 mmol (0.45 g) of stearic acid and 4g (5.0 ml) octadecene (ODE) which was heated to 250 °C to get a colorless solution under N₂ flow. After cooling to room temperature, 3g of octadecyl amine (ODA) and 1g of trioctylphosphine oxide (TOPO) were added. The mixture was then heated to 280 °C. At this temperature, a selenium solution containing 4 mmol of Se, 0.944 g (4.7 mmol, 1.15 ml) of tributylphosphine (TBP) and 2.74 g (3.4 ml) ODE was quickly injected under N₂. The reaction is run at 255 °C. When CdSe nanoparticles reached to the desired size, the reaction mixture was cooled to room temperature. When the reaction mixture reached 100 °C, 5mL of toluene was added to prevent solidification. This synthesis results in monodisperse, highly luminescent particles with quantum yields of about 20%.

Larger Size CdSe NCs (> 3.5 nm diameter)

0.2 mmol of CdO was mixed with 1.2 mmol (0.34 g) of oleic acid and 4.8g (6.0 ml) ODE which was heated to 250 °C to get a colorless solution under N₂ flow. After cooling to room temperature, 1.0 g of ODA and 0.5 g of TOPO were added. The mixture was then heated to 280 °C. At this temperature, a selenium solution containing 1.0 mmol of Se, 0.30 g (1.5 mmol, 0.37ml) of TBP and 1.0 ml of ODE was quickly injected under N₂. The reaction is run at 255 °C for 1 – 2 min. When CdSe nanoparticles reached to the desired size, the reaction mixture was cooled to room temperature. This synthesis results in monodisperse, highly luminescent particles with quantum yields of about 40 - 50%.

Smaller Size CdSe NCs

0.4 mmol of CdO was mixed with 2.4 mmol (0.68 g) of stearic acid and 4.0 g (5.0 ml) ODE which was heated to 250 °C to get a colorless solution under N₂ flow. After cooling to room temperature, 2.0 g of ODA and 0.7 g of TOPO were added. The mixture was then heated to 285 °C. At this temperature, a selenium solution containing 3.0 mmol of Se, 0.90 g (2.4 mmol, 1.1 ml) of trioctylphosphine (TOP) and 1.0 ml of ODE was quickly injected under N₂. The reaction is run at 255 °C for about 1 min. When CdSe nanoparticles reached to the desired size, the reaction mixture was cooled to room temperature. This synthesis results in monodisperse, highly luminescent particles with quantum yields of about 40 - 50%.

The ideas underlying these optimizations are based on the relative rates of nucleation and growth, and are quite straightforward. Larger particles are obtained when nucleation occurs relatively slowly and ceases very early on in the synthesis. These conditions result in relatively few nuclei, and therefore growth of larger particles. The low concentrations used in the large particle synthesis facilitate this type of growth. Conversely, the conditions used for the small particle synthesis result in very rapid nucleation and a high concentration of nuclei. In both cases, the reaction is terminated while still in the strongly focusing regime. We find that this also gives the highest quantum yields, in accord with previous literature reports.¹

Spectral fitting.

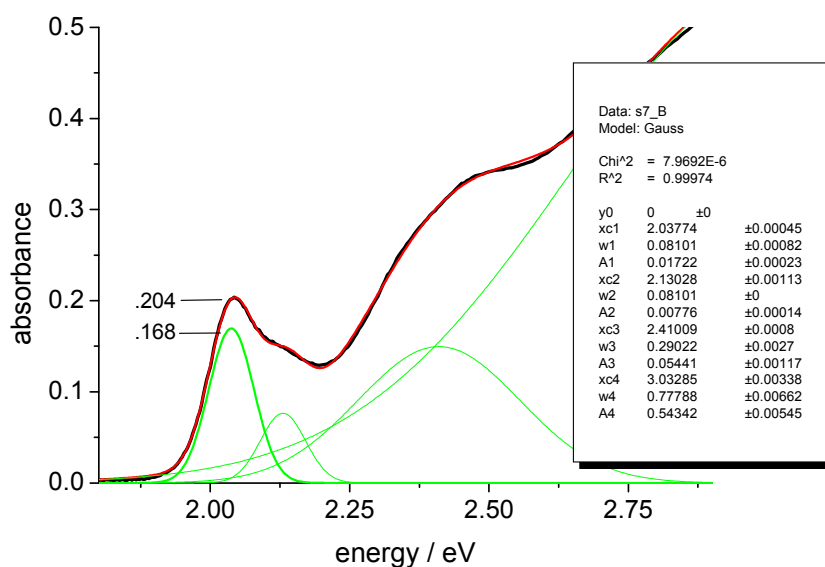


Figure SI-2. An example of a four Gaussian fit to the absorption spectrum of 5.0 nm CdSe QDs. The width of the two lowest transitions have been constrained to be the same. The extinction coefficient correction factor in this case is 0.823 (= .168/.204).

We note that the effect of overlapping transitions becomes more significant for the larger particles, in which the $1S_e-1S_{3/2}$ and $1S_e-2S_{3/2}$ transitions are more closely spaced. The result is that simply taking the product of the maximum extinction coefficient and the spectral width gives a good estimate of the integrated extinction coefficients only for the smallest particles. An increasingly large correction must be applied to this estimate for the larger particles.

References.

- (1) Qu, L.; Peng, X. *J. Am. Chem. Soc.* **2002**, *124*, 2049 - 2055.