Supporting information

Oriented Assembly of CdS nanocrystals via Dynamic Surface Modifications Tailored Particle Interaction

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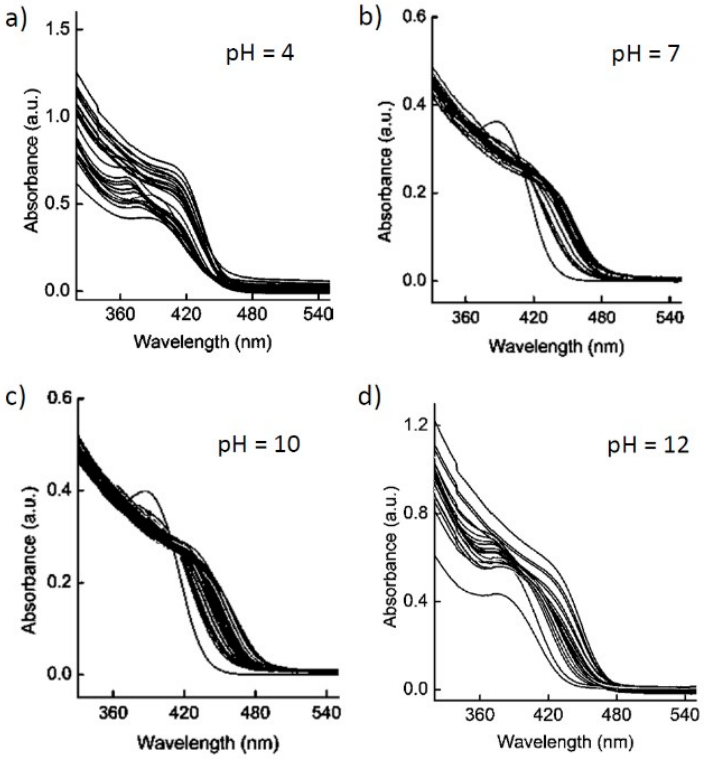
Surporting Figures and Tables

S1. The temporal UV-vis spectra for TGA capped CdS QDs during growth at pH = 4, 7, 10 and 12 at 95 ^{o}C and the method for achieving the average size of the grown CdS QDs.

The UV−vis absorbance data were recorded using a Shimadza UV- 2550 double monochromator UV-vis spectrophotometer at room temperature (298 K).



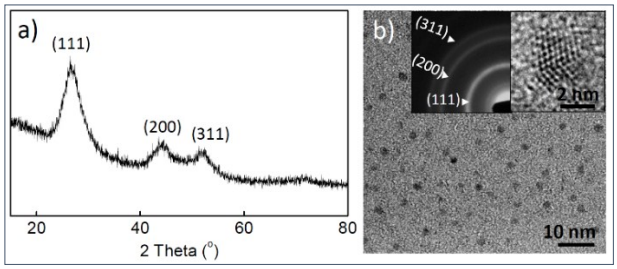
a-d) Temporal UV-vis spectra of TGA-capped CdS QDs during coarsening at 95 ^{o}C at pH = 4, 8 10 and 12.

The average size of the CdS QDs during growth could be calculated from the absorption edge by using the effective mass model:

$$E_R^* = E_g + \frac{h^2\pi^2}{2r^2}\left(\frac{1}{m_0 m_e} + \frac{1}{m_0 m_h}\right) - \frac{1.8e^2}{4\pi\varepsilon\varepsilon_0 r}$$

where E_R* is the band gap of the nanoparticles (E_R* = hc/λ), E_g is the band gap of the corresponding bulk material, r is the particle radius, m_0 is the mass of a free electron, m_e is the effective mass of the electrons, m_h is the effective mass of the holes, ε is the relative permittivity, ε_0 is the permittivity of free space, $\hbar$ is Planck's constant, and e is the charge on the electron.

S2. The XRD pattern SAED and HRTEM images of the as-synthesized TGA capped CdS QDs.



a) The XRD pattern of the as-synthesized TGA capped CdS QDs; b) TEM image, inset SAED and HRTEM images of the as-synthesized CdS QDs

S3. The fitting results of the PL decay curves of CdS samples pH = 4, pH = 12, F-T, A-P 12.

The decay curves of CdS samples pH = 4, pH = 12, F-T, A-P 12 can be well fitted by the biexponential function with different τ_1 and τ_2 values. The detailed parameters of the biexponential function for the four CdS samples are listed in Table. As table illustrated, the shorter decay lifetime τ_1 equals to 0.4–5 ns and the longer decay lifetime and τ_2 ranges from 72 to 131 ns.

The parameter of the fitting for the time-resolved PL of the four CdS samples by using the biexponential function

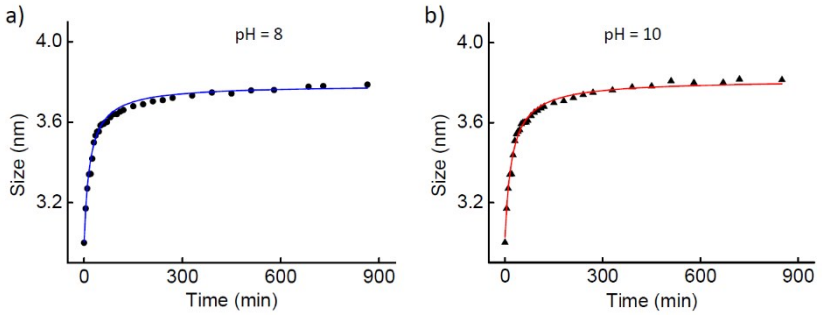
Sample	τ_1 (ns)	τ_2 (ns)	χ^2
pH = 4	4.61	72.69	1.32
pH = 12	4.34	81.12	1.25
F-T	3.94	131.25	1.17
A-P 12	0.41	3.64	1.22

S4. The size Experimental data (scatter) and fitting results (solid line) of the size of CdS QDs as a function of time for CdS at pH = 8 and 10.

The growth of CdS at pH = 8 and 10 can be well fitted by using typical “1+1” OA model:

$$D = \frac{D_0(\sqrt[3]{2}kt + 1)}{kt + 1}$$

Where t is time, k is a rate constant of the OA, D and D_0 is the average particle diameter of particles at time of 0 and t.



a-b) The size Experimental data (scatter) and fitting results (solid line) of the size of CdS QDs as a function of time for CdS at pH = 8 and 10.

S5. Estimated values of kinetic parameters for the growth of TGA-capped CdS at pH = 4, 7 and 10 by fitting the experimental data.

pH	k (1/min)	D_0 (nm)
4	0.062	3.00
7	0.055	3.00
10	0.046	3.00

S6. Estimated values of kinetic parameters for the two growth of TGA-capped CdS at pH = 12 by fitting the experimental data with the established model in main text (i.e. equation 5 and 6).

Step 1		Step 2		
k_1 (1/min)	D_0 (nm)	k_2 (1/min)	D_0 (nm)	t_0 (min)
0.185	2.85	0.012	2.90	20

S7. Photographs of the 0-2 ^oC aging TGA-CdS of pH = 12 (the left) for 1 month and the repeated freezing-defreezing processed TGA-CdS of pH = 12 (the right).

Photographs of the 0 - 2 ^{o}C aging TGA-CdS of pH = 12 (the left) for 1 month and the repeated freezing-defreezing processed TGA-CdS of pH = 12 (the right)