Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Low Temperature Aqueous Synthesis of Size-Controlled Nanocrystals Through Size Focusing: A Quantum Dot Biomineralization Case Study

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Table S1. Estimated particle sizes, HWHM, FWHM, and particle size distributions from TEM analysis for the CdS populations shown in Figure 1.

Growth time (min)	Absorbance peak (nm)	Estimated Diameter (nm)	HWHM (nm)	FWHM (nm)	Diameter from TEM (nm)
30	310	1.47	18.5 ± 2.8	-	-
60	330	1.68	25.5 ± 2.8	128 ± 7.8	2.06 ± 0.52
90	340	1.85	27.7 ± 2.3	127 ± 4.2	-
120	350	2.07	24.2 ± 1.9	128 ± 2.1	2.40 ± 0.51
150	370	2.48	23.3 ± 2.0	133 ± 9.2	-

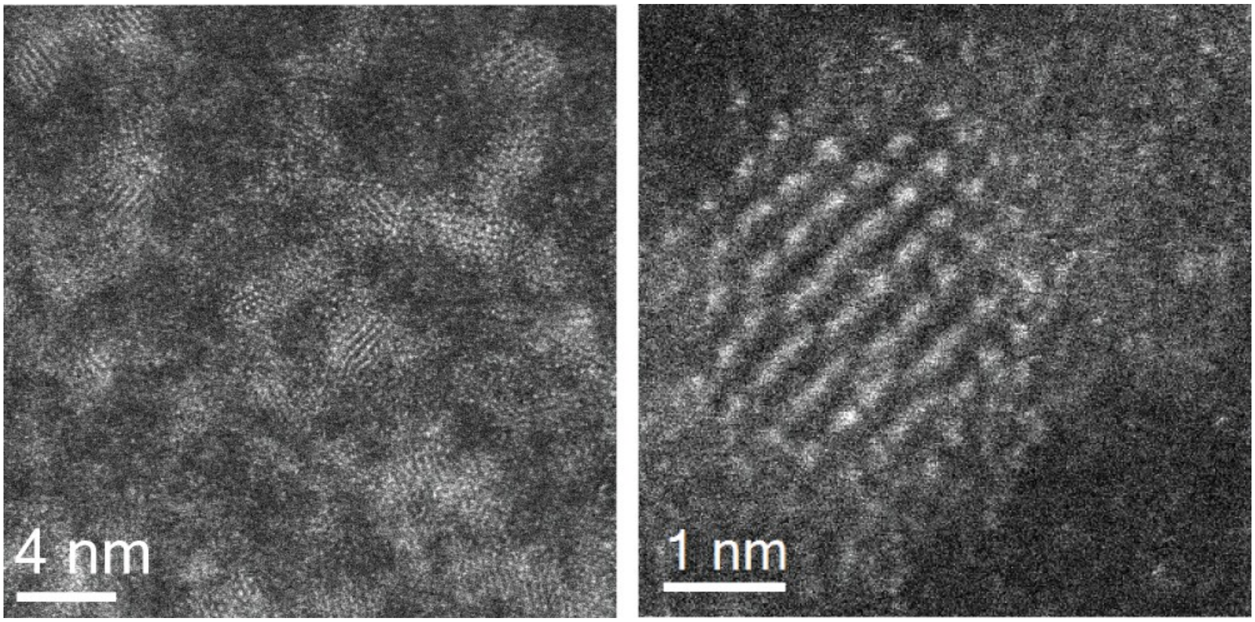

Figure S1. A low magnification (left) and high magnification (right) STEM-HAADF image of CdS nanocrystals biomineralized by CSE at pH 7.5 with an absorbance peak at 350 nm.

Table S2. Compiled estimated particle sizes and HWHM values tabulated for the single-step addition synthesis method results shown in Figure 3.

Figure 3 a) Single-step addition, initial measurement			
NaHS Concentration	Absorbance Peak (nm)	Estimated Diameter (nm)	HWHM (nm)
100 mM	300	1.39	28.1 ± 1.8
200 mM	304	1.42	40 ± 2.56
300 mM	328	1.69	24.9 ± 2.26
400 mM	332	1.75	31 ± 1.1
500 mM	345	1.98	28.2 ± 1.45

Figure 3 b) Single-step addition, 2 hours ripening at 37°C			
NaHS Concentration	Absorbance Peak (nm)	Estimated Diameter (nm)	HWHM (nm)
100 mM	328	1.68	16.5 ± 1.5
200 mM	328	1.69	30.4 ± 2.4
300 mM	340	1.88	26.8 ± 4.25
400 mM	352	2.11	23.5 ± 1.0
500 mM	360	2.29	22.3 ± 1.5

Table S3. Estimated particle sizes, HWHM, FWHM, and particle size distributions from TEM analysis for the CdS populations shown in Figure 6.

NaHS concentration	Absorbance Peak (nm)	Estimated Diameter (nm)	HWHM (nm)	Size from TEM
100 mM	305	1.43	36.2 ± 1.6	-
200 mM	313	1.50	27.5 ± 1.8	-
300 mM	320	1.58	30.2 ± 2.8	2.06 ± 0.45
400 mM	331	1.74	31.2 ± 2.8	-
500 mM	355	2.19	23 ± 2.0	2.44 ± 0.46

Table S4. Estimated particle sizes and HWHM for the CdS populations shown in Figure 7.

Cadmium: Cysteine	Absorbance peak (nm)	Estimated Diameter (nm)	HWHM (nm)
1:8	390	3.08	24.4 ± 4.7
2:8	360	2.29	18.1 ± 0.8
4:8	328	1.70	20.4 ± 3.0
2:16	350	2.28	17.4 ± 3.0
4:32	316	1.54	23.3 ± 4.5

Table S5. Estimated particle sizes, HWHM, and FWHM values for the CdS populations shown in Figure 8.

Growth time (min)	Absorbance peak (nm)	Estimated Diameter (nm)	HWHM (nm)	FWHM (nm)
30	366	2.42	34.1 ± 1.3	-
60	367	2.45	23.6 ± 1.4	121 ± 10.7
90	370	2.52	23.2 ± 1.1	128 ± 19.3
120	371	2.55	22.4 ± 3.7	125 ± 18.2
180	373	2.60	24.3 ± 3.5	125 ± 17.9
240	377	2.71	23.8 ± 2.5	124 ± 13.3

Calculation of K_{obs}

The K_{obs} value used in the calculation of S_∞ was obtained by deriving the observed solubility constant as demonstrated by Xie *et al*.

$$CdS_{bulk} + 2.45Hcys \leftrightarrow 0.45CdH(cys)_2 + 0.1Cd(cys)_2 + 0.45CdH(cys)_3 + HS^- + 0.55H^+$$

H_{cys} represents a protinated L-cysteine. Each of the possible Cd-cysteine chelation species are shown in the above equation: $CdH(cys)_2$, $Cd(cys)_2$, and $CdH(cys)_3$. These species and their relative ratios have been acquired from the supplemental information acquired by Jalilehvand *et al.* Given the reaction above, K_{obs} can be defined.

$$K_{obs} = \frac{[CdH(cys)_2]^{0.45}[Cd(cys)_2]^{0.1}[CdH(cys)_3]^{0.45}[HS^-][H^+]^{0.55}}{[Hcys]^{2.45}}$$

K_{obs} can be rearranged in terms of the solubility constants for each species to yield the final relation

$$K_{obs} = \frac{\beta^{0.45}_{CdH(cys)_2}\beta^{0.1}_{Cd(cys)_2}\beta^{0.45}_{CdH(cys)_3}\left(K^{cys}_a\right)^{2.45}K^{CdS\,bulk}_{sp}}{K^{HS^-}_d}$$

Bulk solubility, S_∞, can then be calculated using this new K_{obs} in terms of HS^-.

References

1 F. Jalilehvand, B. O. Leung and V. Mah, *Inorg. Chem.,* 2009, **48**, 5758-5771.

2 R. Xie, Z. Li and X. Peng, *J. Am. Chem. Soc.,* 2009, **131**, 15457-15466.