

Electronic Supplementary Information for:

**Multivariate optimization of optical properties of CdSe quantum dots obtained by
a facile one-pot aqueous synthesis**

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Table S1 Experimental conditions and results of the syntheses from the two-level full factorial design, with stirring for 120 min.

MSA/Cd molar ratio	Cd/Se molar ratio	pH	Temperature (°C)	PL emission (a. u.)
2:1	1:1	5.0	30	244
6:1	1:1	5.0	30	4
2:1	5:1	5.0	30	833
6:1	5:1	5.0	30	1622
2:1	1:1	12.0	30	127
6:1	1:1	12.0	30	0
2:1	5:1	12.0	30	780
6:1	5:1	12.0	30	19
4:1	3:1	8.5	60	3
4:1	3:1	8.5	60	4
4:1	3:1	8.5	60	1
2:1	1:1	5.0	90	7
6:1	1:1	5.0	90	0
2:1	5:1	5.0	90	11
6:1	5:1	5.0	90	921
2:1	1:1	12.0	90	2
6:1	1:1	12.0	90	0
2:1	5:1	12.0	90	6
6:1	5:1	12.0	90	1

Table S2 Effect estimates summary for the results of PL emission obtained from the two-level full factorial design.

Factor	Effect	Standard error	-95% Confidence limit	+95% Confidence limit
Mean/Intercept	241.32	0.35	239.81	242.82
(1)MSA/Cd molar ratio	69.62	0.76	66.34	72.91
(2)Cd/Se molar ratio	476.12	0.76	472.84	479.41
(3)pH	-338.38	0.76	-341.66	-335.09
(4)Temperature	-335.12	0.76	-338.41	-331.84
1x2	163.62	0.76	160.34	166.91
1x3	-293.38	0.76	-296.66	-290.09
1x4	154.38	0.76	151.09	157.66
2x3	-306.88	0.76	-310.16	-303.59
2x4	-243.62	0.76	-246.91	-240.34
3x4	105.88	0.76	102.59	109.16
1x2x3	-322.88	0.76	-326.16	-319.59
1x2x4	64.88	0.76	61.59	68.16
1x3x4	65.88	0.76	62.59	69.16
2x3x4	76.88	0.76	73.59	80.16

Table S3 Experimental conditions and results of the syntheses from the Doehlert design, with stirring for 60 min.

MSA/Cd molar ratio	Cd/Se molar ratio	pH	Temperature (°C)	PL emission (a. u.)	λ_{abs} (nm)	λ_{ems} (nm)	FWHM (nm)
5:1	6:1	4.0	30	75	452	595	146
5:1	6:1	6.0	30	322	456	587	143
6:1	8:1	5.0	30	2725	413	504	125
6:1	6.5:1	5.0	45	2046	416	511	127
5.1:1	9.7:1	4.8	25	2518	419	511	127
5.1:1	9.7:1	4.8	25	2625	418	511	126
5.1:1	9.7:1	4.8	25	2543	417	510	127
7:1	4:1	4.0	30	77	443	578	145
7:1	4:1	6.0	30	113	473	614	140
7:1	5.5:1	4.0	15	124	433	576	145
7:1	5.5:1	6.0	15	464	450	581	143
8:1	6:1	3.0	30	0	470	-	-
8:1	6:1	5.0	30	2518	415	507	125
8:1	6:1	5.0	30	2241	413	506	126
8:1	6:1	5.0	30	2550	414	505	124
8:1	6:1	7.0	30	45	486	617	142
8:1	4.5:1	5.0	45	2114	420	512	128
8:1	7.5:1	5.0	15	1583	418	513	127
9:1	8:1	4.0	30	90	432	574	147
9:1	8:1	6.0	30	1356	437	560	138
9:1	6.5:1	4.0	45	88	429	573	146
9:1	6.5:1	6.0	45	715	443	573	142
10:1	4:1	5.0	30	2265	418	511	126
10:1	5.5:1	5.0	15	2184	414	506	125
11:1	6:1	4.0	30	65	436	577	146
11:1	6:1	6.0	30	856	440	568	141
6:1	8:1	5.0	30	2745*	411*	503*	125*
6:1	8:1	5.0	30	2789*	410*	501*	125*

*Replicates obtained under optimal conditions, after the statistical treatment of data, and therefore these results were not considered in the effect estimates and ANOVA calculations.

Table S4 Optical features of CdSe QDs synthesized under different experimental conditions of the plateau area of response surfaces of Fig. 2.

Sample	MSA/Cd molar ratio	Cd/Se molar ratio	pH	Temperature (°C)	PL emission (a. u.)	λ_{abs} (nm)	λ_{ems} (nm)	FWHM (nm)
A	6:1	8:1	5.0	30	2725	413	504	125
B	6:1	8:1	5.0	30	2745	411	503	125
C	6:1	8:1	5.0	30	2789	410	501	125
D	8:1	6:1	5.0	30	2518	415	507	125
E	8:1	6:1	5.0	30	2241	413	506	126
F	8:1	6:1	5.0	30	2550	414	505	124
G	10:1	4:1	5.0	30	2265	418	511	126

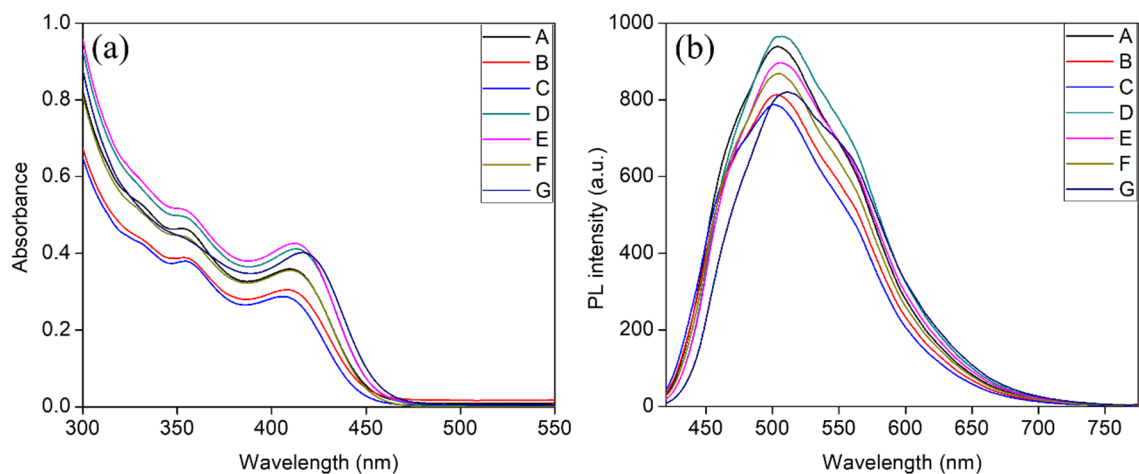


Fig. S1 Absorption and PL emission spectra of suspensions of CdSe QDs synthesized under the experimental conditions specified in Table S4 and stirring for 60 min.

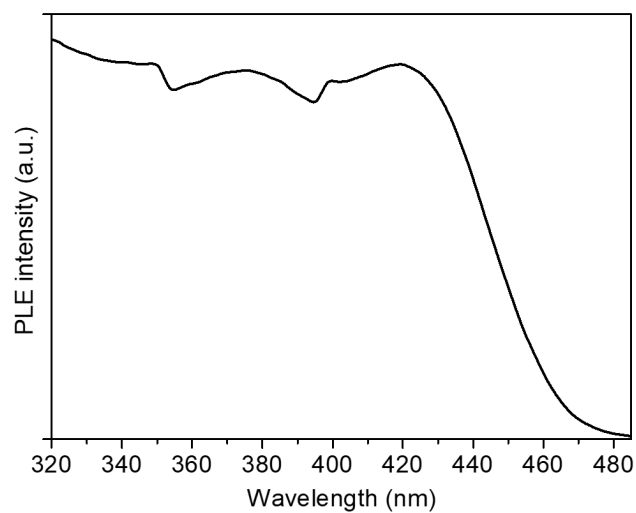


Fig. S2 PL excitation spectra (at emission wavelength of 505 nm) of MSA-capped CdSe QDs synthesized at 30 °C and pH 5.0, with MSA/Cd and Cd/Se molar ratios of 6:1 and 8:1, respectively, and stirring for 60 min.