Supplementary Information for:

Synthesis of hydrophilic Ag_2Se quantum dots optically optimized by multivariate strategies: an easy one-pot approach

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Table S1 Experimental conditions and results of the syntheses from the 2^{4-1} fractional factorial design.

Synthesis code	MSA/Ag molar ratio	Ag/Se molar ratio	pH	Temperature (°C)	Time* (min)	λ_{abs} (nm)	λ_{ems} (nm)	λ_{exc} (nm)
15.1	2:1	2:1	5.0	30	20	550	655	450
15.2	2:1	2:1	5.0	30	60	555	660	450
18.1	8:1	2:1	5.0	60	20	355	393	350
18.2	8:1	2:1	5.0	60	60	365	393	350
14.1	2:1	10:1	5.0	60	20	535	690	450
14.2	2:1	10:1	5.0	60	60	540	700	450
12.1	8:1	10:1	5.0	30	20	515	708	450
12.2	8:1	10:1	5.0	30	60	515	710	450
17.1	2:1	2:1	12.0	60	20	300	455	350
17.2	2:1	2:1	12.0	60	60	293	455	350
13.1	8:1	2:1	12.0	30	20	305	455	350
13.2	8:1	2:1	12.0	30	60	305	455	350
16.1	2:1	10:1	12.0	30	20	310	455	350
16.2	2:1	10:1	12.0	30	60	305	455	350
11.1	8:1	10:1	12.0	60	20	305	455	350
11.2	8:1	10:1	12.0	60	60	305	455	350

*Time at which the aliquots were collected.

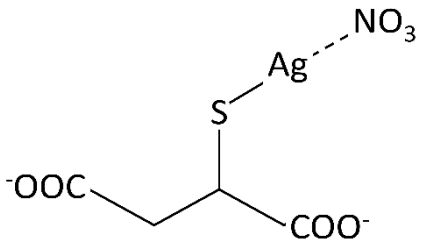

Figure S1 Structure of the MSA–Ag complex in aqueous solution containing nitrate ions at alkaline pH.

Table S2 Experimental conditions and results of the syntheses from the mixed-level factorial design.

Synthesis code	pH	Tempera-ture (°C)	Time* (min)	λ_{abs} (nm)	λ_{ems} (nm)	λ_{exc} (nm)
19.1	5.0	5	20	595	816	484
19.2	5.0	5	60	597	798	484
21.1	5.0	25	20	592	816	484
21.2	5.0	25	60	592	819	484
23.1	5.0	45	20	592	820	484
23.2	5.0	45	60	592	820	484
20.1	12.0	5	20	305	456	350
20.2	12.0	5	60	305	456	350
22.1	12.0	25	20	305	458	350
22.2	12.0	25	60	305	455	350
24.1	12.0	45	20	305	454	350
24.2	12.0	45	60	305	451	350

*Time at which the aliquots were collected.

Table S3 Experimental conditions and results of the syntheses from the 2^4 full factorial design.

Synthesis code	MSA/Ag molar ratio	Ag/Se molar ratio	pH	Tempera-ture (°C)	Time* (min)	PL intensity (a. u.)	λ_{abs} (nm)	λ_{ems} (nm)	λ_{exc} (nm)
31.1	2:1	2:1	5.0	5	20	0	560	–	450
31.2	2:1	2:1	5.0	5	60	0	560	–	450
41.1	2:1	2:1	5.0	5	20	0	555	–	450
41.2	2:1	2:1	5.0	5	60	0	545	–	450
30.1	6:1	2:1	5.0	5	20	23	600	812	450
30.2	6:1	2:1	5.0	5	60	23	600	812	450
36.1	2:1	8:1	5.0	5	20	0	510	–	450
36.2	2:1	8:1	5.0	5	60	0	510	–	450
25.1	6:1	8:1	5.0	5	20	51	515	740	450
25.2	6:1	8:1	5.0	5	60	48	515	732	450
39.1	2:1	2:1	5.0	60	20	0	590	–	450
39.2	2:1	2:1	5.0	60	60	0	590	–	450
33.1	6:1	2:1	5.0	60	20	0	540	–	450
33.2	6:1	2:1	5.0	60	60	0	540	–	450
32.1	2:1	8:1	5.0	60	20	39	550	735	450
32.2	2:1	8:1	5.0	60	60	59	565	737	450
37.1	6:1	8:1	5.0	60	20	168	580	790	450
37.2	6:1	8:1	5.0	60	60	142	585	795	450
29.1	2:1	2:1	12.0	5	20	82	295	415	305
29.2	2:1	2:1	12.0	5	60	23	298	420	305
40.1	6:1	2:1	12.0	5	20	113	305	425	308
40.2	6:1	2:1	12.0	5	60	110	305	425	308
38.1	2:1	8:1	12.0	5	20	526	296	418	308
38.2	2:1	8:1	12.0	5	60	897	296	418	308
28.1	6:1	8:1	12.0	5	20	157	305	425	308
28.2	6:1	8:1	12.0	5	60	104	305	425	308
27.1	2:1	2:1	12.0	60	20	70	305	420	308
27.2	2:1	2:1	12.0	60	60	220	293	420	308
35.1	6:1	2:1	12.0	60	20	0	305	–	305
35.2	6:1	2:1	12.0	60	60	64	305	425	305
26.1	2:1	8:1	12.0	60	20	67	305	420	308
26.2	2:1	8:1	12.0	60	60	453	293	420	308
34.1	6:1	8:1	12.0	60	20	0	305	–	350
34.2	6:1	8:1	12.0	60	60	0	305	–	350
42.1	6:1	8:1	12.0	60	20	0	300	–	308
42.2	6:1	8:1	12.0	60	60	0	300	–	308

*Time at which the aliquots were collected.

Table S4 Experimental conditions and results of the syntheses from the 2^3 full factorial design.

Synthesis code	MSA/Ag molar ratio	pH	Tempera-ture (°C)	Time* (min)	PL intensity (a. u.)**	λ_{abs} (nm)	λ_{ems} (nm)
43.1	5:1	5.0	40	20	21	580	793
43.2	5:1	5.0	40	60	22	577	763
51.1	7:1	5.0	40	20	71	567	805
51.2	7:1	5.0	40	60	72	567	811
44.1	5:1	7.0	40	20	0	692	–
44.2	5:1	7.0	40	60	0	692	–
46.1	7:1	7.0	40	20	0	550	–
46.2	7:1	7.0	40	60	0	550	–
49.1	6:1	6.0	60	20	17	564	723
49.2	6:1	6.0	60	60	11	573	730
53.1	5:1	5.0	80	20	47	590	815
53.2	5:1	5.0	80	60	44	590	825
45.1	7:1	5.0	80	20	87	578	789
45.2	7:1	5.0	80	60	69	575	809
47.1	5:1	7.0	80	20	0	694	–
47.2	5:1	7.0	80	60	0	712	–
48.1	7:1	7.0	80	20	0	805	–
48.2	7:1	7.0	80	60	0	805	–

*Time at which the aliquots were collected.

**All PL spectra were obtained with excitation at 460 nm.

Table S5 Effect estimates summary for the results of the PL intensity of Ag_2Se QDs obtained from the 2^3 full factorial design.

Factor	Effect	Standard error × t	-95% Confidence limit	+95% Confidence limit
Mean	25.61	2.42	23.19	28.03
(1)MSA/Ag molar ratio*	20.63	5.13	15.49	25.76
(2)pH*	-54.13	5.13	-59.26	-48.99
(3)Temperature*	7.63	5.13	2.49	12.76
1x2*	-20.63	5.13	-25.76	-15.49
1x3	-4.38	5.13	-9.51	0.76
2x3*	-7.62	5.13	-12.76	-2.49
1x2x3	4.38	5.13	-0.76	9.51

*Statistically significant factor at 95% confidence level

The main effects of the three factors and the interactions between MSA/Ag molar ratio and pH (interaction 1x2) and between pH and temperature (interaction 2x3) were statistically significant. The effect of pH was the greatest, followed by the effect of MSA/Ag molar ratio. According to the effect estimates, the conditions of the 2^3 factorial design that led to increasing the PL intensity are MSA/Ag molar ratio and temperature at their upper levels (7:1 and 80 °C, respectively) and pH at its lower level (5.0). These conditions correspond to those of syntheses 45.1 and 45.2, whose PL intensities were 87 and 69 a. u., respectively. The absorption and PL spectra of the Ag_2Se QDs obtained in synthesis 45.1 are depicted in Figure S2.

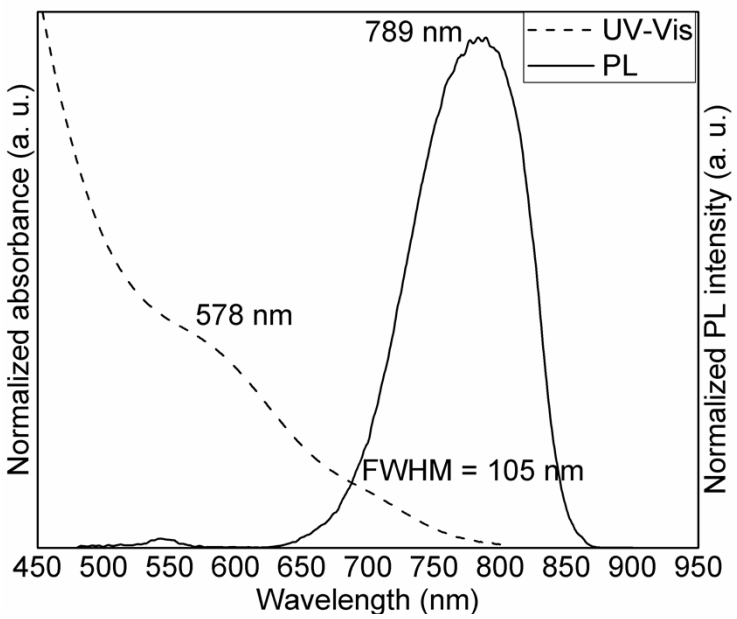

Figure S2 UV-vis absorption and PL spectra (λ_{exc} = 460 nm) of a suspension of MSA–Ag_2Se quantum dots obtained at 80 °C and pH 5.0, with MSA/Ag and Ag/Se molar ratios of 7:1 and 8:1, respectively, and stirring for 20 min.

Table S6 Optical features of Ag_2Se quantum dots synthesized under optimal experimental conditions: MSA/Ag molar ratio of 6:1, Ag/Se molar ratio of 8:1, pH 5.0, and stirring for 20 minutes at 60 °C.

Suspension	**PL intensity (a. u.)**	**λ_{abs} (nm)**	**λ_{ems} (nm)**	**PL FWHM (nm)**
A	168	580	790	103
B	66	582	768	122
C	113	585	813	96
D	93	582	788	113
E	103	586	785	113