

Enhancing the Optical Properties of Hydrophilic Ag₂Se NIR-II Quantum Dots by using Chemometric Approaches Towards (Bio)sensing Applications

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Support Information

1. Data from the 2⁴⁻¹ Fractional Factorial experimental design (experimental design 1)

Assay	Reaction time (1)	[Ag ⁺] (2)	Temperature (3)	Ag:Se (4)	PL Intensity (a. u.)	FWHM PL (nm)
1	-1	1	1	1	12967.64	176
2	1	1	1	1	15049.893	162
3	-1	-1	1	-1	838984.418	290
4	1	-1	1	-1	1355719.47	310
5	-1	-1	-1	1	0	500
6	1	-1	-1	1	0	500
7	-1	1	-1	-1	0	500
8	1	1	-1	-1	5650.2242	171
9	-1	0	0	0	2828.09545	240
10	1	0	0	0	2003.4364	231
11	-1	1	1	1	0	500
12	1	1	1	1	0	500
13	-1	-1	1	-1	268271.605	337
14	1	-1	1	-1	268271.605	337
15	-1	1	-1	-1	235.19229	169
16	1	1	-1	-1	837.8644	201
17	-1	0	0	0	79978.3044	343
18	1	0	0	0	89549.7627	358

PL Intensity = -162375.25*[Ag⁺] + 178190.23* (Temperature) -175528.45* (Ag:Se) + 142092.26

2. Data from the 2³ Full factorial experimental design (experimental design 2)

Assay	Reaction time (1)	Ag:Se (2)	MPA:Ag (3)	PL Intensity (a. u.)	FWHM PL (nm)
1	-1	-1	-1	31380.8715	163

2	1	-1	-1	47156.1969	142
3	-1	1	-1	58885.116	160
4	1	1	-1	59366.1573	139
5	-1	-1	1	8378.60781	312
6	1	-1	1	9230.3339	372
7	-1	1	1	9388.79457	287
8	1	1	1	11092.2467	275
9	-1	0	0	21505.3763	138
10	1	0	0	33022.0713	132
11	-1	-1	-1	8546.97227	170
12	1	-1	-1	30969.1568	158
13	-1	1	-1	71505.3763	146
14	1	1	-1	36078.0985	142
15	-1	-1	1	0	500
16	1	-1	1	8546.97227	270
17	-1	1	1	4981.60724	370
18	1	1	1	11438.8795	138
19	-1	0	0	9230.3339	172
20	1	0	0	12795.6989	175
21	-1	1	-1	85512.1675	166
22	1	1	-1	31692.1336	163

PL Intensity = 7696.3*(2) - 17840.3*(3) - 6230.8*(1*2) - 6353.1(2*3) 6076.1*(1*2*3) + 24405.6

FWHM PL = 78.64*(3) + 220.33

3. Data from the 2³ Central Composite experimental design (experimental design 3)

Assay	pH (1)	Temperature (2)	Reaction time (3)	PL Intensity (a. u.)	FWHM PL (nm)
1	-1	-1	-1	55301.3582	217
2	-1	-1	1	284538.745	200
3	-1	1	-1	284772.653	139
4	-1	1	1	201816.667	138
5	1	-1	-1	59447.0046	181
6	1	-1	1	44789.9968	167
7	1	1	-1	76582.2785	170
8	1	1	1	38457.5967	195
9	-1	0	0	90349.0029	177
10	1	0	0	63226.4529	173
11	0	-1	0	155036.598	176
12	0	-1	0	265126.557	155
13	0	1	0	74008.9994	165
14	0	0	-1	314920.013	136
15	0	0	1	729818.491	136

16	0	0	1	719318.796	141
17	0	0	0	91105.0291	135
18	0	0	0	216611.173	149

$$\text{PL Intensity} = -244782.66*(1)^2 - 140122.50*(2)^2 + 263928.18*(3)^2 + 265666.30$$

$$\text{FWHM PL} = 26.49*(1)^2 - 11.73*(2) + 146.34$$