Supplementary Information

Effect of Manganese Doping on the Hyperthermic Profile of Ferrite Nanoparticles using Response Surface Methodology

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Table S1: Results of experimental runs (20 reactions).

Run order	Fe^{3+}/Mn^{2+} ratio A	Temperature B (°C)	Time C (h)	Saturated Magnetization R1 (emu/g)		Temperature Rise R2 (°C)	
				Experimental value	Predicted value	Experimental value	Predicted value
1	13	100	4	68.30	63.57	5.7	4.71
2	31	150	7	74.5	74.22	4.0	3.73
3	31	65.9	7	71.43	77.52	2.6	3.31
4	49	200	4	77.46	78.42	0.7	0.49
5	31	150	7	74.5	74.22	3.9	3.73
6	13	100	10	64.58	56.80	2.2	2.42
7	49	100	10	77.19	77.20	3.2	2.70
8	13	200	4	76.84	70.01	1.0	1.52
9	49	200	10	82.99	80.89	1.6	2.40
10	31	234	7	82.49	86.05	1.1	0.37
11	13	200	10	66.74	63.19	3.9	3.82
12	0.7	150	7	40.76	50.32	3	3.21
13	31	150	7	74.5	74.22	3.8	3.73
14	31	150	2	65.05	70.01	4.0	4.36
15	31	150	7	74.5	74.22	3.8	3.73
16	31	150	12	61.7	66.39	4.4	4.03
17	31	150	7	74.5	74.22	3.5	3.73
18	31	150	7	74.5	74.22	3.4	3.73
19	61	150	7	75.21	74.54	2.8	2.58
20	49	100	4	77.95	74.68	5.3	5.39
Optimal	42	100	4	73	75	8.4	5

Table S2: Characterization of Mn-doped Ferrite Nanoparticles ($Mn_xFe_{3-x}O_4$).

Experimental Run Order	Dopant (x)	Surface Charge (mV)	Hydrodynamic Size (nm)	Crystallite size (nm)	Lattice constant (nm)
1	0.21	-16.7 ± 0.8	273.1 ± 36.6	14.8	0.8367
2	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
3	0.1	-8.2 ± 0.7	294.6 ± 66.5	18.3	0.8398
4	0.05	-13.2 ± 0.9	310.5 ± 46.0	14.4	0.8359
5	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
6	0.21	-14.9 ± 0.9	218.7 ± 24.1	15.9	0.8408
7	0.05	-13.8 ± 0.6	313.3 ± 1.2	26.9	0.8392
8	0.16	-11.1 ± 1.4	187.5 ± 52.5	16.6	0.8440
9	0.07	-12.5 ± 0.7	210.5 ± 117.8	14.9	0.8392
10	0.09	-10.2 ± 0.5	256.0 ± 34.1	24.6	0.8407
11	0.21	-12.0 ± 1.1	151.9 ± 26.8	15.2	0.8376
12	0.07	-12.2 ± 0.3	225.0 ± 54.9	14.7	0.8522
13	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
14	0.09	-9.9 ± 0.7	216.8 ± 47.5	17.3	0.8366
15	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
16	0.1	-7.6 ± 0.5	215.9 ± 90.5	10.3	0.8407
17	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
18	0.08	-11.3 ± 1.1	307.1 ± 8.5	24.4	0.8378
19	0.05	-11.8 ± 0.5	388.2 ± 23.8	17.6	0.8366
20	0.06	-14.9 ± 0.8	173.6 ± 58.8	15.4	0.8376
Optimal sample	0.07	-11.3 ± 0.4	278.2 ± 14.8	19.2	0.8292

Table S3: Magnetic and hyperthermic properties of Mn-doped Ferrite Nanoparticles ($Mn_xFe_{3-x}O_4$).

Experimental Run Order	**Ms (emu/g)**	**Mr (emu/g)**	**Hc (Oe)**	**SAR (W/g)**	**ILP (nHm^2/kg)**
1	68.30	0	0.43	41.85	0.58
2	74.5	4.91	10.34	6.98	0.096
3	71.43	3.64	75.25	6.98	0.096
4	77.46	12.73	152.86	3.49	0.048
5	74.5	4.91	35.85	6.98	0.096
6	64.58	2.35	67.26	6.98	0.096
7	77.19	2.71	9.33	13.95	0.19
8	76.84	4.97	84.32	20.93	0.29
9	82.99	6.62	130.0	6.98	0.096
10	82.49	12.97	50.98	3.49	0.048
11	66.74	0.78	17.82	13.95	0.19
12	40.76	13.53	156.12	6.98	0.10
13	74.5	4.91	14.32	6.98	0.10
14	65.05	0	69.38	13.95	0.19
15	74.5	4.91	65.53	6.98	0.10
16	61.7	7.2	135.0	20.93	0.29
17	74.5	4.91	32.97	6.98	0.10
18	74.5	4.91	73.27	6.98	0.10
19	75.21	4.5	69.5	10.46	0.14
20	77.95	0	66.7	20.93	0.29
PEG-coated Optimal sample	73	9.28	140	76.73	1.12

Table S4: The results of ANOVA analysis for R1 response model.

Source	Sum of Squares	df	Mean Square	F-value	p-value
Model	1306.28	9	145.14	4.01	0.0205
A-Fe/Mn ratio	708.21	1	708.21	19.58	0.0013
B-Temperature	87.71	1	87.71	2.42	0.1505
C-Time	15.79	1	15.79	0.4364	0.5238
AB	3.63	1	3.63	0.1004	0.7579
AC	43.20	1	43.20	1.19	0.3001
BC	0.0010	1	0.0010	0.0000	0.9959
A^2	250.66	1	250.66	6.93	0.0251
B^2	102.93	1	102.93	2.85	0.1225
C^2	65.41	1	65.41	1.81	0.2084

Table S5: The results of ANOVA analysis for R2 response model.

Source	Sum of Squares	df	Mean Square	F-value	p-value
Model	31.25	9	3.47	8.15	0.0015
A-Fe/Mn ratio	0.4711	1	0.4711	1.11	0.3178
B-Temperature	10.41	1	10.41	24.43	0.0006
C-Time	0.1290	1	0.1290	0.3028	0.5942
AB	1.44	1	1.44	3.39	0.0953
AC	0.0800	1	0.0800	0.1878	0.6740
BC	10.58	1	10.58	24.84	0.0006
A^2	1.27	1	1.27	2.99	0.1144
B^2	6.44	1	6.44	15.12	0.0030
C^2	0.3795	1	0.3795	0.8909	0.3675

Table S6: Structure coordinates of the $Mn_xFe_{3-x}O_4$ system.

Elements	A	B	O
Coordinates	0,0,0	0.625, 0.625, 0.625	0.375, 0.375, 0.375

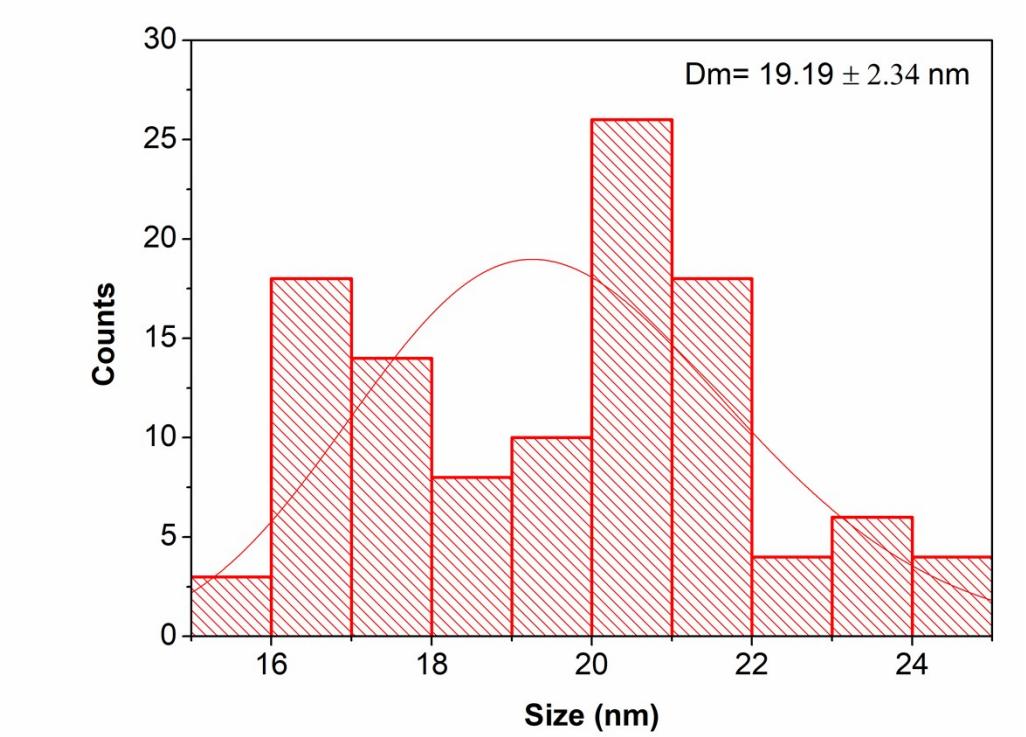

Figure S1: Size distribution histogram of the optimal sample synthesized. Dm represents the mean diameter of the particles.

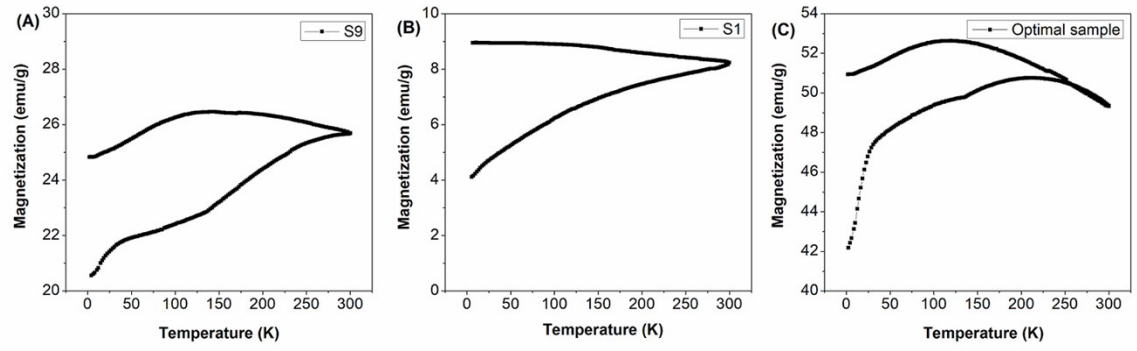

Figure S2: Magnetization as a function of temperature on application of 100 Oe field for $Mn_xFe_{3-x}O_4$ nanoparticles exhibiting (A) maximum magnetization (run order 9; S9); (B) maximum temperature rise (run order 1; S1) and (C) optimal sample synthesized.

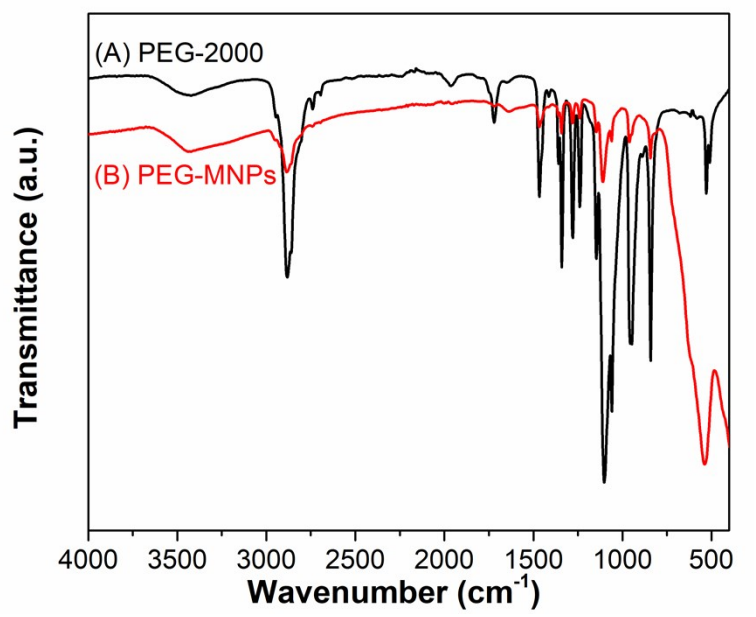

Figure S3: FTIR analysis of (A) PEG-2000 and (B) PEG-coated optimal MNPs.