

Supporting Information

Ecofriendly Synthesis, Crystal Chemistry, and Magnetic Properties of Manganese Substituted CoFe_2O_4 Nanoparticles

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1. XRD

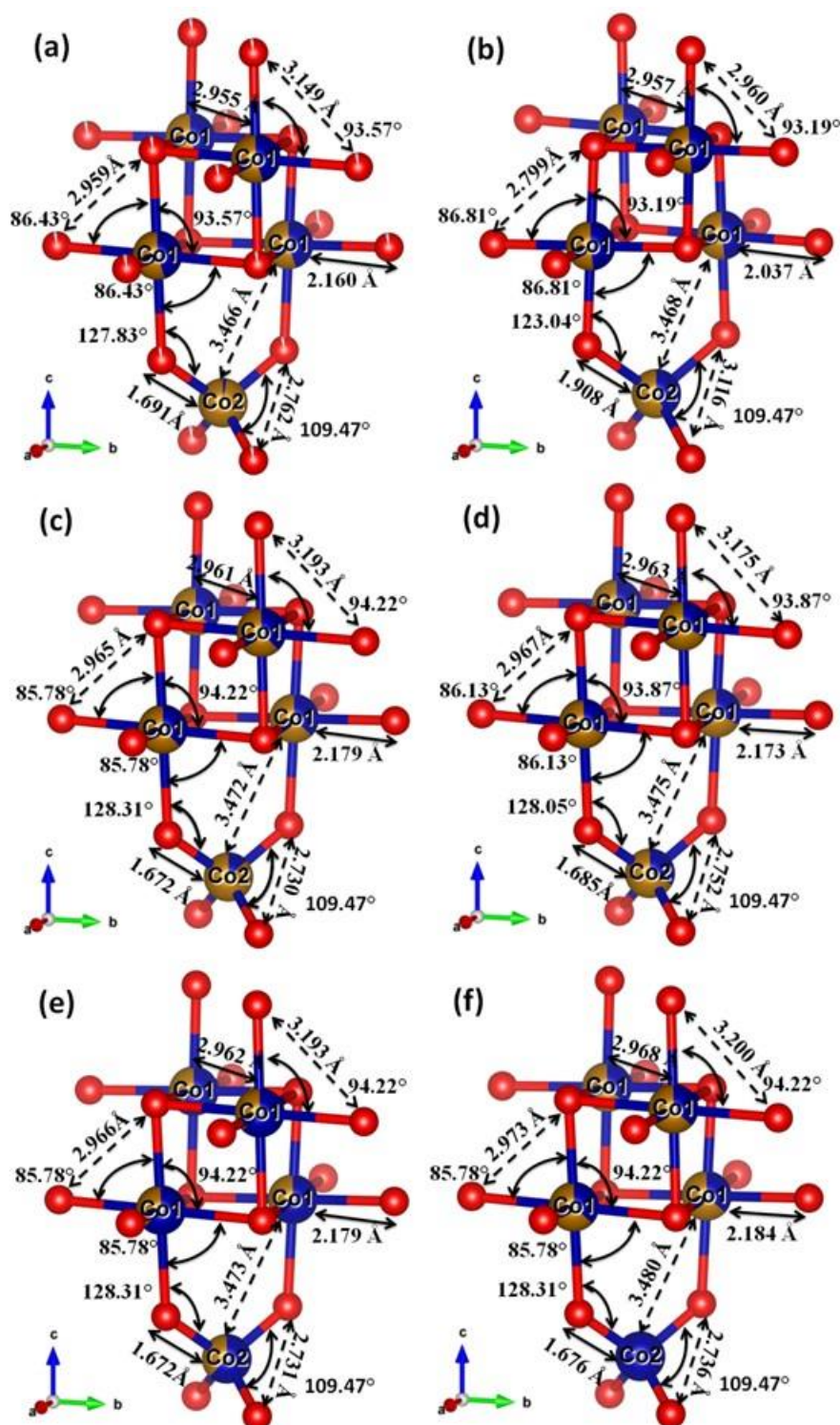


Figure S1. Bond angle, Bond length and interaction among the octahedral and tetrahedral sites are shown for (a) CF, (b) CMF15, (c) CMF25, (d) CMF30, (e) CMF40, and (f) CMF50 NPs, as

derived from the XRD refinement data; where Co1 and Co2 represents the cation present at octahedral and tetrahedral site and red ball shows the oxygen.

2. Raman Analysis:

In order to get more accurate information from the experimental data, Raman data of the samples were fitted by superposition of Lorentz peaks expressed by equation

$$I(\omega) = I_o + \frac{2A}{\Pi} \frac{W}{W^2 + 4(\omega - \omega_o)^2}$$

where ω_o is phonon frequency of the peak, W is its FWHM, A is a constant, and I_o is intensity of the background. The parameters obtained from the deconvoluted Raman spectra for all the major peaks observed for as-synthesized CMFO samples and are listed in Table S1.

Table S1: Raman mode parameters obtained by fitting the Raman spectra

Sample	A _{1g} (1)		A _{1g} (2)		T _{2g} (1)		T _{2g} (2)		T _{2g} (3)		E _g		P ₁	P ₂
	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^a	Area	$\bar{\nu}$ (cm ⁻¹) ^b	$\bar{\nu}$ (cm ⁻¹) ^b
CF	673.24	64163	599.34	144468 1	520	9330	454.37	82358	188.48	32471	290.36	77288	-	120.43
CMF15	671.58	10355 7	595.50	135082	546	1139 9	459.14	124488	168.86	56843	289.68	100673	-	115.48
CMF-25	677.00	44781	595.00	101741	-	-	457.72	56709	169.99	35553	295.16	65239	-	-
CMF-30	674.41	61077	596.79	174809	-	-	457.62	92679	167.65	44717	290.43	123830	-	-
CMF-40	671.78	70345	597.95	109864	520	4346 6	460.00	81213	166	46025	283.42	123250	216.48	115.47
CMF-50	666.10	21093	597.33	116019	-	-	460.77	29674	158.30	22393	373.00	14187	213.36	117.43

^a Raman mode position

^b Additional non-indexed Raman mode

P1 and P2: unassigned mode

3. FE-SEM analysis

The diameter varying distribution can be fitted to a normalized log-normal distribution function as:

$$P(D) = \frac{A}{D\sqrt{2\pi\sigma}} \exp\left[\frac{-\ln(D / D_{FESEM})^2}{2\sigma^2}\right]$$

where ‘D’ is the diameter of NPs; D_{FESEM} is the mean diameter of NPs; ‘A’ is the normalization constant; and ‘ σ ’ is the polydispersity index of size distribution of NPs.

Table S2 parameters obtained from the FE-SEM analysis

Samples Parameter	CF	CMF15	CMF25	CMF30	CMF40	CMF50
Adjusted R-square (R)	0.937	0.941	0.951	0.967	0.970	0.957
Median diameter (D_{FESEM})	10.86	13.97	13.58	11.70	14.41	16.10
Polydispersity index (σ)	0.33	0.32	0.31	0.21	0.25	0.25
Normalization constant (A)	886.55	1036.45	1207.00	877.06	1064.55	682.61

4. EDS Analysis:

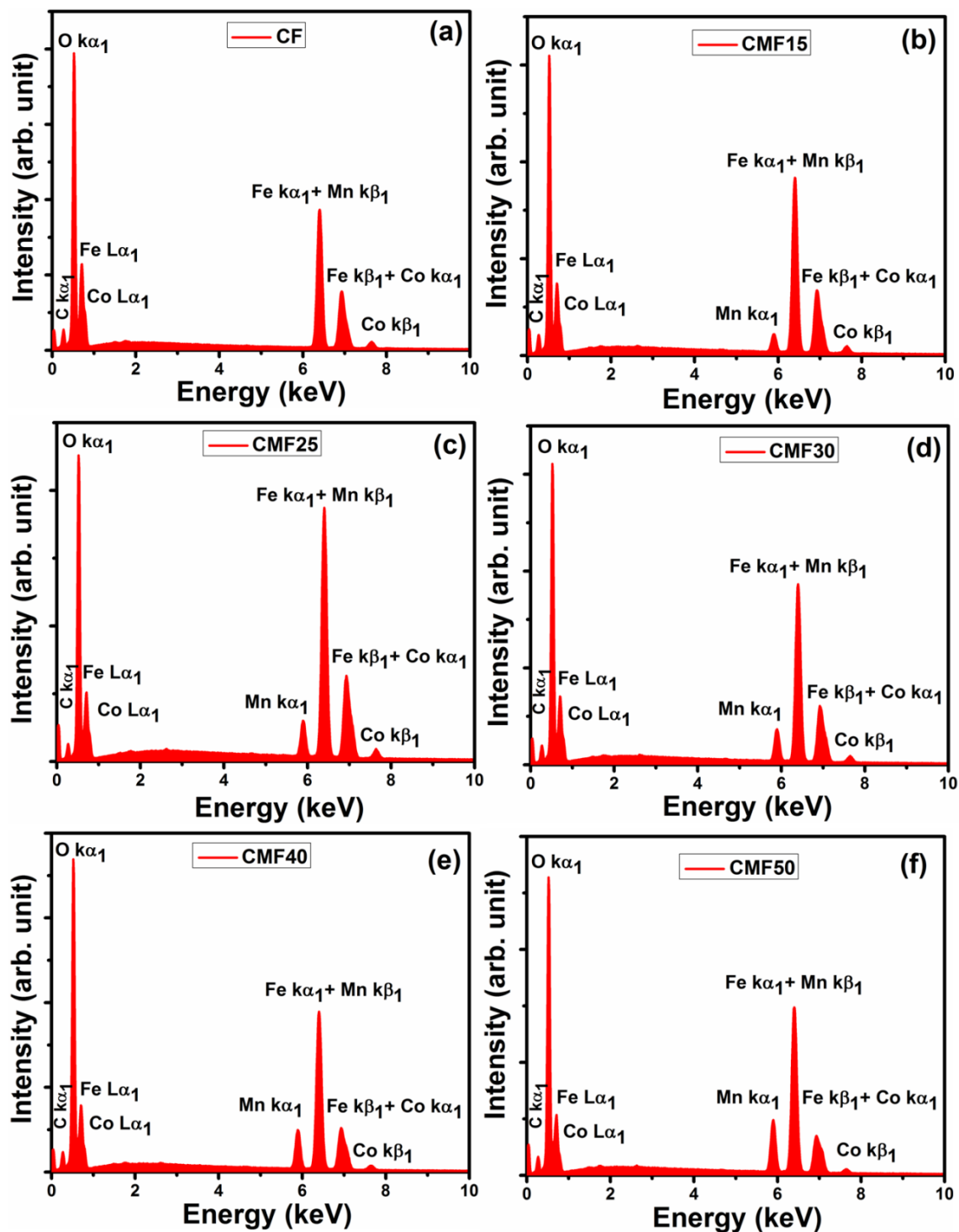


Figure S2. EDS data of the $\text{Co}_{1-x}\text{Mn}_x\text{Fe}_2\text{O}_4$ magnetic nanoparticles. The EDS spectra of (a) CF, (b) CMF15, (c) CMF25, (d) CMF30, (e) CMF40 and (f) CMF50 samples are shown.

5. Magnetic properties:

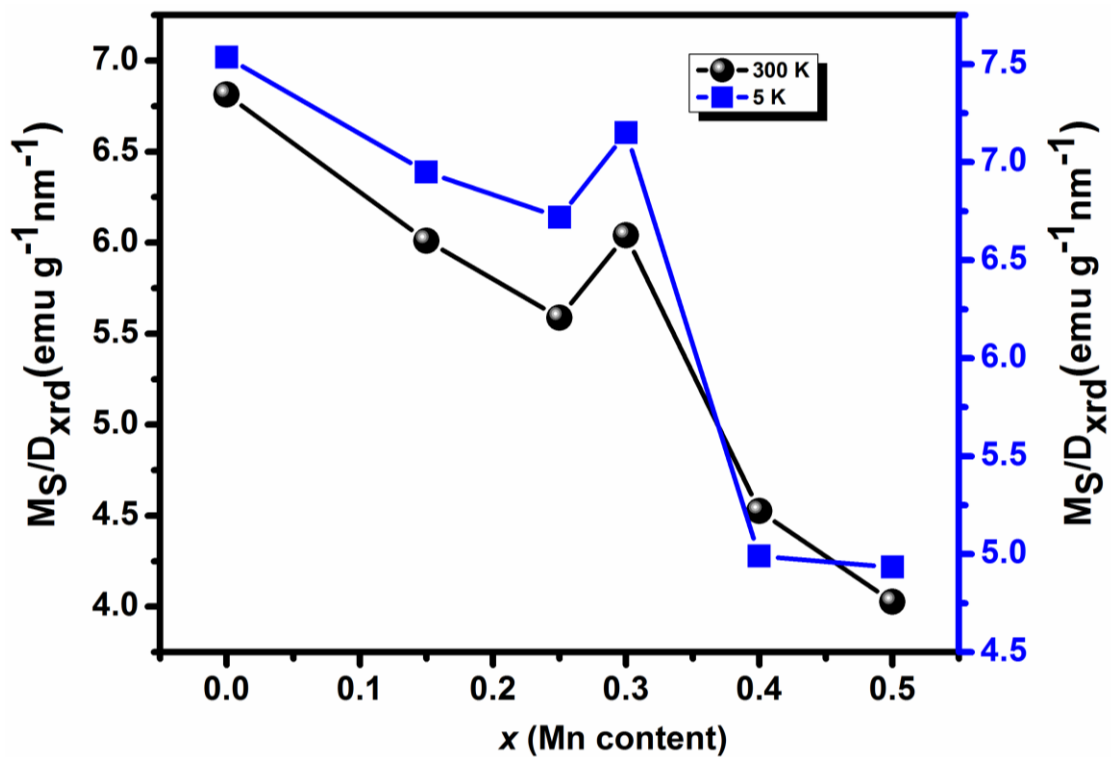


Figure S3. Saturation magnetization (M_S) normalized by the particle size (determined by XRD) as a function of Mn content for $\text{Co}_{1-x}\text{Mn}_x\text{Fe}_2\text{O}_4$ magnetic nanoparticles at 5 K and 300 K