

SUPPORTING INFORMATION

Crystal/magnetic structure and cation inversion in hydrothermally synthesized MnFe_2O_4 , CoFe_2O_4 , NiFe_2O_4 , and ZnFe_2O_4 nanoparticles: A neutron powder diffraction study

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MnFe_2O_4 - STEM-HAADF images

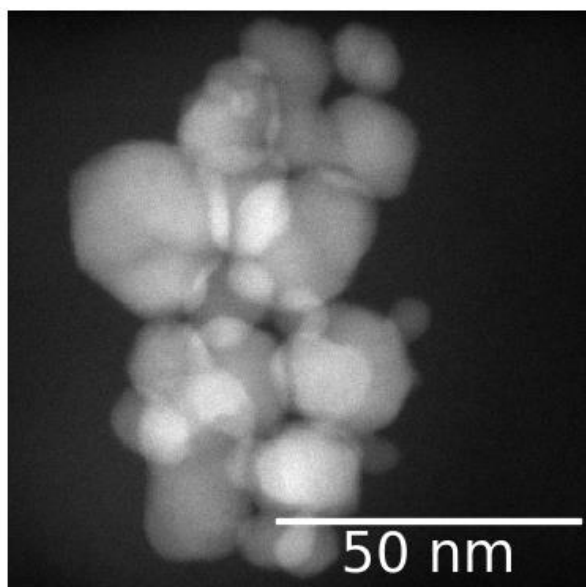
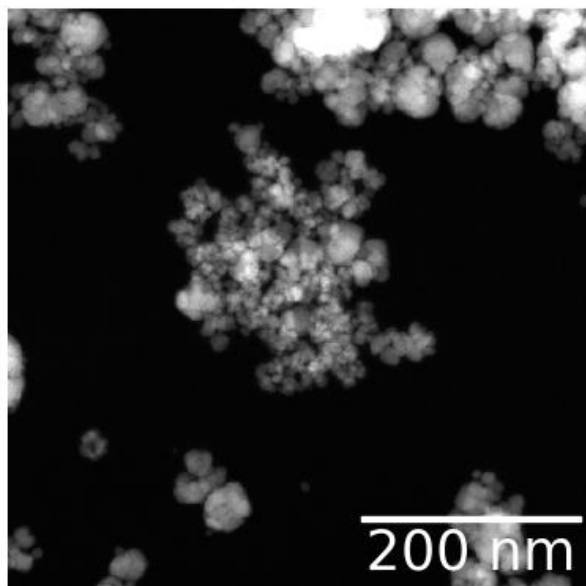


Figure S1: Representative STEM-HAADF images for the MnFe_2O_4 sample.

MnFe₂O₄ – EDS spectrum

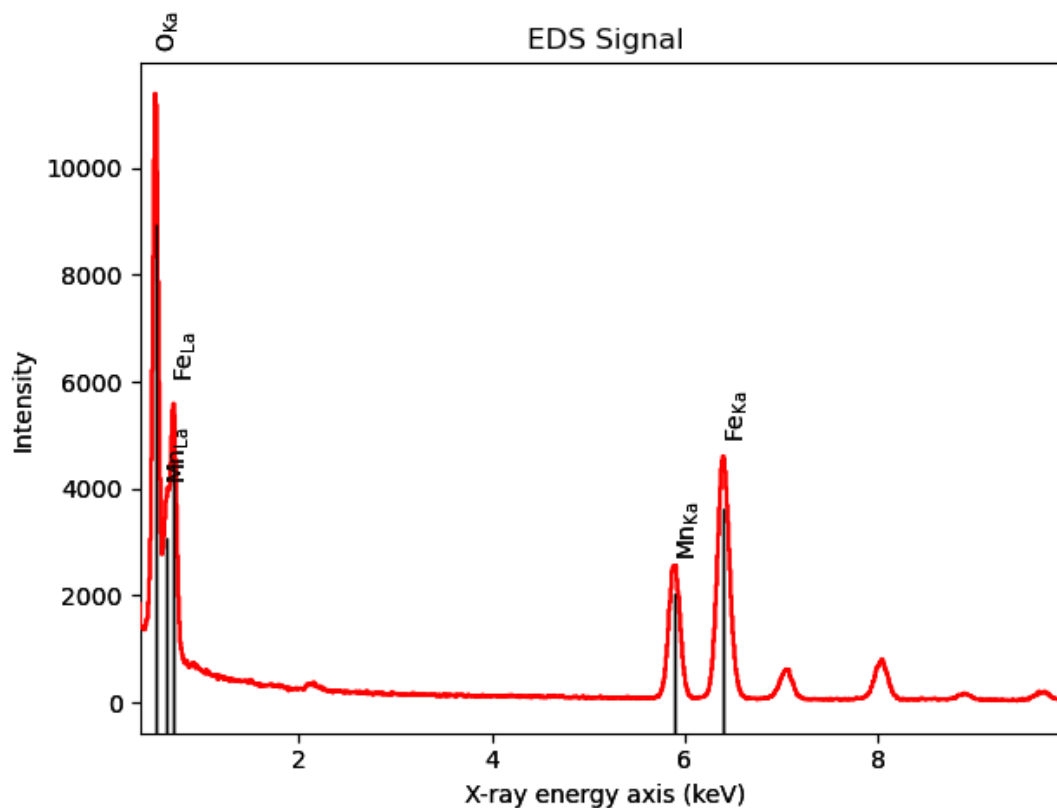


Figure S2: EDS spectrum for the MnFe₂O₄ sample.

Table S1: Quantitative analysis of EDS data for the MnFe₂O₄ sample.

MnFe ₂ O ₄					
Spectrum Image	0951	0932	1000		Average
O	2.28	2.95	3.07		2.77
Error O	0.46	0.60	0.62		0.33
Fe	0.75	1.02	0.98		0.92
Error Fe	0.10	0.14	0.13		0.07
Mn	0.33	0.58	0.54		0.48
Error Mn	0.05	0.08	0.07		0.04
Fe:Mn	2.00	1.75	1.86		1.87
Error Fe:Mn	0.46	0.34	0.34		0.24
O:Fe	3.04	2.89	3.13		3.02
Error O:Fe	0.74	0.71	0.76		0.44
O:Mn	6.91	5.09	5.69		5.89
Error O:Mn	1.74	1.25	1.36		1.71
O:(Fe+Mn)	2.11	1.84	2.02		1.99
Error O:(Fe+Mn)	0.48	0.42	0.45		0.28

CoFe_2O_4 - STEM-HAADF images

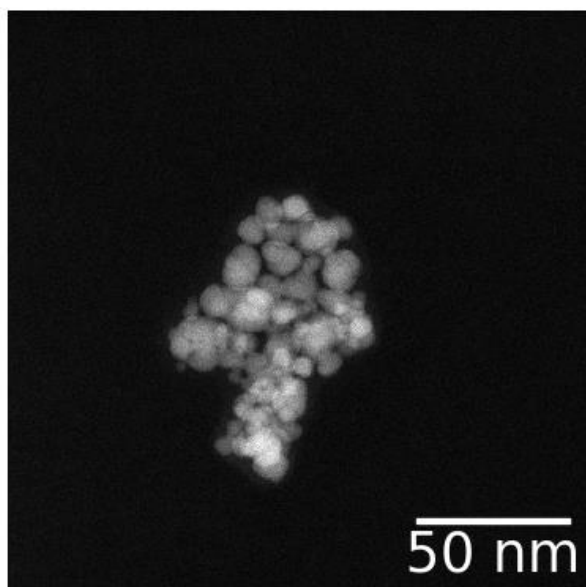
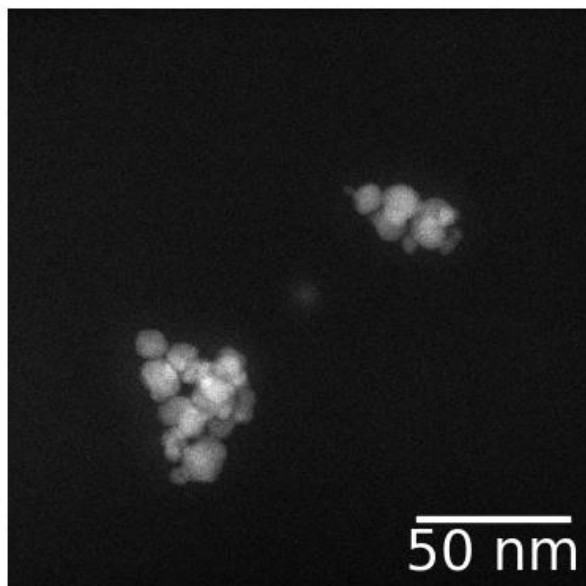


Figure S3: Representative STEM-HAADF images for the CoFe_2O_4 sample.

CoFe₂O₄ – EDS spectrum

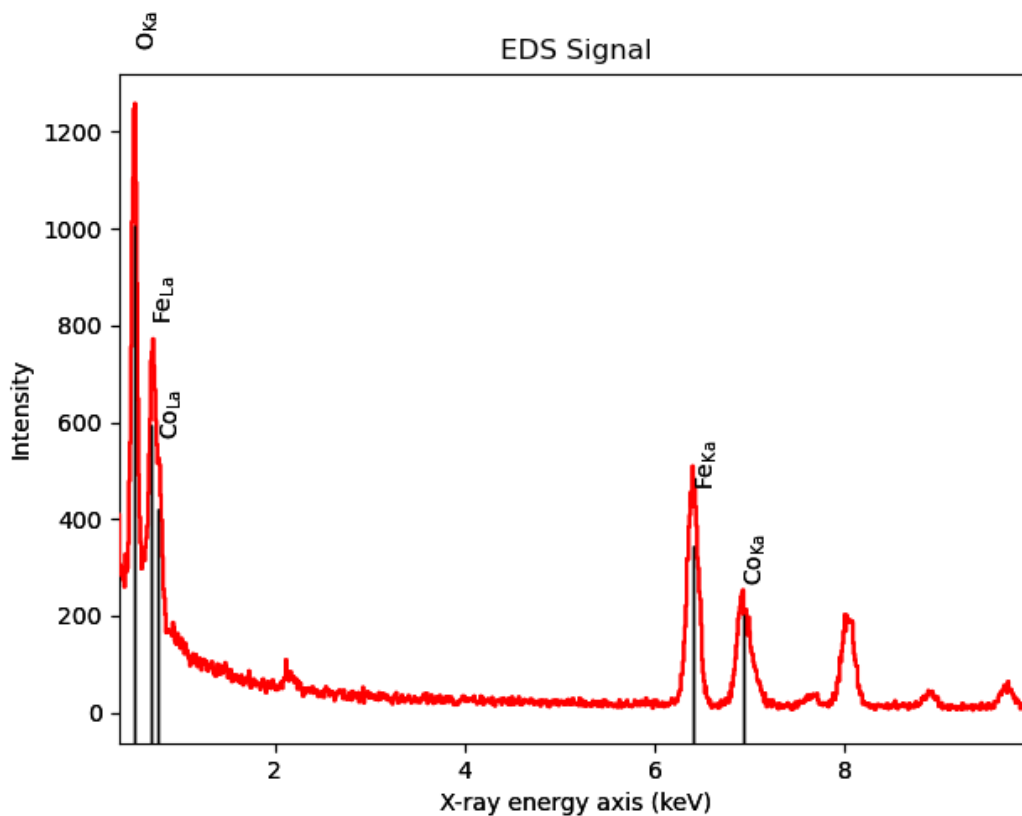


Figure S4: EDS spectrum for the CoFe₂O₄ sample.

Table S2: Quantitative analysis of EDS data for the CoFe₂O₄ sample.

CoFe ₂ O ₄					
Spectrum Image	1038	1053	1117		Average
O	2.18	4.52	2.64		3.11
Error O	0.44	0.92	0.53		0.38
Fe	0.68	1.61	0.78		1.02
Error Fe	0.09	0.22	0.11		0.09
Co	0.29	0.80	0.38		0.49
Error Co	0.04	0.11	0.05		0.04
Fe:Co	2.25	2.00	2.20		2.15
Error Fe:Co	0.45	0.39	0.40		0.26
O:Fe	3.21	2.81	3.38		3.13
Error O:Fe	0.77	0.69	0.83		0.53
O:Co	7.52	5.65	6.95		6.70
Error O:Co	1.84	1.39	1.67		1.86
O:(Fe+Co)	2.25	1.88	2.28		2.13
Error O:(Fe+Co)	0.51	0.43	0.51		0.33

NiFe_2O_4 - STEM-HAADF images

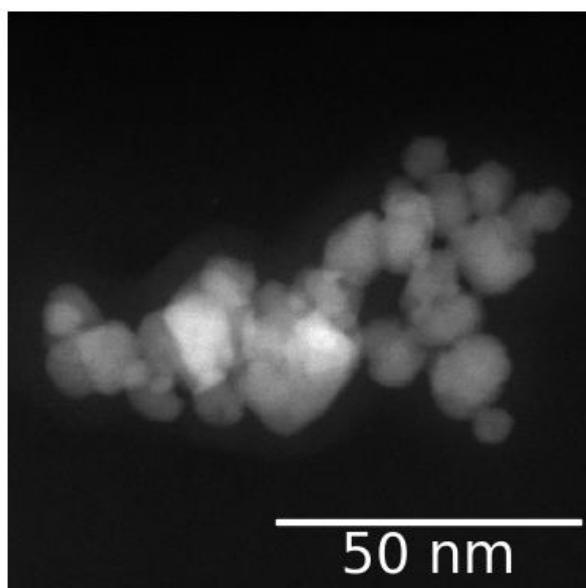
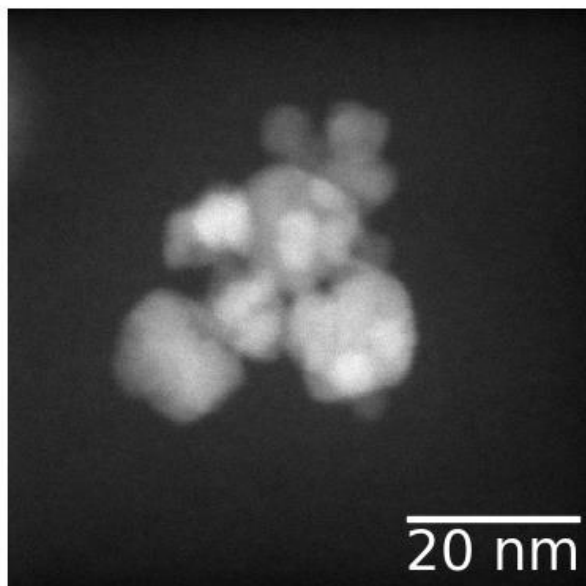


Figure S5: Representative STEM-HAADF images for the NiFe_2O_4 sample.

NiFe₂O₄ – EDS spectrum

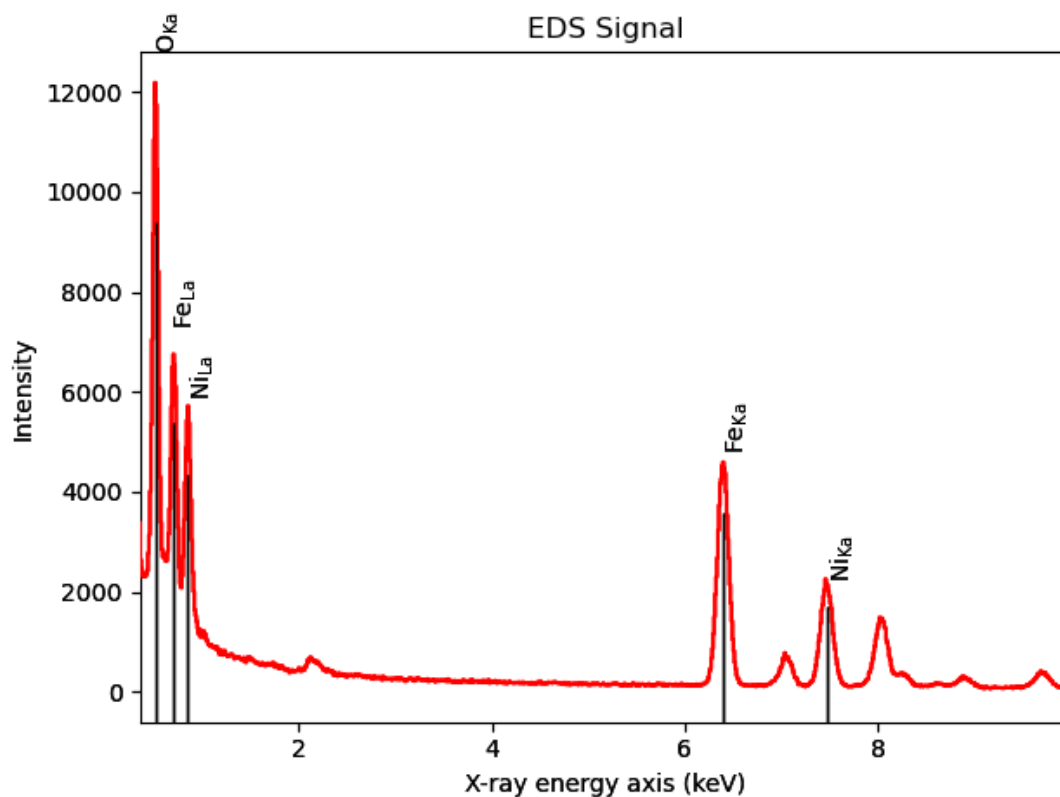


Figure S6: EDS spectrum for the NiFe₂O₄ sample.

Table S3: Quantitative analysis of EDS data for the NiFe₂O₄ sample.

NiFe ₂ O ₄					
Spectrum Image	0900	0932	1026		Average
O	2.86	1.89	2.40		2.38
Error O	0.58	0.38	0.49		0.28
Fe	0.94	0.57	0.72		0.74
Error Fe	0.13	0.08	0.10		0.06
Ni	0.46	0.29	0.39		0.38
Error Ni	0.06	0.04	0.05		0.03
Fe:Ni	2.17	2.00	2.00		2.06
Error Fe:Ni	0.39	0.39	0.35		0.23
O:Fe	3.04	3.32	3.33		3.23
Error O:Fe	0.75	0.81	0.82		0.49
O:Ni	6.22	6.52	6.15		6.30
Error O:Ni	1.50	1.59	1.48		0.92
O:(Fe+Ni)	2.04	2.20	2.16		2.13
Error O:(Fe+Ni)	0.46	0.50	0.49		0.29

ZnFe_2O_4 - STEM-HAADF images

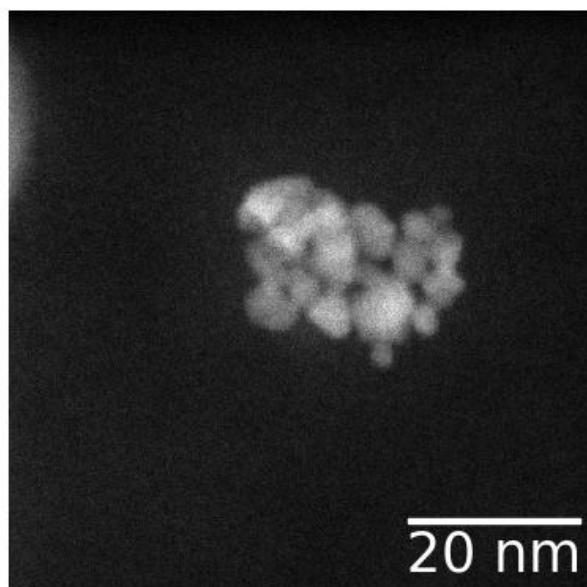
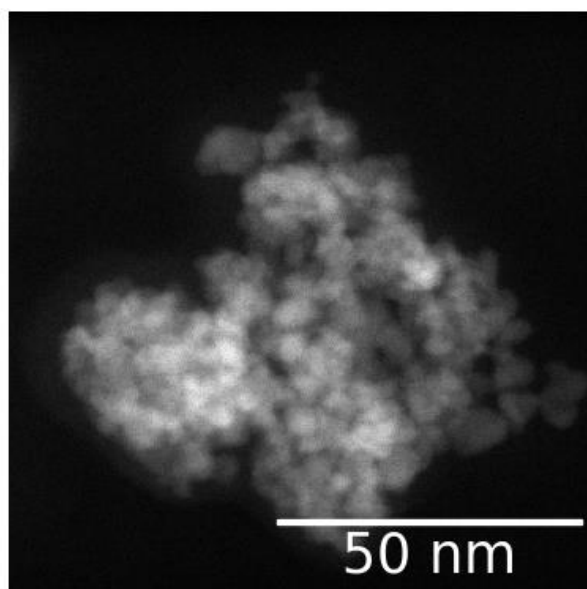


Figure S7: Representative STEM-HAADF images for the ZnFe_2O_4 sample.

ZnFe₂O₄ – EDS spectrum

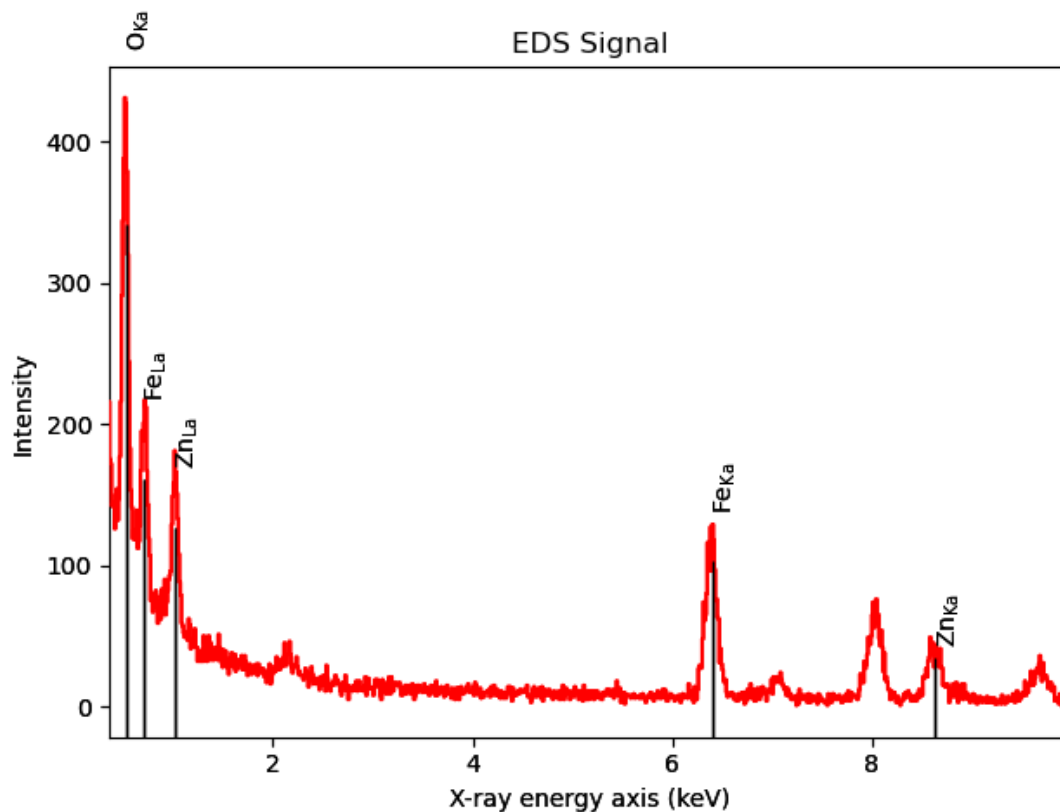


Figure S8: EDS spectrum for the ZnFe₂O₄ sample.

Table S4: Quantitative analysis of EDS data for the ZnFe₂O₄ sample.

ZnFe ₂ O ₄					
Spectrum Image	0951	0932			Average
O	2.46	1.40			1.29
Error O	0.49	0.28			0.19
Fe	0.78	0.34			0.37
Error Fe	0.10	0.05			0.04
Zn	0.40	0.14			0.18
Error Zn	0.05	0.02			0.02
Fe:Zn	2.00	2.50			2.25
Error Fe:Zn	0.35	0.50			0.43
O:Fe	3.15	4.12			3.64
Error O:Fe	0.75	1.02			1.10
O:Zn	6.15	10.00			8.08
Error O:Zn	1.45	2.46			8.84
O:(Fe+Zn)	2.08	2.92			2.50
Error O:(Fe+Zn)	0.46	0.67			0.75

MnFe₂O₄ data - Test model 1: Mn_xFe_{2-x}O₄

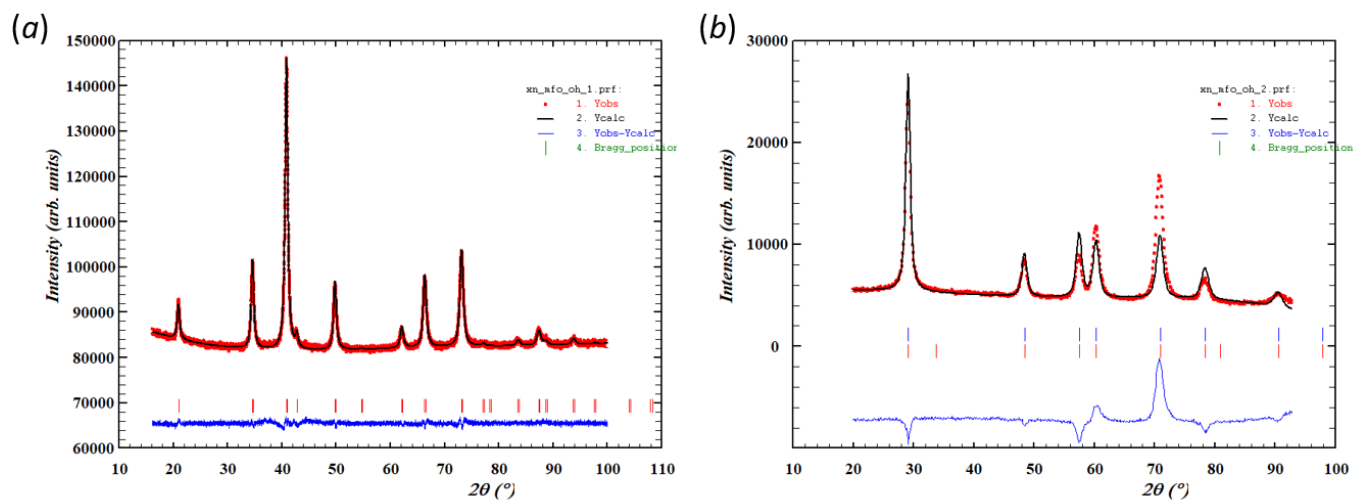


Figure S9: a) PXR data, $R_{\text{Bragg}}=1.84\%$, $R_F=1.64\%$. b) NPD data, $R_{\text{Bragg}}=33.5\%$, $R_F=16.5\%$, $R_{\text{magn}}=18.7\%$.

MnFe₂O₄ data - Test model 2: Fe₃O₄

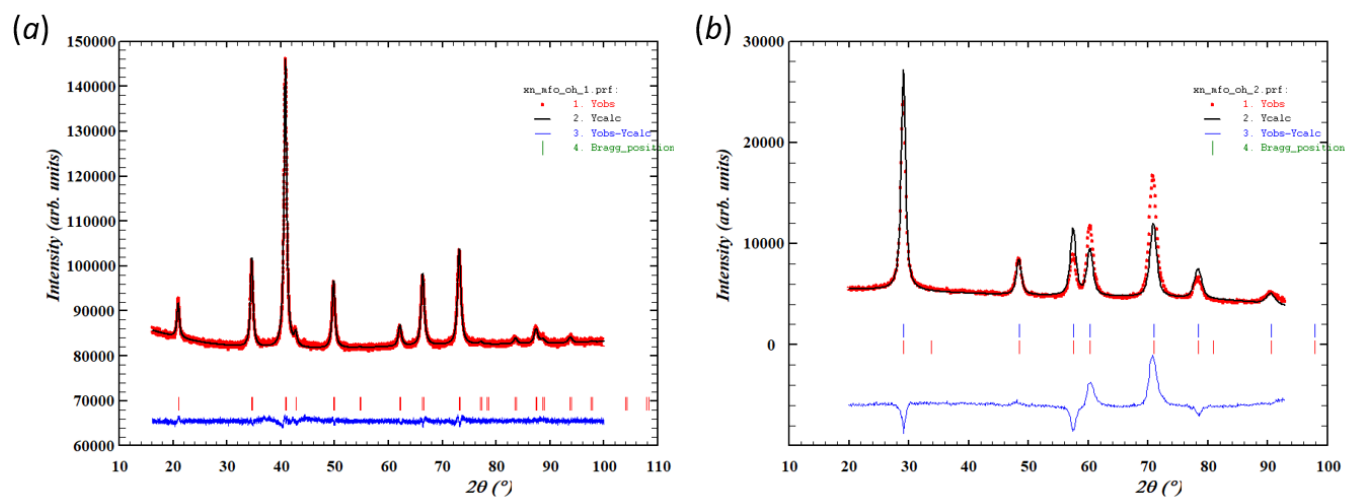


Figure S10: a) PXR data, $R_{\text{Bragg}}=2.00\%$, $R_F=1.75\%$. b) NPD data, $R_{\text{Bragg}}=34.2\%$, $R_F=15.2\%$, $R_{\text{magn}}=18.0\%$.

MnFe₂O₄ data - Test model 3: γ -Fe₂O₃

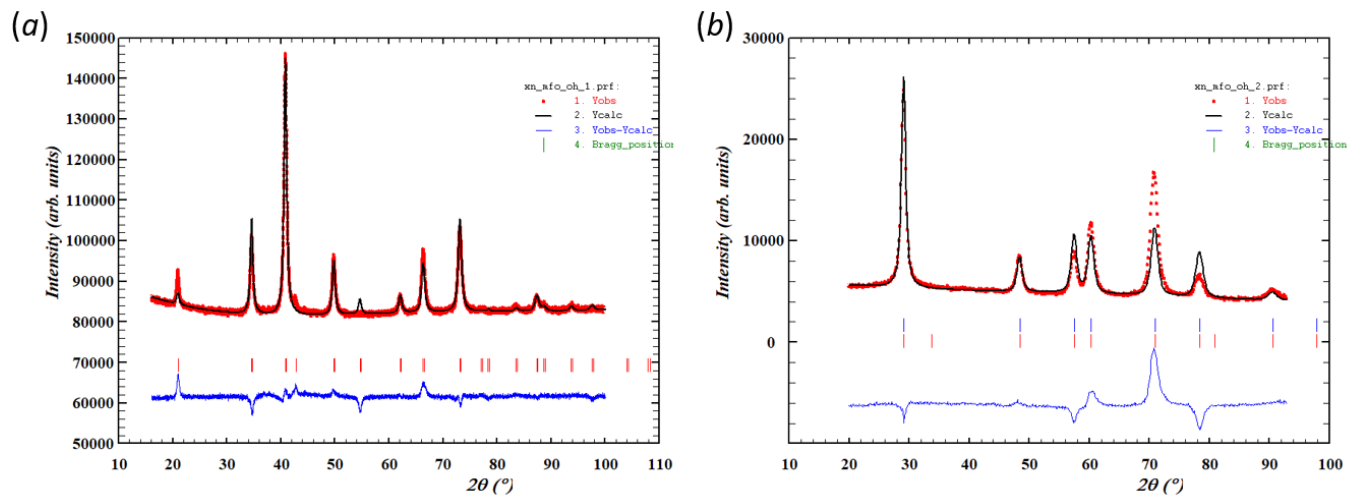


Figure S11: a) PXRD data, $R_{\text{Bragg}}=12.7\%$, $R_F=10.2\%$. b) NPD data, $R_{\text{Bragg}}=36.2\%$, $R_F=16.7\%$, $R_{\text{magn}}=18.8\%$.

MnFe₂O₄ data - Test model 4: γ -Mn_{0.67}Fe_{1.33}O₃

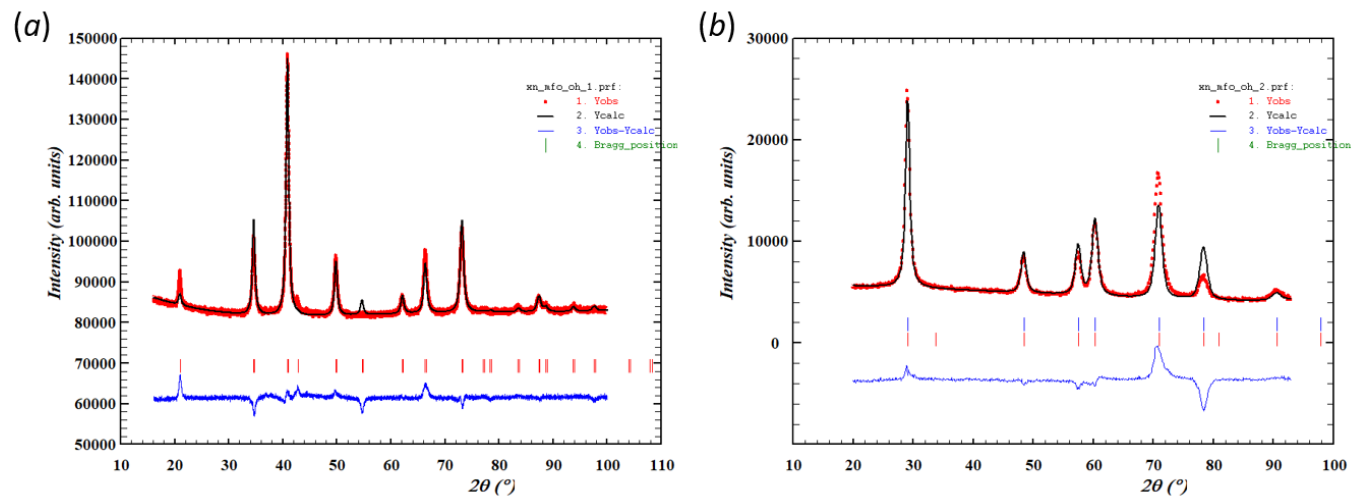


Figure S12: a) PXRD data, $R_{\text{Bragg}}=12.5\%$, $R_F=10.1\%$. b) NPD data, $R_{\text{Bragg}}=22.2\%$, $R_F=11.2\%$, $R_{\text{magn}}=15.5\%$.

MnFe₂O₄ data - Test model 5: Mn³⁺ in magnetic model

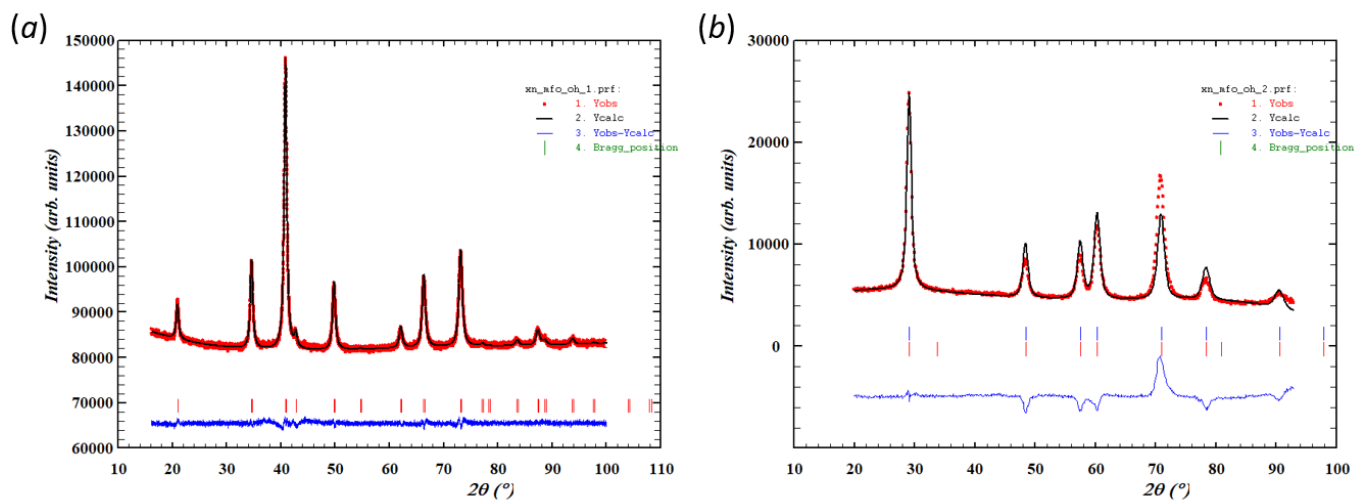


Figure S13: a) PXRD data, $R_{\text{Bragg}}=1.88\%$, $R_{\text{F}}=1.59\%$. b) NPD data, $R_{\text{Bragg}}=21.6\%$, $R_{\text{F}}=11.5\%$, $R_{\text{magn}}=13.0\%$.