SUPPLEMENTARY CONTENT (S1)

Revealing the influence of Fe substitution on structural and magnetic features of orthomanganite $DyMn_2O_5$

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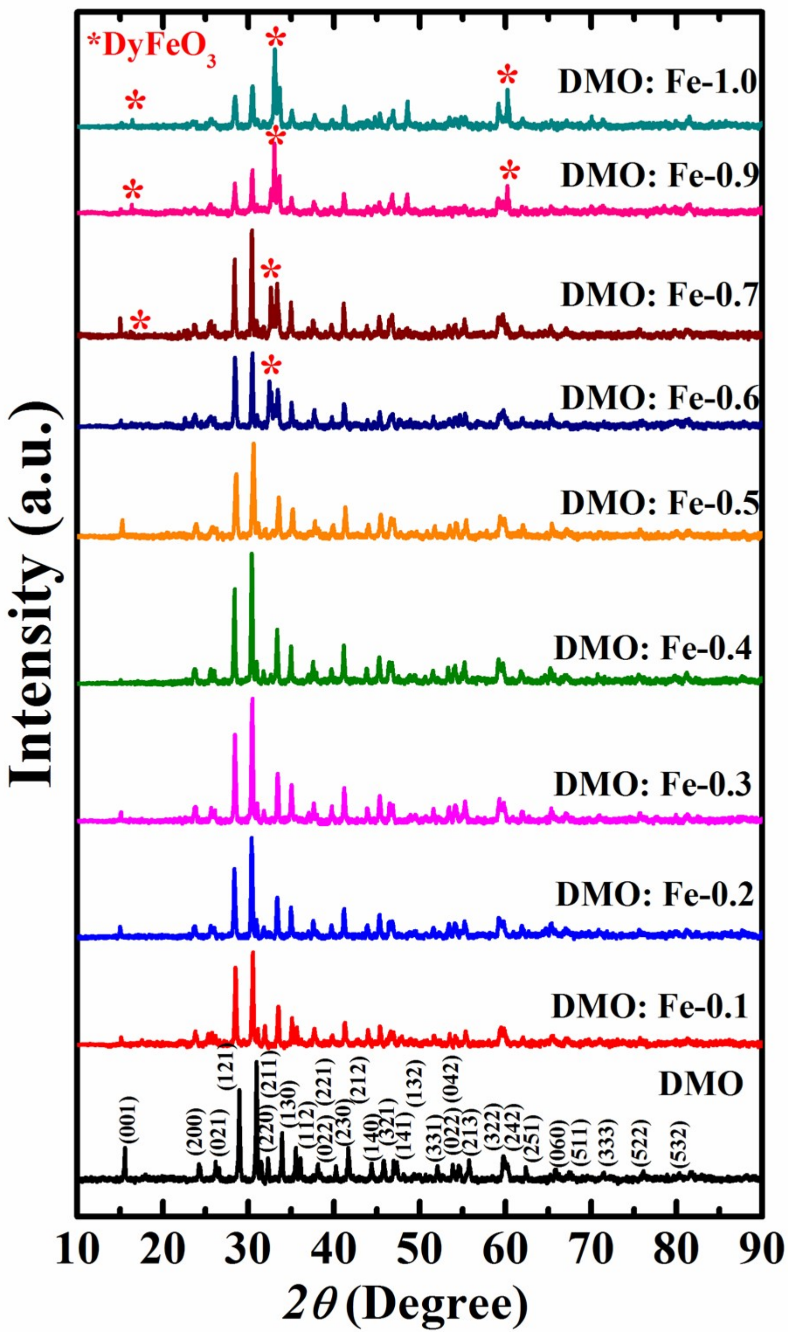

FIG.S1. XRD patterns of $DyMn_{2-x}Fe_xO_5$ (x = 0 to 1).

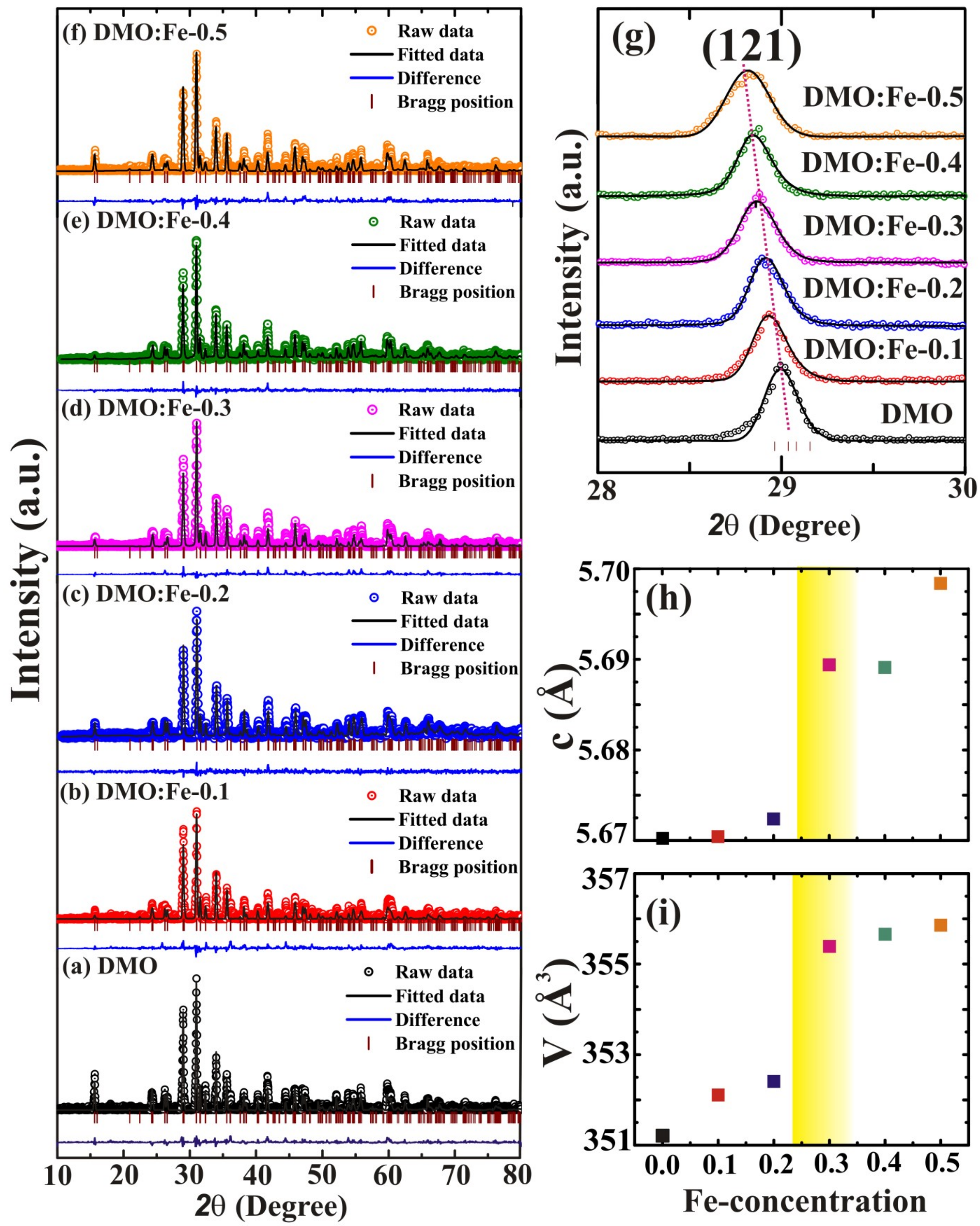

FIG.S2. (a-f) Refined XRD patterns of $DyMn_{2-x}Fe_xO_5$ (x=0-0.5) (g) Magnified view of (121) reflection (h,i) Variation of lattice constant 'c' and cell volume (V) with Fe composition.

Sample	Bond angles (°)	M_s (μ_B)	K_1 (erg/cm^3)
DMO	Mn1-O3-Mn2 ~122.28 (2) Mn1-O4-Mn2 ~121.51(1) Mn2-O1-Mn2 ~99.97(3) Mn1-O3-Mn1 ~115.18(1)	13.36	0.50×10^6
DMO:Fe-0.1	Mn1-O3-Fe/Mn2 ~122.26(3) Mn1-O4-Fe/Mn2 ~108.72(2) Fe/Mn2-O1-Fe/Mn2 ~130.31(2) Mn1-O3-Mn1 ~102.43(1)	12.89	0.47×10^6
DMO:Fe-0.2	Mn1-O3-Fe/Mn2 ~121.6(2) Mn1-O4-Fe/Mn2 ~106.2(1) Fe/Mn2-O1-Fe/Mn2 ~98.5(3) Mn1-O3-Mn1 ~94.8(1)	11.74	0.43×10^6
DMO:Fe-0.3	Mn1-O3-Fe/Mn2 ~134.41(1) Mn1-O4-Fe/Mn2 ~127.10(2) Fe/Mn2-O1-Fe/Mn2 ~122.25(1) Mn1-O3-Mn1 ~90.24(3)	10.78	0.40×10^6
DMO:Fe-0.4	Mn1-O3-Fe/Mn2 ~136.81(1) Mn1-O4-Fe/Mn2 ~129.86(2) Fe/Mn2-O1-Fe/Mn2 ~114.79 (1) Mn1-O3-Mn1 ~84.30(2)	14.18	0.53×10^6
DMO:Fe-0.5	Mn1-O3-Fe/Mn2 ~131.39(1) Mn1-O4-Fe/Mn2 ~124.16(1) Fe/Mn2-O1-Fe/Mn2 ~110.75(2) Mn1-O3-Mn1 ~93.88(3)	13.78	0.52×10^6

TABLE.S1. Values of bond angles present in the unit cell of $DyMn_{2-x}Fe_xO_5$ (x=0-0.5) samples along with magnetic parameters like saturation magnetization (M_s) and magnetic anisotropy constant (K_1).

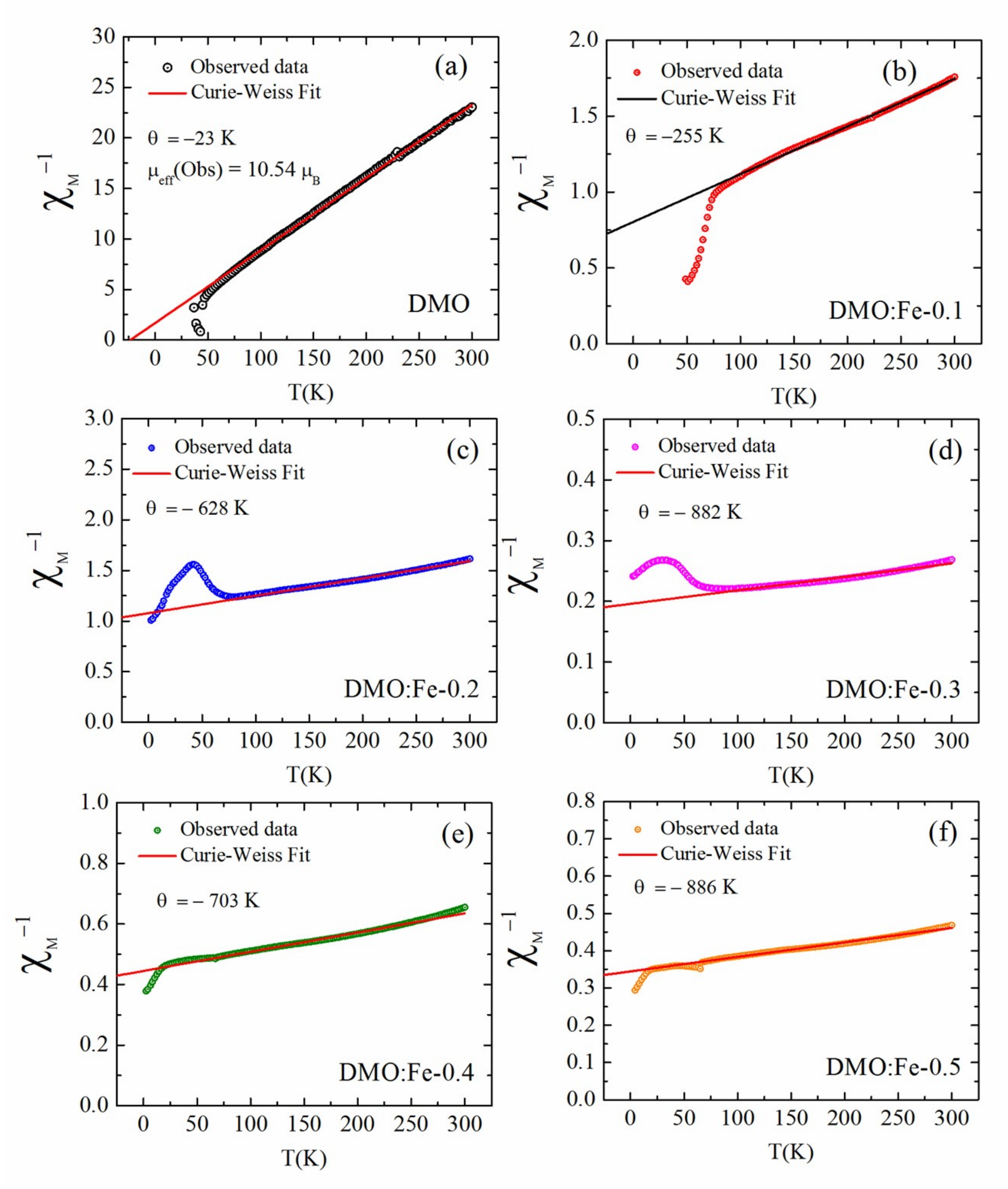

FIG.S3. (a-f) Inverse of susceptibility versus temperature curves of $DyMn_{2-x}Fe_xO_5$ (x=0-0.5) samples along with Curie-Weiss fit.

To explore the exact magnetic nature of $DyMn_{2-x}Fe_xO_5$ (x=0-0.5) samples, Curi-Weiss law ($\chi = C/T\text{-}\theta$) was applied to the plot of the inverse of susceptibility versus temperature (Fig. S3).

Curie-Weiss fit yields Weiss temperature (*θ = -23 K*) and the observed effective magnetic moment of 10.54 μ_B for DMO sample. The small value of Weiss temperature (*θ = -23 K*) reflects anti-ferromagnetic (AFM) character of DMO samples as already confirmed through M-T studies (Fig. 8). The theoretical value of *μeff* (th) is also calculated by considering the magnetic moments of Dy^{3+} (10.62 *μB*), Mn^{3+} (4.9 *μB*) and Mn^{4+} (3.87 *μB*) ***(AIP Adv. 7, 055830 (2017))***. *μeff* (obs) (10.54 *$\mu B/f.u.$)* is found to be lower than *μeff* (th) (12.32 *$\mu B/f.u.$)*. This difference could be due to the analysis carried out near T_N and short-range AFM ordering ***(Materials Chemistry and Physics 317 (2024) 129198)***. Curie-Weiss fit suggests that Fe substitution lead to enhance Weiss temperature (*θ*) from -255 K >> T_N (for Fe: 0.1) to -882 K >> T_N (for for Fe: 0.3). The large magnitude of Weiss temperature at the negative side depicts frustrated AFM behaviour of Fe-substituted samples that found to be similar to the Fe substituted $BiMn_2O_5$ as reported in ***(Journal of Magnetism and Magnetic Materials 452 (2018) 120–128).*** The value of Weiss temperature is found to be reduced for Fe: 0.4 and not escalated at that extent for Fe: 0.5 substituted samples. This is because for Fe: 0.4 and 0.5 samples, Fe^{3+} substitution is sufficient to enhance the strength of Mn^{4+}-O-Fe^{3+}-O-Mn^{4+} interaction as already discussed in section of low temperature (5K) M-H analysis. The effective magnetic moment for Fe-substituted samples cannot be correctly predicted due to the frustrated AFM behaviour of the samples.