Electronic Supplementary Information (ESI)

Implications of including a magnetic ion (Cr^{3+} and Fe^{3+}) at the vanadium site in geometrically frustrated spinel MgV_2O_4: Magnetic and Catalytic properties

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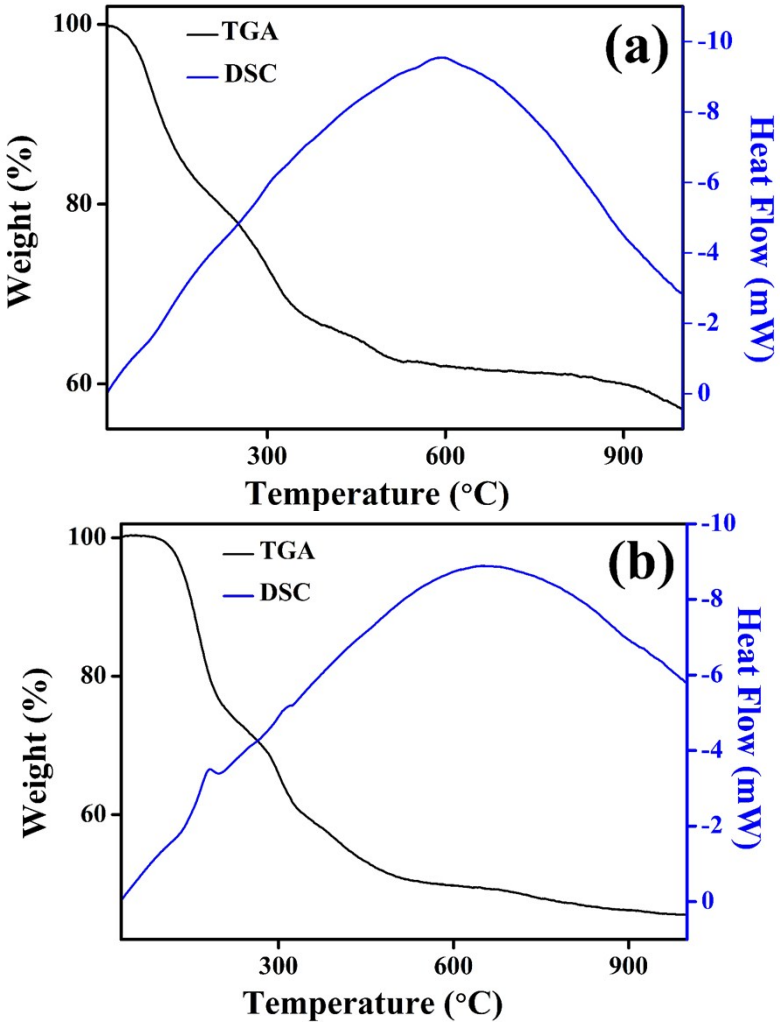

Fig. S1 Thermogravimetric (TG) and Differential Scanning Calorimetric (DSC) traces of xerogel obtained from the reaction of propylene oxide with (a) $MgCl_2.6H_2O$, VCl_3, $CrCl_3.6H_2O$ and (b) $MgCl_2.6H_2O$, VCl_3, $Fe(NO_3)_3.9H_2O$.

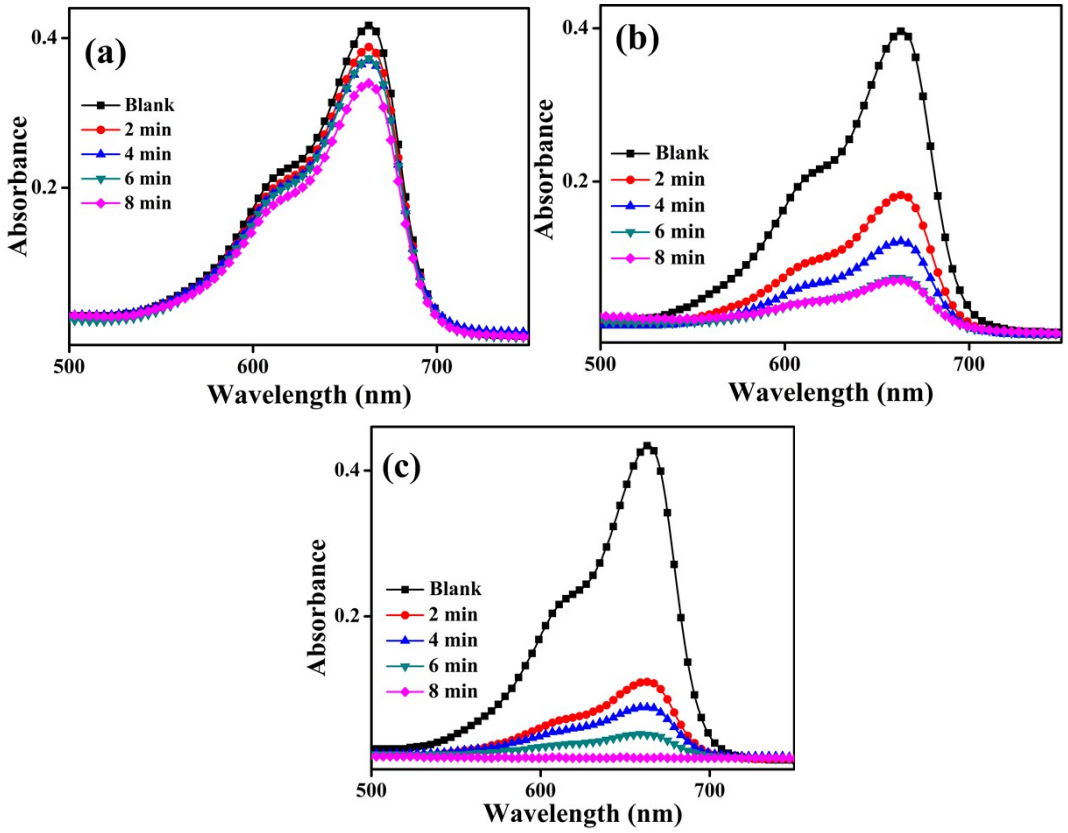

Fig. S2 Temporal changes in the absorbance characteristics of 50 mL MB dye solution (10 μM) in the presence of 5 mL H_2O_2 and 50 mg of (a) MgV_2O_4, (b) $MgVCrO_4$ and (c) $MgVFeO_4$ as catalyst.

Table S1 Summary of the crystallographic details from the Rietveld refinement of PXRD patterns

Formula	**MgV_2O_4**	**$MgVCrO_4$**	**$MgVFeO_4$**
Crystal system	Cubic	Cubic	Cubic
Space group	$Fd\bar{3}m$ (#227)	$Fd\bar{3}m$ (#227)	$Fd\bar{3}m$ (#227)
a (Å)	8.3990 (4)	8.3497 (5)	8.3957 (27)
Cell volume (Å^3)	592.49 (8)	582.12 (10)	591.81 (6)
Formula weight (g/mol)	187.64	184.04	189.12
Z	8	8	8
ρ calc (g/cm^3)	4.207	4.200	4.246
Temperature (°C)	25	25	25
No. of data points	2250	2250	1875
2θ range	10-100°	10-100°	25-100°
R_p (%)	7.38	6.54	3.10
R_{wp} (%)	9.57	8.22	3.99
χ^2	1.461	1.343	1.318

Table S2: Atomic parameters after the final cycle of refinement of MgV_2O_4, $MgCrVO_4$, and $MgVFeO_4$.

Atoms	*Wyck*	*x/a*	*y/b*	*z/c*	SOF	U(iso)Å^2
V	*16c*	0	0	0	0.971 (8)	0.0264 (8)
Mg	*8b*	0.375	0.375	0.375	1.015 (9)	0.0286 (14)
O	*32e*	0.2411 (4)	0.2411 (4)	0.2411 (4)	1	0.025
V	*16c*	0	0	0	0.437 (8)	0.0197 (10)
Cr	*16c*	0	0	0	0.496 (7)	0.0197 (10)
Mg	*8b*	0.375	0.375	0.375	0.986 (8)	0.0344 (21)
O	*32e*	0.2409 (6)	0.2409 (6)	0.2409 (6)	1.0	0.025
V	*16c*	0	0	0	0.520 (27)	0.022(4)
Fe	*16c*	0	0	0	0.397 (19)	0.0322 (32)
Mg	*8b*	0.375	0.375	0.375	0.992 (18)	0.0209 (30)
O	*32e*	0.2402 (8)	0.2402 (8)	0.2402 (8)	1.0	0.025