Electronic Supplementary Information (†ESI)

Modulating the optical and magnetic properties of geometrically frustrated ZnV_2O_4 by the introduction of indium (nonmagnetic) and iron and chromium (magnetic ions)

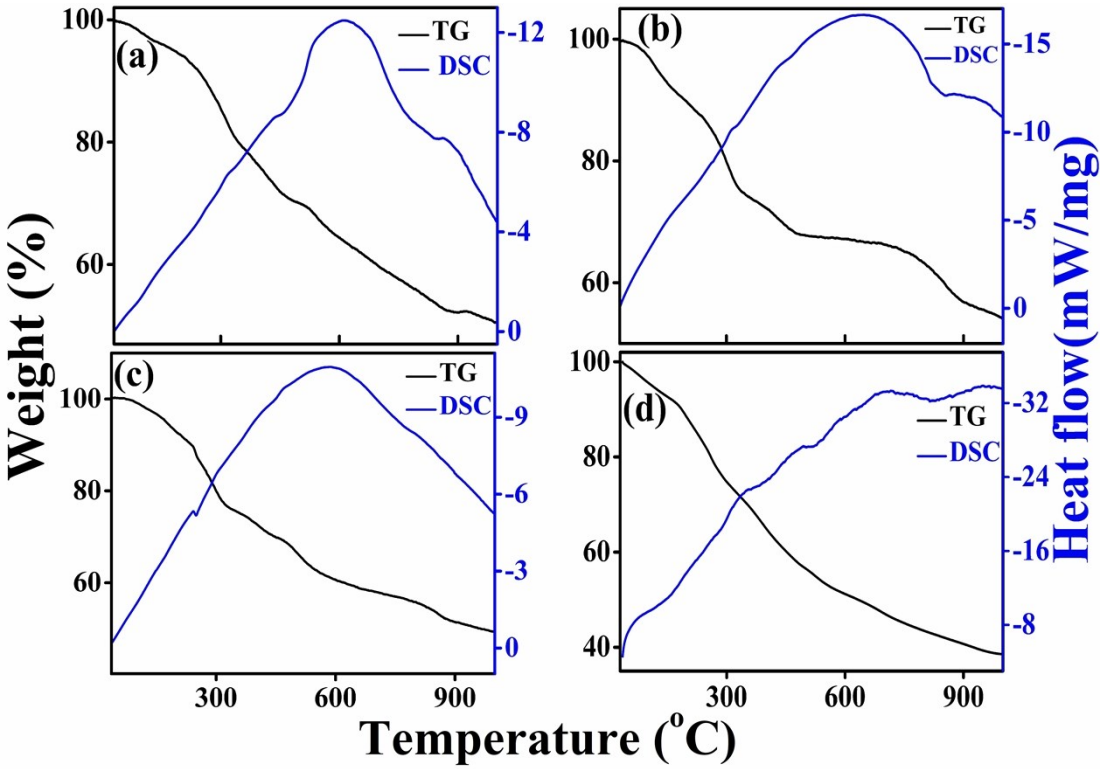

Fig. S1 shows thermogravimetric (TG) and differential scanning calorimetric (DSC) traces of xerogels formed from the reaction of propylene oxide with chloride salts of zinc and vanadium with $In(NO_3)_3.xH_2O$ to yield $ZnV_{2-x}In_xO_4$ series where (a) x = 0.00, (b) x = 0.25, (c) x = 0.50, and (d) x = 1.00.

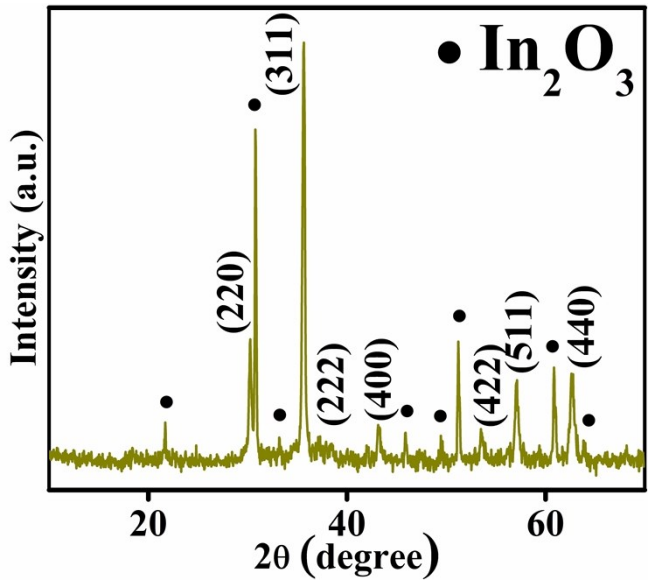

Fig. S2 shows PXRD pattern of calcined xerogel with a composition of $ZnV_{0.50}In_{1.50}O_4$.

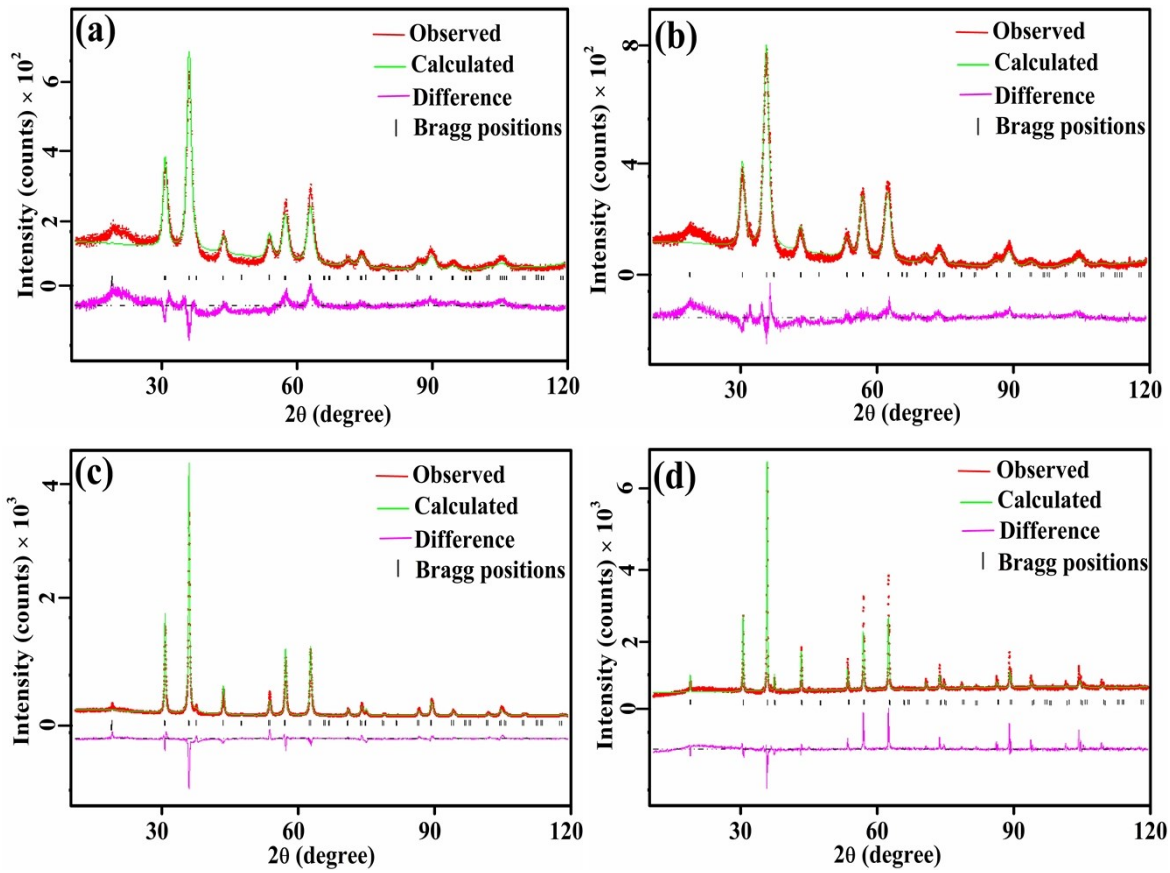

Fig. S3 shows (a)-(c) structural refinement trials of the PXRD patterns of compositions of the series $ZnV_{2-x}In_xO_4$ (x = 0.25, 0.50, and 1.00) by the Rietveld method considering 10 mol % of In^{3+} occupying tetrahedral sites in addition to octahedral sites, (d) structural refinement of the PXRD pattern of $ZnVFeO_4$ in which mixed occupancy of Fe at the tetrahedral and octahedral sites is considered.

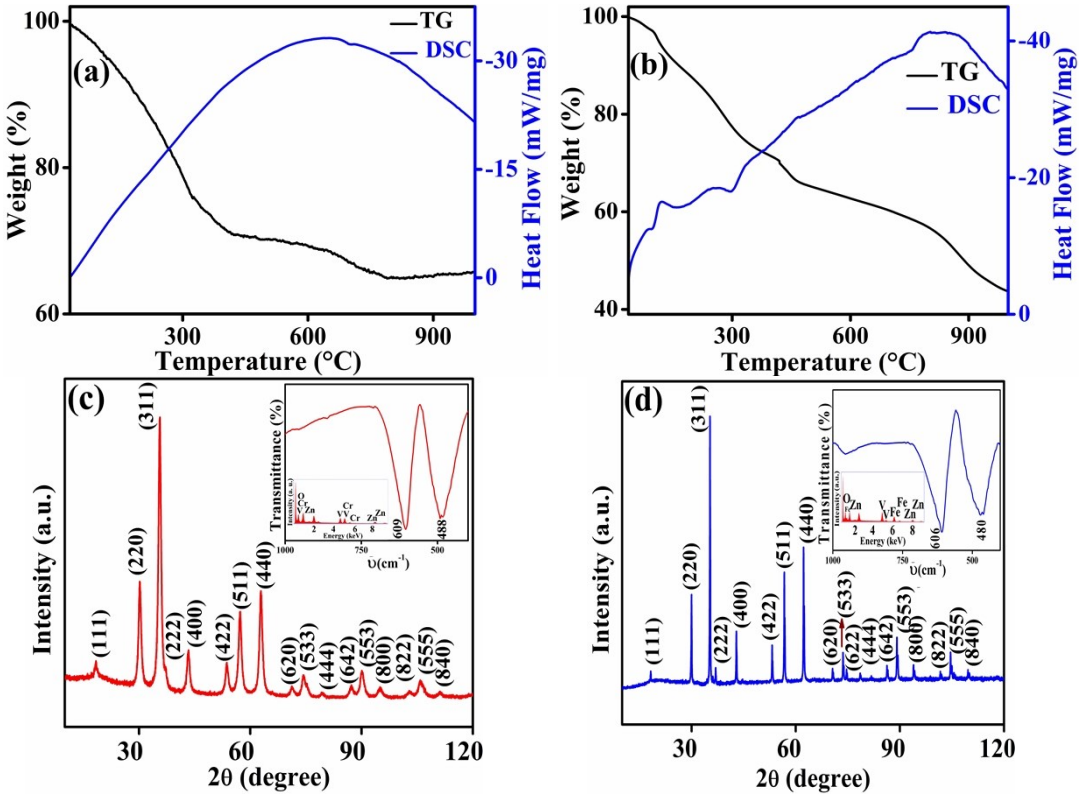

Fig. S4 shows (a) and (b) show thermogravimetric (TG) and differential scanning calorimetric (DSC) traces of xerogels obtained from the reaction of propylene oxide with chloride salts of Zn, V and Cr (1:1:1) and chloride and nitrate salts of zinc, vanadium, and iron (1:1:1), respectively, (c) and (d) PXRD pattern obtained after calcining the xerogels containing zinc, vanadium with chromium and zinc, vanadium with iron at 700 °C and 850 °C, respectively in flowing argon atmosphere for 2 h. Insets of (c) and (d) show their respective FTIR and energy dispersive spectra.

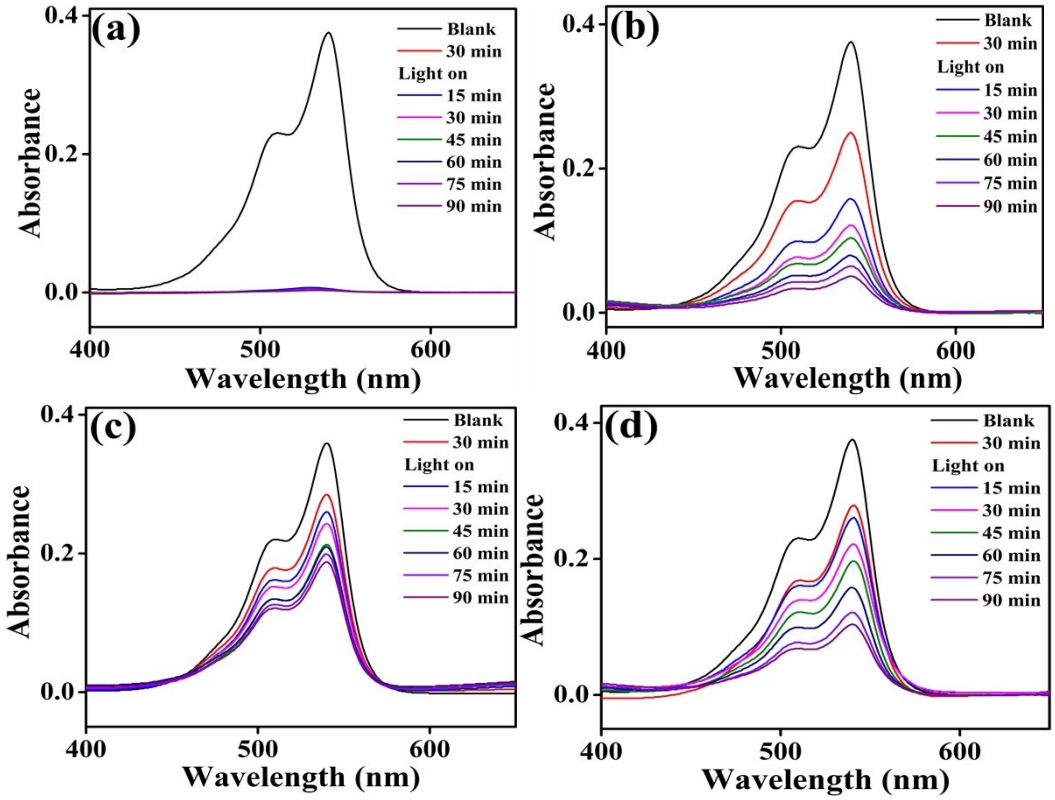

Fig. S5 shows temporal changes of Rh-6G dye solution (10×10^{-5} M) in the presence of 50 mg of (a) ZnV_2O_4, (b) $ZnVInO_4$, (c) $ZnVCrO_4$, and (d) $ZnVFeO_4$ under UV-visible light.

Table S1 Summary of the crystallographic details from the Rietveld refinement of PXRD patterns of $ZnVCrO_4$ and $ZnVFeO_4$.

Formula	**$ZnVCrO_4$**	**$ZnVFeO_4$**
Crystal system	Cubic	Cubic
Space group	$Fd\bar{3}m$ (#227)	$Fd\bar{3}m$ (#227)
a (Å)	8.3567 (23)	8.40665 (7)
Cell volume (Å^3)	583.5 (5)	594.112 (14)
Formula weight (g/mol)	232.12	235.92
Z	8	8
ρ calc (g/cm^3)	5.284	5.275
Temperature (°C)	25	25
No. of data points	11001	11001
2θ range	10-120°	10-120°
R_p (%)	5.44	9.32
R_{wp} (%)	7.46	11.49
χ^2	1.178	1.498

Table S2 Atomic parameters after the final cycle of refinement of $ZnVCrO_4$ and $ZnVFeO_4$.

Atoms	***Wyck***	***x/a***	***y/b***	***z/c***	**SOF**	**U(iso)Å²**
V	*16c*	0	0	0	0.517 (6)	0.0205 (7)
Cr	*16c*	0	0	0	0.491 (6)	0.0219 (11)
Zn	*8b*	0.375	0.375	0.375	0.983 (5)	0.0224 (8)
O	*32e*	0.2438 (5)	0.2438 (5)	0.2438 (5)	1.0	0.025
V	*16c*	0	0	0	0.526 (6)	0.0168 (12)
Fe	*16c*	0	0	0	0.477 (5)	0.0238 (13)
Zn	*8b*	0.375	0.375	0.375	0.996 (5)	0.0245 (7)
O	*32e*	0.2493 (5)	0.2493 (5)	0.2493 (5)	1.0	0.025