

Supplementary information

Exploring the Structural, Magnetic, and Optical properties of multifunctional $\text{Ni}_{0.4}\text{Mn}_{0.6}\text{Cr}_2\text{O}_4$ Spinel Chromite compound toward Optoelectronic Innovation

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Table SI.1. Structural parameters of chromite $\text{Ni}_{0.4}\text{Mn}_{0.6}\text{Cr}_2\text{O}_4$ sample.

Sample				$\text{Ni}_{0.4}\text{Mn}_{0.6}\text{Cr}_2\text{O}_4$
Structure				Cubic
Space group				$\text{Fd}\bar{3}m$
Unit cell parameter	$a(\text{Å})$			8.3872(7)
	$V(\text{Å}^3)$			590.016
Atoms	Tetrahedral A-site (Ni/Mn)	<i>Wykoff position</i>	$x = y = z$	8a
		<i>Site symmetry</i>		-43m
		<i>Atomic positions</i>		0.125
		$B_{\text{iso}}(\text{Å}^2)$		0.19819
		<i>Occupancy (Ni)</i>		0.0500(1)
		<i>Occupancy (Mn)</i>		0.0749(8)
	Octahedral B-site (Cr)	<i>Wykoff position</i>	$x = y = z$	16d
		<i>Site symmetry</i>		-3m
		<i>Atomic positions</i>		0.5
		$B_{\text{iso}}(\text{Å}^2)$		0.02140
		<i>Occupancy</i>		0.2499(8)
		<i>Wykoff position</i>		32e
<i>Site symmetry</i>			3m	

	O	<i>Atomic positions</i>	x = y = z	0.26251
		$B_{iso}(\text{Å}^2)$		0.21150
		<i>Occupancy</i>		0.4999(2)
	D_{SSP} (nm)			96.54
	D_{AL}(Å)			0.1817(3)
	L_{A-A} (Å)			3.6317(9)
	L_{B-B} (Å)			2.9653(4)
	D_{BL}(Å)			3.3202(0)
	D_{AE}(Å)			0.2967(7)
	D_{BE} (Å)			5.6339(2)
	d_{BEU} (Å)			3.5148(1)
	$d_{X-ray} (\text{g.cm}^{-3})$			5.053
	$\delta(10^{-4}\text{nm}^{-2})$			1.07
	$\langle Mn/Ni - O - Cr \rangle (^{\circ})$			120.9647(15)
	$\langle Cr - O - Cr \rangle (^{\circ})$			95.9073(11)
	r_A (Å)			0.6176(3)
	r_B (Å)			1.6603(0)
Agreement Factors	R_p (%)			2.62
	R_{exp}(%)			1.16
	R_{wp} (%)			1.36
	R_F (%)			2.64
	R_{Bragg} (%)			1.86
	χ^2			1.37