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**Structural, Electronic, Vibrational and Magnetic Properties of Zn2+ Substituted MnCr2O4 Nanoparticles**

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**Abstract**

In the present investigation, we report the structural, vibrational, electronic and magnetic properties of Mn0.5Zn0.5Cr2O4 nanoparticles fabricated by the solution combustion method and complemented by Density Functional theory (DFT) calculations. X-ray diffraction (XRD), Neutron diffraction, X-ray photoelectron spectroscopy and Raman analysis confirms the formation of single-phase with spinel cubic structure. The average crystallite size was found to be 8 nm. The theoretical calculations suggest that Zn-doping on the MnCr2O4 matrix induces a unit cell contraction associated with structural distortions along both [AO4] (A = Mn, Zn) and [CrO6] clusters, in agreement with the experimental evidence. These structural distortions contribute to narrowing the band-gap of Mn0.5Zn0.5Cr2O4 from disturbed energy levels in the vicinity of Fermi level. Field dependent magnetization confirms that the samples exhibit paramagnetic nature at 300 K and antiferromagnetic nature at 3 K. In the theoretical context, the exchange coupling constant for pure and Zn2+ substituted MnCr2O4 materials were calculated confirming the dominant antiferromagnetic character of Cr-Cr interactions. The temperature dependent susceptibility reveals that the magnetic transition from paramagnetic phase to antiferromagnetic phase occurs at 19 K (TN). The spin frustration factor of Mn0.5Zn0.5Cr2O4 is found to be 22 K. Hence, our experimental and theoretical result suggests that synthesized materials are useful for low and high frequency applications.

**Keywords:**

Neutron diffraction, Solution combustion method, Raman spectra, Antiferromagnetic, DFT calculations

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