Abstract

The nanocrystalline MnX_2O_4 (X=Ce, Nd, Ho) are prepared through the sol–gel route. The structural, magnetic and vibrational properties of rare earth-based spinels have been reported. The crystallinity, phase structure, and structural parameters of the synthesized samples have been determined through X-ray diffraction (XRD). FTIR study reveals that in the wavenumber range of 400 to 740 cm^{-1}, two vibrational bands were observed for each sample, thereby confirming the spinel structure. The complete evacuation of the nitrates and citric acid from the incorporated samples was avowed by the FTIR spectra. Fitting the Raman spectrums of the compounds (Gaussian deconvoluted) reveals six wide Raman bands at 204, 305, 460, 525, 668, 759 cm^{-1}. The distinctive bands of the crystalline cubic spinel MnX_2O_4 (X=Ce, Nd, Ho) with Fd3m are responsible for the six Raman bands. The sample's remanence ratios (Mr/Ms) are less than 0.5, this implies that all the samples have a single domain and magnetic isotropy. All the powders showed ferromagnetic characteristics, according to VSM testing.

First-principle calculations were carried to demonstrate the structural, electronic, magnetic, and thermoelectric properties of the manganese-based ternary spinel oxides MnX_2O_4 (X=Ce, Nd, Ho) by utilizing density functional theory with Perdew–Burke–Ernzerhof Generalized-Gradient Approximation as exchange and correlation functional. The spin polarized band structure and density of states illustrate that MnX_2O_4 (X=Ce, Nd, Ho) have a half metallic nature with indirect bandgap of 1.24 eV in spin up and metallic in spin down for $MnCe_2O_4$ whereas $MnNd_2O_4$ and $MnHo_2O_4$ have direct bandgaps of 0.0007 eV and 1.44 eV in spin up channel. Under the impact of the octahedral environment, the strong hybridization of Nd/Ho/Ce-d states with the O-p state increases the magnetic moment of the Ce/Nd/Ho and produces a fraction of the magnetic moments at the Mn and O sites. To evaluate the transport performance of compounds at different temperatures, thermoelectric (TE) properties such as power factor (PF), Seebeck coefficient (S), thermal conductivity (k/τ), electrical conductivity (σ/τ), power factor, and figure of merit (ZT) is established. Results reveal that, MnX_2O_4 (X=Ce, Nd, Ho) exhibit higher ZT values up to 0.006, 0.87 and 0.97, respectively. Hence, findings indicate that MnX_2O_4 (X=Ce, Nd, Ho)'s 100% spin polarization at the Fermi level makes it a competitive candidate in spintronics.