Experimental and Theoretical Investigation of Structural, Magnetic and Optical Properties of Nd_2FeCrO_6 and Gd_2FeCrO_6 Perovskites Synthesized by Sol-gel Technique

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Abstract

The first-principles predictions on the structural stability, magnetic behaviour and electronic structure of B-site ordered double perovskite Nd_2FeCrO_6 have been reported. The thermodynamic, mechanical, and dynamic stability analyses suggest the possibility of the synthesis of Nd_2FeCrO_6 double perovskite at ambient pressure. This compound shows ferrimagnetic (FiM) nature with 2 μB net magnetic moment and the magnetic ordering temperature has been estimated to be ~265 K. Electronic structure indicates a higher probability of direct photon transition over the indirect transition with a band gap of ~ 1.85 eV. Based on the theoretical prediction, Nd_2FeCrO_6 and Gd_2FeCrO_6 nanoparticles were synthesized for the first time using a facile citrate-based sol-gel method, and their structural, magnetic, and optical characteristics were thoroughly studied. Rietveld refinement analysis of the powder X-ray diffraction pattern of the synthesized Nd_2FeCrO_6 and Gd_2FeCrO_6 nanoparticles confirmed their single-phase monoclinic structure with $P2_1/n$ space group. X-ray photoelectron spectroscopy confirmed the presence of mixed-valence states of Fe and Cr. The temperature dependent magnetization curves exhibited magnetic reversal behavior in Nd_2FeCrO_6 double perovskite at temperature 6 K in the field cooled mode. Interestingly, exchange bias effect was observed in this double perovskite material while the sample was cooled down from 300 K to 10 K and magnetic fields were applied during cooling. The zero-field cooled (ZFC) and field cooled (FC) curves of Gd_2FeCrO_6 perovskite largely diverged below 20 K. A downturn was observed in the ZFC curve at 15 K which corresponds to an antiferromagnetic, Néel transition. The narrow magnetic hysteresis loop of Gd_2FeCrO_6 recorded at 5 K was nearly saturated and demonstrated an asymmetric shift along the magnetic field axis indicating the concurrence of ferromagnetic and antiferromagnetic domains in Gd_2FeCrO_6 nanoparticles. The optical band gap of Nd_2FeCrO_6 and Gd_2FeCrO_6 nanoparticles are found to be 1.95 eV and 2.00 eV, evaluated experimentally from the UV–visible and photoluminescence spectroscopic analyses. Here, by employing experimentally obtained structural parameters of Gd_2FeCrO_6 perovskite in first-principles calculation, the spin-polarized electronic band structure, density of states and optical absorption property of Gd_2FeCrO_6 double perovskite were also investigated and compared the results with experimental outcomes. Therefore, due to the lower band gap and magnetically tunable exchange bias, it is anticipated that the newly synthesized Nd_2FeCrO_6 and Gd_2FeCrO_6 double perovskite could be a promising material for spintronic and visible-light-driven energy device application.