


Abstract

Multifunctional materials are greatly appealed in both electronic and magnetic devices, which are being developed by many researchers for the fabrication of future devices. Among these materials, the double perovskites own good magnetic properties such as, magnetic ordering, multiferroicity, half metallicity, and magnetoresistance, which make them favorable for energy storage devices, memory components, and spintronics devices. In the present work, we have successfully synthesized A_2NiCrO_6 ($A=Ce, Pr$ and Nd) double perovskites by using hydrothermal synthesis and investigated their structural, electronic, magnetic, and optical properties. X-ray diffraction analysis confirmed that all the compounds have orthorhombic crystal structures and belong to the Pbnm space group. The values of the unit cell parameters for Ce_2NiCrO_6 are calculated as ($a = 5.41, b = 5.43, c = 7.70$). Similarly, in the case of Pr_2NiCrO_6 and Nd_2NiCrO_6 double perovskites these values are found as ($a = 5.41, b = 5.44, c = 7.71$) and ($a = 5.44, b = 5.45, c = 7.71$) respectively. SEM micrographs show well-shaped particles. EDS mapping depicts the homogeneity and stoichiometry of the elements in the synthesized compounds. The investigated electronic structures and density of states (DOS) results under the framework of Density Functional Theory (DFT) reveals that all the three compounds have half metallic nature. In the spin up channel, it is observed that both the conduction and valance bands are overlapping at the fermi level and compounds are behaving like metals, while in the down spin channel, all the three compounds A_2NiCrO_6 ($A=Ce, Pr$ and Nd) show semiconducting nature, having band gaps of 1.32 eV, 1.21 eV and 1.12 eV respectively. The presence of a magnetic hysteresis curve and coercivity clearly indicates that ferromagnetism is present in the synthesized compounds at room temperature. The calculated values of the magnetic saturation for A_2NiCrO_6 ($A=Ce, Pr$ and Nd) were found to be 5.96 emu/g, 7.93 emu/g and 11.51 emu/g respectively. The reflectivity spectrum shows maximum values of the reflectivity in the electromagnetic spectrum visible region. Optical conductivity was found to increase by increasing the photon energy up to a maximum value and then it starts decreasing. The half-metallic nature and suitable values of magnetic saturation demonstrate the applicability of A_2NiCrO_6 ($A=Ce, Pr$ and Nd) double perovskites in spintronic applications.  (Ctrl) ▾