

Robust Half-Metallicity and Magnetic Properties of Cubic PrMnO₃ Perovskite

Authors : B. Bouadjemi, S. Bentata, W. Benstaali, A. Abbad, T. Lantri, A. Zitouni

Abstract : The purpose of this study was to investigate the structural, electronic and magnetic properties of the cubic praseodymium oxides perovskites PrMnO₃. It includes our calculations based on the use of the density functional theory (DFT) with both generalized gradient approximation (GGA) and GGA+U approaches. The spin polarized electronic band structures and densities of states as well as the integer value of the magnetic moment of the unit cell (6 μ_B) illustrate that PrMnO₃ is half-metallic ferromagnetic. The study shows that the robust half-metallicity makes the cubic PrMnO₃ a promising candidate for application in spintronics.

Keywords : Perovskite, DFT, electronic properties, Magnetic moment, half-metallic

Conference Title : ICCIS 2015 : International Conference on Chemical Industry and Science

Conference Location : Jeddah, Saudi Arabia

Conference Dates : January 26-27, 2015