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Theoretical Investigation on Electronic and Magnetic Properties of Cubic PrMnO3 Perovskite

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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 μB) illustrate that PrMnO3 is half-metallic ferromagnetic. The study prove that the compound is half-metallic ferromagnetic however the results obtained, make the cubic PrMnO3 a promising candidate for application in spintronics.

Keywords : cubic, DFT, electronic properties, magnetic moment, spintronics
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