

Evidence of Half-Metallicity in Cubic PrMnO₃ Perovskite

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Abstract : The electronic and magnetic properties of the cubic praseodymium oxides perovskites PrMnO₃ were calculated using the density functional theory (DFT) with both generalized gradient approximation (GGA) and GGA+U approaches, where U is on-site Coulomb interaction correction. The results show a half-metallic ferromagnetic ground state for PrMnO₃ in GGA+U approached, while semi-metallic ferromagnetic character is observed in GGA. The results obtained, make the cubic PrMnO₃ a promising candidate for application in spintronics.

Keywords : first-principles, electronic properties, transition metal, materials science

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