Study of Half-Metallic Ferromagnetism in CeFeO3

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Abstract : Using first-principles calculations based on the density functional theory and generalize gradient approximation, we predict electronic and magnetic properties of CeFeO3 orthorhombic perovskite. The calculated densities of states presented in this study identify the metallic behavior CeFeO3 when we use the GGA scheme, whereas when we use the GGA+U, we see that its exhibits half-metallic character with an integer magnetic moment of $24\mu B$ per formula unit at its equilibrium volume which makes this compound promising candidate for applications in spintronics.

Keywords : CeFeO3, magnetic moment, half-metallic, electronic properties

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