

Electronic and Magnetic Properties of the $\text{Dy}_{0.0625}\text{Y}_{0.9375}\text{FeO}_3$ and $\text{Dy}_{0.125}\text{Y}_{0.875}\text{FeO}_3$ Perovskites

Authors : Sari Aouatef, Larabi Amina

Abstract : First-principles calculations within density functional theory based are used to investigate the influence of doped rare earth elements on some properties of perovskite systems $\text{Dy}_{0.0625}\text{Y}_{0.9375}\text{FeO}_3$ and $\text{Dy}_{0.125}\text{Y}_{0.875}\text{FeO}_3$. The electronic and magnetic properties are studied by means of the full-potential linearized augmented plane wave method with Vasp code. The calculated densities of states presented in this work identify the semiconducting behavior for $\text{Dy}_{0.125}\text{Y}_{0.875}\text{FeO}_3$, and the semi-metallic behavior for $\text{Dy}_{0.0625}\text{Y}_{0.9375}\text{FeO}_3$. Besides, to investigate magnetic properties of several compounds, four magnetic configurations are considered (ferromagnetic (FM), antiferromagnetic type A (A-AFM), antiferromagnetic type C (C-AFM) and antiferromagnetic type G (G-AFM). By doping the Dy element, the system shows different changes in the magnetic order and electronic structure. It is found that $\text{Dy}_{0.0625}\text{Y}_{0.9375}\text{FeO}_3$ exhibits the strongest magnetic change corresponding to the transition to the ferromagnetic order with the largest magnetic moment of 4.997.

Keywords : DFT, Perovskites, multiferroic, magnetic properties

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