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Electronic and Magnetic Properties of the $Dy_{0.0625}Y_{0.9375}$ FeO_3 and $Dy_{0.125}$ $Y_{0.875}$ FeO_3 Perovskites

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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 $Dy_{0.0625}Y_{0.9375}FeO_3$ and $Dy_{0.125}$ $Y_{0.875}$ 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 $Dy_{0.125}$ $Y_{0.875}$ FeO_3, and the semi-metallic behavior for $Dy_{0.0625}Y_{0.9375}$ 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 $Dy_{0.0625}Y_{0.9375}$ 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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