First Principles Calculation of Magnetic and Optical Properties of Dy0.0625Y0.9375Fe03 and Ce0.0625Y0.9375Fe03 Perovskites: A Comparative Study

Aouatef Sari
Laboratory of Materials Discovery, Unit of Research Materials and Renewable Energies, LEPM-URMER, University of Tlemcen, Algeria
Institute of Science and Technology, University Center of Maghnia – Tlemcen, Algeria

S. Benmansour
Institute of Science and Technology, University Center of Maghnia – Tlemcen, Algeria

Abstract

A comparative study of structural, magnetic and optical properties of YFe03, Dy0.0625Y0.9375Fe03 and Ce0.0625Y0.9375Fe03 perovskite systems is investigated. First-principles calculations based on density functional theory are carried out to achieve the study. Further, full-potential linearized augmented plane wave method implemented in VASP code is used. First, calculated formation enthalpies approve a thermodynamic stability of several compounds. Then, magnetic properties are considered in four magnetic configurations (FM, A-AFM, C-AFM, and G-AFM). Optical properties are examined through analysis absorption specter coefficient and calculated reflectivity. Results obtained in this work predict a semiconductor behavior of YFe03 and a semi-metallic behavior of Dy0.0625Y0.9375Fe03 and Ce0.0625Y0.9375Fe03. Moreover, by doping rare earth element Dy, system exhibits different changes in magnetic order and electronic structure. Besides, results of optical properties show that Ce0.125Y0.875Fe03 is a superior photoabsorber compared to other systems since it exhibits an upper absorption coefficient and a higher reflectivity.