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ORIGINAL PAPER

Ab Initio Investigation on Electronic, Magnetic, Mechanical, and Thermodynamic Properties of AMO_3 (A = Eu, M = Ga, In) Perovskites

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Abstract The structural, electronic, magnetic, elastic, and thermodynamic properties of cubic AMO_3 perovskites (A = Eu, M = Ga, In) have been successfully studied within density functional theory using full-potential linearized augmented plane wave (FP-LAPW). The structural study reveals that both the compounds are stable in ferromagnetic states. The GGA + U calculated spin-polarized electronic band and density of states present the half-metallic nature of both the compounds. The magnetic moments calculated with different approximations were found to be approximately 6 μ_B for $EuGaO_3$ and approximately 7 μ_B for $EuInO_3$. From elastic calculation, the three independent elastic constants (C_{11}, C_{12}, C_{44}) have been acquired to yield the mechanical properties like Young modulus (Y), shear modulus (G), Poisson ratio (ν), and anisotropic factor (A). The calculated values of B/G show that both the compounds are ductile in nature. The thermodynamic study was also accomplished by exploring the thermodynamic parameters like specific heat, heat capacity, thermal expansion, Grüneisen parameter, Debye temperature, etc. within the temperature range 0 to 900 K and pressure range 0 to 50 GPa.

Keywords Perovskite oxides · Half metallic · Ferromagnetic · Mechanical properties · Thermodynamic properties

1 Introduction

The perovskite oxide structure has a general formula of ABO_3, where "A" and "B" are cations and "O" is an anion. In the ideal cubic structure, the B cation is six-fold coordinated, surrounded by an octahedron of anions, and the A cation has a 12-fold cub octahedral coordination. Perovskites represent a broad class of materials occupying maximum elements in the periodic table having a wide range of properties and crystal structure. They show a wide range of interesting and fascinating properties stretching from spintronics to multiferroic materials [1–6]. Oxide-based perovskites and their derivatives especially those having a cubic structure have remained a vital subject to researchers all over the globe because of their simple structure and unique dielectric, ferromagnetic, and ferroelectric properties. These solid materials have currently gained importance in geo-physics [7], superconductivity [8], catalytic action [9], colossal magneto resistance [10], etc.

During the last few years, many experimental and theoretical works have been carried out on perovskites especially oxide based to check their structural, electronic, magnetic, properties, etc, in order to have a look on their possible applications and device fabrications. Exploring new materials and their study for modifying them is the thrust area of present-day research. Transition element-based perovskites

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