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First principle studies on structure, magneto-electronic and elastic properties of photovoltaic semiconductor halide ($RbGeI_3$) and ferromagnetic half metal oxide ($RbDyO_3$)

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By using density functional theory (DFT) in terms of ab-initio investigation, we examined the structural, electronic and magnetic properties of cubic, halide perovskite ($RbGeI_3$) and oxide perovskite ($RbDyO_3$) for the first time. Structural stability of cubic $RbGeI_3$ and $RbDyO_3$ compounds were determined by optimizing the structure in ferromagnetic (FM), non-magnetic (NM), and Anti-ferromagnetic (AFM) phases by using PBE generalized gradient approximation (GGA) functional to find the exchange-correlation potential. From structural optimizations, the nonmagnetic phase of $RbGeI_3$ and the ferromagnetic phase of $RbDyO_3$ was observed to be stable. From the stability curve, we calculated the equilibrium lattices, bulk moduli and their pressure derivatives and equilibrium volume. Moreover, the calculation of tolerance factor for these compounds ($\tau \approx 1$) demonstrates the formation of the cubic perovskite structure. The spin magnetic moments of these compounds have been obtained to explore the magnetic properties of $RbDyO_3$. Since, $RbGeI_3$ is nonmagnetic material with zero magnetic moment as also observed from the structural optimization. Rare earths like Dysprosium (Dy) possess strongly localized f-electronic states which are responsible for their strong magnetic properties and other delocalized f-electron states arising from the hybridization of p-d states which determine the electronic properties within the material. The latter situation suits well for $RbGeI_3$ compound. We report a detailed analysis of the different ground state properties for the two compounds using GGA and GGA-modified Becke–Johnson computational approaches.

1. Introduction

Perovskites with general structural formula ABX_3 are a continuing research theme due to the variety of ground state properties and their technological applications. Owing to their remarkable properties like optoelectronic, multiferroic, semiconducting, superconducting, photocatalytic etc., [1–10] perovskite semiconductors are used in varied applications such as sensors, photocatalysis, photodiodes, LEDs, solar photovoltaics, spintronic devices, and solid-state memory devices [11–20]. Rare earth and alkaline earth metal based perovskites are interesting because of their potential applications in green energy harvesting as electrocatalysts for state-of-the-art fuel cells, and catalysts for hydrogen generation and hydrocarbons oxidation. Moreover, studies of organometal halide perovskites for their applications in solar photovoltaic devices have taken a giant leap in terms of solar cell performance in the recent past [21]. These studies are driven by the goal of manufacturing highly stable, more efficient and cost-effective solid-state solar cells [22]. Innovative halide perovskite materials like $RbGeI_3$ have found wide-ranging applications as solar cell absorbers, topological insulators, superconductors, LEDs etc. [23,24] Furthermore, oxide perovskites (ABO_3) are formed from divalent A^{2+} (1b site – cuboctahedral) and tetravalent B^{4+} (1a site – octahedral) metal cations while as halide perovskites e.g. (ABX_3)

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