

Unveiling the Properties of FrBX_3 ($\text{B} = \text{Pb, Zr}$; $\text{X} = \text{Br, Cl}$) Inorganic Metal Halide Perovskites: Electronic, Optical, and Mechanical Perspectives

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Abstract—This study provides a comprehensive investigation into the structural, optoelectronic, and elastic properties of inorganic metal halide perovskites FrBX_3 ($\text{B} = \text{Pb, Zr}$; $\text{X} = \text{Br, Cl}$) using first-principles calculations based on density functional theory (DFT). Structural analysis confirms the stability of these perovskite phases through optimized lattice parameters and positive formation energies. Electronic band structure calculations reveal that FrZnX_3 compounds exhibit direct band gaps, while FrPbX_3 compounds possess indirect band gaps. Using the GGA-PBE functional, the band gaps are found to decrease in the order: FrPbCl_3 (2.237 eV), FrPbBr_3 (1.795 eV), FrZnCl_3 (1.185 eV), and FrZnBr_3 (0.057 eV), highlighting their potential for photovoltaic applications, particularly in solar energy harvesting. The optical properties, evaluated via dielectric functions, absorption coefficients, and refractive indices, demonstrate strong absorption in the visible region, suggesting their suitability as efficient light-absorbing materials. Furthermore, the elastic properties, including elastic constants, bulk modulus, shear modulus, and Poisson's ratio, confirm the mechanical stability and ductility of all studied compounds, as they satisfy the Born stability criteria. Moreover, the calculated elastic anisotropy indicates that these materials exhibit moderate directional dependence in their mechanical response, which is advantageous for thin-film fabrication processes. Overall, the combination of favorable electronic, optical, and mechanical properties makes these Fr-based perovskites promising candidates for use in next-generation photovoltaic devices and other optoelectronic applications.

Keywords: inorganic metal halide perovskites, electronic and optical properties, mechanical stability

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1. INTRODUCTION

Halide perovskites (HPs), usually expressed by the general formula ABX_3 , where A stands for a monovalent cation (such as methylammonium (MA^+), formamidinium (FA^+), or cesium (Cs^+)), B for a divalent metal cation (lead (Pb^{2+}) or tin (Sn^{2+})), and X for a halide anion (chloride (Cl^-), bromide (Br^-), or iodide (I^-)) have emerged as a versatile and highly promising class of materials due to their exceptional optoelectronic properties [1–4]. These materials have revolutionized the field of photovoltaics, achieving remarkable progress in solar cell efficiency due to their intrinsic properties, such as high absorption coefficients [5], tunable bandgaps, long carrier diffusion lengths, and low exciton binding energies. Beyond their application

in photovoltaics, HPs exhibit a range of multifunctional properties, including strong photocatalytic activity [6], exceptional photovoltaic performance [7], piezoelectricity [8], and ferroelectricity [9]. These characteristics have catalyzed extensive research into their potential applications across various fields such as light-emitting diodes (LEDs) [10], lasers [11], field-effect transistors (FETs) [12], and photodetectors [13]. Despite impressive advancements, particularly in achieving power conversion efficiencies (PCE) of 25.7% in solar cells and LED efficiencies up to 23.4% [14], halide perovskite technologies continue to confront critical challenges. Key areas requiring further improvement include long-term stability of devices under operational and environmental stress, reducing the toxicity linked to lead-based compounds, and