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RESEARCH

# State of Art in Lead Free Double Perovskite Ceramics, $X_2MgTeO_6$ (X = Sr, Ba): Structural Stability and their Potential Energy Harvesting Applications

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**Abstract**
The present first principles calculations regarding lead-free double perovskite ceramics $X_2MgTeO_6$ (X = Sr, Ba) have discovered their structural, thermal, and thermodynamic stability in the rock-salt phase. The lattice constants were calculated to be in close agreement with experimental values. The dynamical properties were explored in terms of phonon dispersion spectra, vibrational internal energy, Debye temperature, vibrational Helmholtz free energy, lattice thermal conductivity, specific heat, and vibrational entropy. It was found that both perovskites follow the Dulong-Petit law at high temperatures and Debye's law at low temperatures. The electronic properties revealed the direct band gap nature of both double perovskites, with band gap values of 3.18 eV for $Sr_2MgTeO_6$ and 2.42 eV for $Ba_2MgTeO_6$. The optical properties predicted that the most active absorption occurs in the ultra violet (UV) region with an absorption coefficient greater than $10^5$ $cm^{-1}$. Therefore, the $X_2MgTeO_6$ double perovskites are proposed for optoelectronic devices operating in the UV region. The positive values of the Seebeck coefficients indicate the p-type conductivity in both ceramics. The values of the figure of merit (0.609 for $Sr_2MgTeO_6$ and 0.594 for $Ba_2MgTeO_6$ at 800 K) suggest that both ceramics are suitable for thermoelectric-based applications at high temperatures.

**Keywords** First Principles Calculations · Double Perovskite Ceramics · Dynamical Properties · Absorption Coefficient · P-Type Conductivity · Lattice Thermal Conductivity

## 1 Intoduction

The lead containing perovskites $XPbY_3$ (X = Rb, Cs, Ba, Sr, MA, FA, Y = O, I, Br, Cl) have been effectively demonstrated during last decade [1]. These perovskites have attracted the research interest because of their high defect tolerance, high carrier mobility, low binding energy of exciton, high optical absorption; low effective masses of the carriers, readily tunable band gaps and high photoluminescence quantum yield [2–5]. Because of these unique properties, these perovskites are applied for LEDs (light emitting diodes), solar cells, lashing, photo-detectors and x-ray detectors [6–9]. Despite these remarkable applications, the toxic nature of lead content is a point of concern for the factory workers and consumers. European Union has restricted lead-based technology, and in the future, other countries are bound to control the use of the toxic materials for device based applications [10]. These disquiets are accredited to further essential and applied research on alternatives to $XPbY_3$ materials within the perovskite family. Therefore, several lead free perovskites were fabricated. Where, in one type, lead free double perovskites (LFDPs) $X_2BB'Y_6$, Pb is replaced by B and B′ [11–13]. The average possible oxidation state of B and B′ is four which can be accomplished by a combination of $B^{2+}/B'^{6+}$, $B^{3+}/B'^{5+}$and $B^{4+}/B'^{4}$ [14].

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