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Theoretical investigation of the lead-free K_2InBiX_6 (X = Cl, Br) double perovskite compounds using first principle calculation

D. Behera[1)], *S. K. Mukherjee*[1)]

Department of Physics, Birla Institute of Technology, Mesra, 835215 Ranchi, India

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The need for energy has grown dramatically over the past few years, which has intensified efforts to find non-fossil fuel and unconventional energy sources. As a result, emphasis is diverted to seeking for renewable energy sources on a global scale [1]. Through the direct conversion of thermal to electrical energies, thermoelectricity could be employed to produce renewable energy that allows for the efficient utilization of waste heat [2]. The efficiency of thermoelectric (TE) material is governed by the figure of merit (ZT), as ZT = $= (S^2\sigma T)/(\kappa_e + \kappa_l)$, where S is the Seebeck coefficient, σ – electrical conductivity, T – absolute temperature, and κ_e, κl are electronic and lattice contributions to the thermal conductivity [3]. Due to their outstanding potential for contemporary applications, double perovskites have garnered a lot of attention. The double perovskite has the formula $A_2BB'X_6$, where X can be an oxide or a halide, the B and B′ sites are inhabited by transition or non-transition cations and the A site is occupied by a rare-earth or alkaline-earth metal. A variety of unique double perovskite compounds have recently been developed. The double perovskite compounds with A – such as K, Cs, Rb, B^+ cation – as Cu, Ag, In, B^{3+} cation – as Bi, Sb, and X – as Cl, Br, I were thoroughly described in this context, revealing their optoelectronics and transport properties [4]. However, based on literature review, halide double perovskite K_2InBiX_6 (X = Cl, Br) have not been thoroughly examined. In this study, first-principles computations were employed to investigate the structural, elastic, electrical, optical, and thermoelectric properties of K_2InBiX_6 (X = Cl, Br) compounds.

The K_2InBiX_6 (X = Cl, Br) compounds possess a cubic face-cantered (Fm3m) atomic configuration and space group 225. The constituent atoms K, In, Bi, and X are located at $(0.25, 0.25, 0.25)$, $(0.5, 0.5, 0.5)$, $(0, 0, 0)$, and $(y, 0, 0)$, respectively ($y = 0.247$) [5]. The negative formation energy of the studied K_2InBiX_6 (X = Cl, Br) compounds (−1.63 eV/atom, −1.40 eV/atom) confirms its stability [6]. When designing solids for industrial manufacturing, mechanical properties such as the second-order elastic constants (C_{ij}), bulk modulus (B), shear modulus (G), Pung ratio (B/G), and anisotropy (A) must be taken into account. The computed Poisson ratio ν for K_2InBiX_6 (X = Cl, Br) compounds is 0.27, 0.32, showing that materials are ductile by nature. Using various potentials, including Perdew-Burke-Ernzerhof – Generalized Gradient Approximation (PBE-GGA) and modified Becke Johnson Potential (mBJ), we estimated the electronic band structure of K_2InBiX_6 (X = Cl, Br) compounds. Bandgap about 1.81, 1.29 eV were obtained using mBJ. Optical properties were studied in terms of real and imaginary dielectric function, refractive index and reflectivity, etc. No absorption has been observed between 1.41 and 1.17 eV that would indicate the optical bandgap is about equivalent to the electrical bandgap. The variation in peak intensities results from light photons reflecting off the surface of the material at various angles. The various peaks are observed for absorption coefficient $\alpha(\omega)$ plot that resulted due to material absorption [7]. Absorption peaks in the visible spectrum show that the investigated substances have strong absorption performance.

The variation of S with temperature is shown in Fig. 1a, which suggests p type behavior with a positive magnitude of the Seebeck coefficient. For the investigated K_2InBiX_6 (X = Cl, Br) compounds at room temperature, the magnitude of S was determined to be 252 μV/K and 248 μV/K, respectively, Furthermore, an ideal TE material has Seebeck coefficient more than 200 μV/K suggesting good thermoelectric response of investigated compounds. The σ/τ ratio for $K_2InBiCl_6$ is $0.13 \times 10^{18}\,(\Omega ms)^{-1}$ at 200 K and becomes $9.01 \times 10^{18}\,(\Omega ms)^{-1}$ at 800 K. For $K_2InBiBr_6$ it is $0.35 \times 10^{18}\,(\Omega ms)^{-1}$ at 200 K and reaches $9.35 \times 10^{18}\,(\Omega ms)^{-1}$ when temperature goes to 800 K. For

[1)]e-mail: sanat_aphy@yahoo.co.in

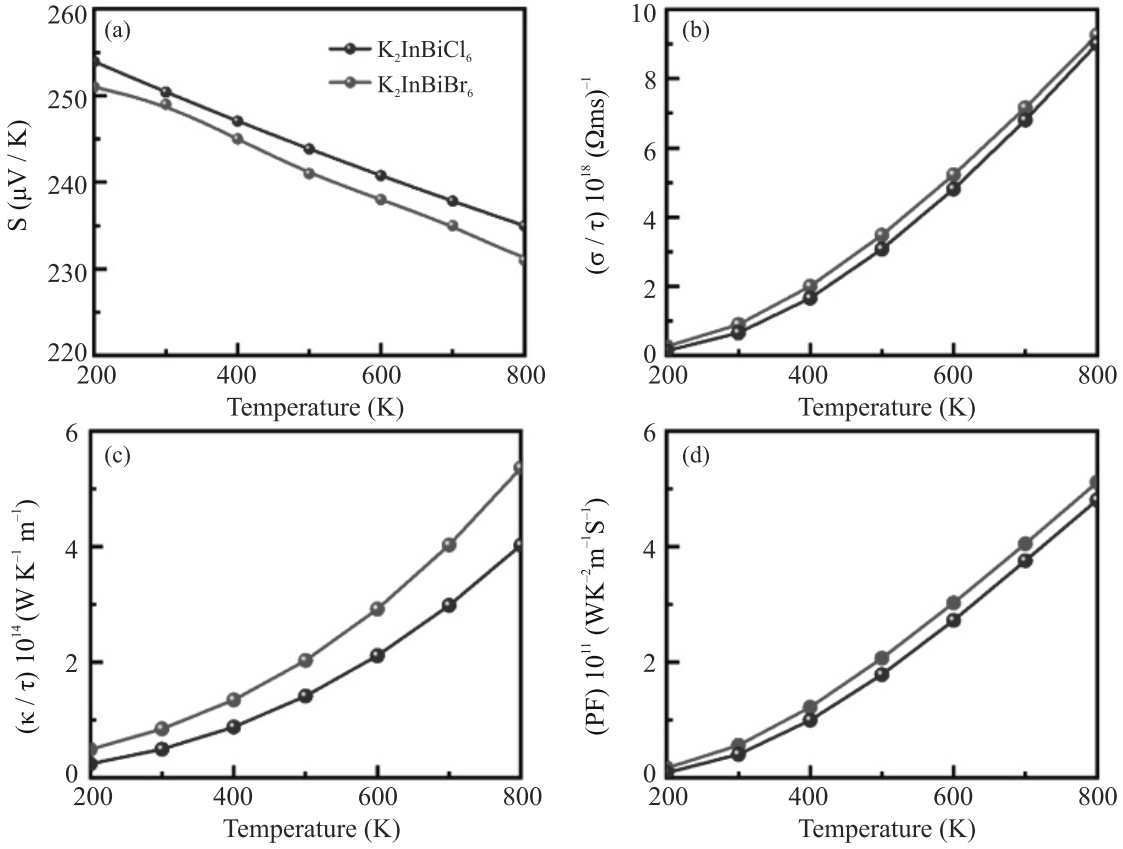

Fig. 1. (Color online) Computed values of (a) – Seebeck coefficient (S), (b) – electrical conductivity (σ/τ), (c) – thermal conductivity (κ/τ), (d) – power factor "PF" ($S^2\sigma$) with temperature for K_2InBiX_6 (X = Cl, Br) compounds

K_2InBiX_6 (X = Cl, Br) compounds, the computed PF at 800 K is determined to be 4.81×10^{11} W/K^{2}ms and 5.13×10^{11} W/K^{2}ms. Such a high-power factor at high temperatures signifies that the compounds are suitable for thermoelectric device applications.

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