ABSTRACT

The primary basis of renewable energy is the transformation of light energy in the form of electrical energy, which has been highly analyzed in the past decade. Using Quantum espresso code that is based on density functional theory, we have elucidated mechanical, electronic, and optical properties of organic $(CH_3NH_3)_2AgMBr_6$ (M = Sb, Bi) halides. In order to treat the exchange-correlation functional, we employed PBE generalized gradient approximations (GGA) to execute the mechanical and optoelectronic parameters. Our calculated results of Pugh's ratio and Poisson's ratio of both halides recommended the quality of ductility. In addition, electronic and optical properties are obtained by using GGA+U in-order-to deliberate the accurate band gap. The required indirect band gaps for optoelectronic applications are calculated as 0.1 eV/0.88 eV for $(CH_3NH_3)_2AgSb/BiCl_6$. Interestingly, significant absorption coefficients for both halides endorse that these are appropriate optoelectronic devices in near-visible and infra-red regions. Double perovskite halides, being a trustworthy source of renewable energy, play an important role in solving all requirements of energy scarcity problems. As a result, these perovskite halides are finding new uses in thermoelectric and optoelectronics.

We recently examined the physical properties of Rb_2KScI_6 and Cs_2KScI_6 double perovskite (DP) halides for use in renewable energy devices using DFT calculations based on the FP-LAPW+lo approach for all electrons. The calculated Goldsmith's tolerance factor and enthalpy of the formation of studied halides show structural and thermodynamic stability in the cubic phase. Moreover, analyzing the elastic characteristics of the Poison and Pugh ratio reveals its ductile nature. We estimated band structure in addition to studying their electrical characteristics. Therefore, for bandgap calculations of Rb_2KScI_6 (E_g = 2.75 eV) and Cs_2KScI_6(E_g = 2.65 eV), we employed modified Becke-Johnson (mBJ) potentials to achieve corrected band gap values compared to experimental values. Likewise, we looked at the optical characteristics of the halides under study in terms of complicated dielectric functions. The estimated optical characteristics certainly define optimal light absorption in visible zones, demonstrating the suitability of these halides for usage in optoelectronic devices. The electrical-conductivity (EC), the figure of merit, Seebeck-coefficient (SC) as well as thermal-conductivity (TC) of thermoelectric properties were also investigated. Impatiently, our results would support evaluating Rb_2KScI_6 and Cs_2KScI_6 for future experimental investigations for renewable energy device applications.

As a result of their exceptional optoelectronic properties, the growing need for renewable and sustainable energy has heightened interest in perovskites. Using DFT, mechanical, optoelectronic, and thermoelectric properties of double perovskites Cs_2CuScX_6 (X = Cl, Br, I)" were analyzed to gain a comprehensive understanding of these materials. To ensure structural and thermal stability, permissible values for the tolerance factor (t_G) and energy formation (ΔH_f) have been determined. The indirect band gaps of anions Cl, Br, as well as I-based double perovskites, are 1.9 eV, 1.80 eV, and 1.70 eV, respectively, according to band structure (BS) simulations. A band gap of 1.70 eV makes Cs_2CuScI_6 an attractive material for solar cell applications. The optical properties of the compounds studied, including dielectric constants, optical absorption, and refractive index, in the 0-10 eV energy range, indicate visible and ultraviolet absorption. The investigated compound Cs_2CuScI_6 exhibited the highest visible spectrum absorption, making it an ideal candidate for solar cell applications. Boltzmann's theory also accounted for the lattice thermodynamic and electrical conductivities, Seebeck coefficient, and the Figure of merit (ZT) against temperature and chemical potential, making them optimal for thermoelectric uses.