Abstract

Double-perovskite materials have acquired a lot of attention recently in the field of optoelectronics because of their novel optical and thermoelectric characteristics. In this study, we used the antisolvent recrystallization technique to synthesize K2CuBiBr6 nanoparticles. The XRD analysis indicated that the materials belong to the Fm3m group. The lattice parameters of K2CuBiBr6 were determined to be 10.56 Å, respectively. A scanning electron microscope (SEM) was utilized to examine the surface morphology of the sample, yielding an average particle size of 0.69 μm. The EDX examination gave an extensive evaluation of the elemental composition of K2CuBiBr6, including both qualitative and quantitative aspects. For theoretical investigation, we used Wien2K code in the framework of DFT to explore the structural, electrical, optical, thermoelectric, and elastic features of potassium(K) based double-halide perovskite K2MBiBr6 (M = Na, Ag, Cu). Various factors, including negative formation energy, structural optimization, tolerance, and octahedral factors, verify the stability of perovskites. The generalized gradient approximation (GGA) tends to investigate the structural phase and elastic properties. We also used the Tran-Balaha modified Becke-Johnson (TB-mBJ) function to obtain improved results for electronic, optical, and thermoelectric properties, based on closed experimental findings. The electrical parameters, such as bandgap and density of states, were calculated. The findings showed that K2NaBiBr6, K2AgBiBr6, and K2CuBiBr6 have semiconductor order, with indirect bandgaps of 4.01eV, 2.36eV, and 1.26eV, respectively. For optical properties, the current study examines characteristics such as energy loss, refractive index, light energy absorption, and polarization through the entire energy spectrum, which ranges from 0 to 8eV. The BoltzTraP code was used to examine thermoelectric factors such as the Seebeck coefficient, power factor, thermal conductivity, electrical conductivity, and figure of merit. Furthermore, the stability of each DP, the Born Criteria, and formation energy are assessed. The study emphasizes the elastic constants of cubic symmetry to figure out the variation between ductile and brittle nature, anisotropy, and the large melting temperature of these materials. The theoretical findings given in the present article have substantial impacts on the future renewable energy sector.