Abstract

Double perovskites have emerged as a potential new material for optoelectronic and thermoelectric applications. In the present work, Ba_2YBiO_6 double perovskites have successfully synthesized by using hydrothermal synthesis and theoretically investigated their structural, electronic, optical and thermoelectric properties. X-ray diffraction analysis confirmed that Ba_2YBiO_6 have cubic crystal structures and belong to the Fm3m space group. The values of lattice parameters of Ba_2YBiO_6 are calculated as 8.31 Å. SEM micrographs show well-shaped particles. The average particle size is 0.89 μm. EDS mapping depicts the homogeneity and stoichiometry of the elements in the synthesized compounds. Through density functional theory the most stable structure, according to the optimized structural parameters, is a cubic Fm3m (225) symmetry with a nonmagnetic (NM) state. The TB-mBJ approximation is used to estimate the band structure and density of states. The semiconductor nature is predicted with indirect bandgap values of 2.21eV, 2.01 eV, and 1.61eV for Mg_2YBiO_6, Ca_2YBiO_6, and Ba_2YBiO_6, respectively. Notable optical responses such as higher absorption ($>10^5$ cm^{-1}) and low reflectivity for A_2YBiO_6 suggest appropriate candidates for optoelectronic applications. Furthermore, the thermoelectric properties have been evaluated through BoltzTraP code, revealing the larger value of figure of merit value of 0.75, 0.80, and 0.81, respectively, at 300K. Consequently, the investigated results show that the investigated compounds could be good alternatives for thermoelectric and photovoltaic applications.