Abstract

The remarkable efficiency of double perovskite materials has recently attracted significant interest in optoelectronics and thermoelectric devices. In this article, density functional theory (DFT) is used to investigate the physical aspects of the halide double perovskites Na_2AgAsZ_6 (Z = F, Cl, Br, I). These substances have a cubic arrangement and are classified under space group Fm3m (225) based on their octahedral and tolerance factors values. All the perovskites are determined to be thermodynamically stable, as indicated by their negative formation energies. These double perovskite materials are semiconductors based on their electronic band structure. The energy band gaps of Na_2AgAsF_6, $Na_2AgAsCl_6$, $Na_2AgAsBr_6$, and Na_2AgAsI_6 were determined to be 2.96 eV, 1.93 eV, 1.28 eV, and 0.68 eV, respectively. We also calculated and examined the optical properties of these substances in the photon energy range of 0–8 eV. Our results indicate that most of the absorption occurs in the visible-ultraviolet spectrum, which makes the materials well-suited for solar systems. We employed the BoltzTraP algorithm to compute the thermoelectric properties of the materials and establish their thermoelectric behavior. These materials demonstrated figures of merit values of 0.55, 0.71, 0.74, and 0.75, respectively. Thus, these materials are appropriate for application in photovoltaic and thermoelectric devices.