ABSTRACT

In this study, the structural, electronic, mechanical, optical, and thermoelectric properties of the cubic half-Heusler compound ZrCoY(Y—Sb and Bi) obtained using first-principles calculations are presented. The following exchange-correlation functionals have been employed: Generalized Gradient Approximation with Perdew-Burke-Ernzerhoff (GGA-PBE), Generalized Gradient Approximation with Perdew-Burke-Enzerhoff for solids (GGA-PBESol) and Local Density Approximation (LDA). Both ZrCoSb and ZrCoBi compounds are mechanically and dynamically stable, based on the elastic and phonon properties analysis. The calculated electronic band gaps for both compounds are about 1 eV, as predicted by all the three functionals. Since it is noted that GGA-PBE functional is most favourable for predicting structural properties and the energetic stability of ZrCoSb and ZrCoBi compounds, it is further used to calculate their thermoelectric properties. Within the energy range of 0–40 eV, the refractive index, dielectric constant, and energy loss function of ZrCoSb and ZrCoBi compounds are calculated. The possibility of electronic transition from the valence band maximum (VBM) to the conduction minimum band (CBM) is confirmed by the occurrence of absorption peaks in the visible range. For the evaluation of thermoelectric properties, the p-type and n-type doping attained Seebeck coefficients of 1800 and -1800 μVK 1 at 300 K, respectively. The maximum peak of 17 × 1011 W/m s K2 is attained in n- type doping, according to the power factor results.

Keywords: First principles: Electronic: Mechanical: Optical and thermoelectric properties: Half-Heusler alloys: ZrCoY (Y = Sb and Bi)