Abstract

The structural, electronic, elastic, magnetic, and thermoelectric characteristics of three novel Ta-based Half-Heusler alloys, CsTaC, CsTaSi, and CsTaGe, have been investigated using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method within the density functional theory (DFT). The volume-optimization graphs show that all compounds are stable in the ferromagnetic (FM) phase. Half-Metallicity of these compounds is confirmed by the density of states (DOS) and band structures. The total magnetic moment for CsTaC is $6\mu_B$, and for CsTaX (X=Si, Ge) is $2\mu_B$. The negative pd exchange energy and exchange constants confirm ferromagnetism. The values of Pugh's ratio (B/G) and Poisson's ratio (v) reveal that CsTaC is ductile and CsTaX (Si, Ge) is brittle. The thermoelectric response is estimated using the BoltzTraP code, demonstrating that at room temperature, maximum *ZT* values for CsTaC, CsTaSi, and CsTaGe are 0.99, 0.97, and 0.90, respectively. Consequently, CsTaX (X=C, Si, and Ge) are suitable candidates for spintronic and thermoelectric applications.