Half metallic materials have attracted significant attention from scientists due to their extensive use in magneto-electronics and spintronics devices. This thesis primarily focuses on the theoretical investigation of Half metallic materials (HMM) FeCoSi (Z=Si, Ge, Pb). Theoretical research focuses on examining the structural, electrical, magnetic, thermoelectric, thermodynamic, and elastic properties of half-metallic (HH) compounds FeCoSi, FeCoGe, and FeCoPb using Density Functional Theory (DFT). The computations utilize the first principle technique within the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. Perdew-Burke-Ernzerhof Generalized Gradient Approximations (PBE-GGA) have been used for the exchange and correlation potential by employing Wien 2K code. The structural parameters we have estimated align well with the findings of earlier studies. Our investigation reveals that these chemicals exhibit indirect band gap values specifically in the spin-up channel. The computed values of band gaps exhibit strong concordance with other theoretical studies. The electronic characteristics of these compounds confirm the presence of half-metallicity (HM). The magnetic characteristics provide evidence of the ferromagnetic nature of these substances. The thermoelectric properties of these compounds are determined by utilizing the BoltzTraP code within a temperature range of 200-800 K. Suggest that these materials are suitable for thermoelectric devices. The thermodynamic property examines the thermodynamic stability of certain substances. The ductile nature of these half Heusler alloys is further indicated by their elastic properties. Moreover, a comprehensive examination of these compounds reveals their enhanced suitability for spintronics and magnetoelectronics devices.