J Laser Opt Photonics 2019, Volume 06
DOI: 10.4172/2469-410X-C2-050

Calculation of structural, electronic, magnetic and elastic properties of Half-Heusler Alloys CrNiZ (Z=Al, Si, Ge and As)

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Structural, elastic, and electronic properties of Half-Heusler Alloys CrNiZ with Z=Al, Si, Ge and As in three different atomic configurations α, β, and γ phases are studied using both full potential linearized augmented plane wave (FP-LAPW) and plane-wave pseudopotential (PW-PP) methods. Exchange–correlation effects are treated by the generalized gradient approximation (GGA). The band structure calculations show that the majority spin is strongly metallic, while the minority spin shows an insulating behavior. For our compounds the total magnetic moment calculated equal to 1, 2, 2 and 3 μB, is an integral, in agreement with the Slater-Pauling curve for Half-Heusler alloys. For elastic constants,Young modulus, and Poisson ratio, to our knowledge, no data are available in literature for comparison.