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First principles study of the new half-metallic ferromagnetic full-Heusler alloys $\text{Co}_2\text{CrSi}_{1-x}\text{Ge}_x$: An ab-initio study

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Abstract : We have studied the structural, electronic, elastic, magnetic, thermal and thermodynamic property of the quaternary Heusler alloys $\text{Co}_2\text{CrSi}_{1-x}\text{Ge}_x$ ($x = 0, 0.25, 0.5, 0.75, 1$) with the linearized augmented plane wave method based on density functional theory (DFT) and implemented in wien2k code. For exchange correlation potential we have used the generalized gradient approximation (GGA) of Perdew et al. Our results provide a theoretical study for the mixed Heusler $\text{Co}_2\text{CrSi}_{1-x}\text{Ge}_x$ ($0 < x < 1$) in which no experimental or theoretical data are currently available. In their equilibrium L2₁ structure, all concentrations are magnetic and metallic. However, there is linear variation of the lattice parameter. The bulk modulus, the elastic constants and the Debye temperature was studied with variation of composition x of Ge. A regular solution model is used to investigate the thermodynamic stability of the alloy which essentially shows a miscibility gap phase by calculating the critical temperatures of the alloys. In addition, the quasi-harmonic Debye model is applied to determine the thermal properties of the alloy.

Keywords : DFT, wien2k, GGA, Heusler, Debye