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First principles study of the new half-metallicferromagnetic full-Heusler alloysCo2CrSi1_xGex: 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 Co2CrSi1-xGe(x = 0, 0.25, 0.5, 0.75, 1) with the linearized augmented plane wave method based ondensity functional theory (DFT) and implemented in wien2kcode. For exchange correlation potential we have used the generalized gradient approximation (GGA) of Perdew et al. Our esults provide a theoretical study for the mixed HeuslerCo2CrSi1-xGexx(0 < x < 1) in which no experimental or theoretical data are currently available. In their equilibrium L2structure, 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 withvariation of composition x of Ge. A regular solution model is used to investigate the thermodynamic stability of the alloy which is applied to determine the thermal properties of the alloy.

Keywords : DFT, wien2k, GGA, Heusler, Debye