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Magneto-electronic and thermodynamic properties of $Cr_2GdGe_{1-x}Sn_x$ Heusler alloys

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The main investigation's goal of this work is to give a report on the structural, mechanical, magneto-electronic and thermodynamic properties of the quaternary full-Heusler alloys $Cr_2GdGe_{1-x}Sn_x$ for different concentrations x ($0 \leq x \leq 1$). The present result was done by means of DFT calculations. The effect of concentration x on the calculated lattice parameters and bulk modulus, shows a linear dependence for the lattice parameters with marginal downward bowing parameters equal to 0.0457 Å, while a nonlinear behavior is observed for the variation of bulk modulus with disorder parameter equal to 4.696 GPa. The estimated elastic constants confirm the mechanical stability of our compounds. The thermodynamic stability was explored on the basis of the regular solution model. Furthermore, the temperature and pressure effects on the bulk modulus, heat capacities and Debye temperatures are also computed and discussed in details. The magneto-electronic calculations reveal that all the presented compounds exhibit a HMF behavior. Finally, we can report that due to the potential half-metallicity exhibited by our investigated alloys, these compounds could be used for spintronic application.

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