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# The Structural, Elastic, Thermal, Electronic, and Magnetic Properties of Intermetallic rmn$_2$ge$_2$ (R=CA, Y, ND)

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**Abstract :** The structural, elastic, Thermal, electronic, and magnetic properties of intermetallic $RMn_2Ge_2$ (R= Ca, Y, Nd) are investigated by density functional theory (DFT), using the full potential –linearised augmented plane wave method (FP-LAPW). In this approach, the local-density approximation (LDA) is used for the exchange-correlation (XC) potential. The equilibrium lattice constant and magnetic moment agree well with the experiment. The density of states shows that these phases are conductors, with contribution predominantly from the R and Mn d states. We have determined the elastic constants $C_{11}$, $C_{12}$, $C_{13}$, $C_{44}$, $C_{33}$, and$C_{66}$ at ambient conditions in, which have not been established neither experimentally nor theoretically. Thermal properties, including the relative expansion coefficients and the heat capacity, have been estimated using a quasi-harmonic Debye model.

**Keywords :** $RMn_2Ge_2$, intermetallic, first-principles, density of states, mechanical properties
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