

# Pressure-Dependent Structural, Elastic, and Mechanical Properties of Half-Metallic Heusler Compounds

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# Letter to Editor

The structural, electrical, elastic, and optical characteristics as a function of hydrostatic pressure are explored using first-principles computations. The estimated and observed values of these compounds' lattice properties accord well in the current investigation. Up to the specified pressure range of 0-30 GPA, the steady decrease in lattice parameter and unit cell volume with increasing pressure excludes the possibility of phase transition. The density of states and the pressuredependent band structure computations show that and behave half-metallic and near half-metallic up to 20 respectively, before disappearing at pressures around 30 GPa [1]. The changes in optical constants as a function of pressure are consistent with the electronic structure calculations. Both compounds have a high reflectivity making them suitable for optoelectronic device applications. Despite being discovered in 1903, a class of intermetallic compounds known as Heusler alloys remains appealing in the twenty-first century. Due to the widespread interest in Heusler alloys in numerous domains, particularly spintronics, several of them have been researched experimentally and theoretically in recent decades.

This means that the contribution of bond bending to strength raises with pressure The Machinability Index is a metric that measures how easy it is to make something. is a metric for determining a compound's industrial viability. When the machinability index of a material is high, it is considered suitable for cutting [2-5]. Respectively, is more machinable than, according to this data. For machinability increases gradually with pressure, but, machinability increases abruptly over the pressure range examined.

Kleinman parameter indicates the type of bonding in a compound. The contribution of bond bending or bond stretching to withstand the external pressure is determined by the value of the value corresponds to the dominance of bond stretching while corresponds to the dominance of bond bending. Strength of is dominated by bond bending which is evident from the value. On the other hand, almost equal contribution of bond bending and bond stretching to the strength of is expected from the value of is pressure dependent. A gradual increase of this parameter with hydrostatic pressure is observed for while anomalous behaviour is observed. This implies that bond bending contribution to the strength of increases progressively with pressure.

## Conclusion

The influence of hydrostatic pressure on the structural, elastic, mechanical, electrical, and optical characteristics of the Heusler compounds and is investigated using DFT simulations. These chemicals' calculated ground state lattice constants match those found in earlier experimental and computational research. The structural stability of the examined compounds under elevated pressures up to 30 GPa is indicated by the increasing decrease of lattice parameters and unit cell volume with pressure. The lack of an imaginary frequency in our predicted phonon dispersion curves indicates that these compounds are dynamically stable at pressures up to 30 GPA.

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## **Conflict of Interest**

The authors declare that they are no conflict of interest.

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