

Accepted Manuscript

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PII: S0925-8388(18)30395-5

DOI: [10.1016/j.jallcom.2018.01.377](https://doi.org/10.1016/j.jallcom.2018.01.377)

Reference: JALCOM 44841

To appear in: *Journal of Alloys and Compounds*

Received Date: 5 September 2017

Revised Date: 16 January 2018

Accepted Date: 29 January 2018

Please cite this article as: I. Asfour, H. Rached, D. Rached, M. Caid, M. Labair, Magneto-electronic, mechanical and thermodynamic properties of full-Heusler alloys $\text{Cr}_2\text{GdGe}_{1-x}\text{Sn}_x$, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.01.377.

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Magneto-electronic, Mechanical and thermodynamic properties of full-Heusler alloys $\text{Cr}_2\text{GdGe}_{1-x}\text{Sn}_x$

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Abstract

In this work we have used the density functional theory (DFT) to investigate the ground state properties, mechanical and magneto-electronic properties of the quaternary full-Heusler alloys $\text{Cr}_2\text{GdGe}_{1-x}\text{Sn}_x$ in $L2_1$ structure. The system are treated in ferromagnetic order. The electronic structure report that, our compounds have half-metallic (HM) nature. The mechanical results show that these compounds are mechanically stable. The thermodynamic stability of these compounds are also determined. In addition the temperature and pressure effects on the bulk modulus, heat capacities, Debye temperatures and entropy are computed and discussed in details.

KEYWORDS: Heusler alloys, Magneto-electronic properties, Thermodynamic properties, HM-FM characters

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