



## Structural, electronic and magnetic properties of new full Heusler alloys $Rh_2CrZ$ ( $Z = Al, Ga, In$ ): First-principles calculations



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### ARTICLE INFO

#### Keywords:

First-principles calculations  
Heusler alloys  
Structural properties  
Magnetic properties  
Half metallicity

### ABSTRACT

First-principles calculations based on the density functional theory (DFT) within full-potential linearized augmented plane wave method (FP-LAPW) were carried out to investigate the structural, electronic and magnetic properties of  $Rh_2CrZ$  ( $Z = Al, Ga, In$ ) Heusler alloys. The electron exchange-correlation energy is described by the generalized gradient approximation (GGA-PBE), Tran and Blaha modified Becke-Johnson (TB-mBJ) potential and GGA + U (U is Hubbard correction). The present work reveals the stability of  $Rh_2CrZ$  ( $Z = Al, Ga, In$ ) Heusler in  $Cu_2MnAl$ -type structure. The negative value of formation energy in  $Rh_2CrZ$  ( $Z = Al, Ga, In$ ) alloys indicates that these compounds can be synthesized experimentally.  $Rh_2CrZ$  ( $Z = Al, Ga$ ) are half metal ferromagnets and expected to be potential candidates for application in spintronics. However,  $Rh_2CrIn$  is nearly half metallic behavior.

### 1. Introduction

Half-metallic (HM) materials are considered to be the most promising one, characterized by a metallic behavior in one spin channel and semiconducting nature for the other leads to 100% spin polarization at the Fermi level. The HM materials are the key in terms of technological importance and a prospective component of spintronic devices, in particular, as a resource of spin-injection into semiconductor substrates. Spintronic is a new form of electronics which utilizes the spin degree of freedom of electrons as well as

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<https://doi.org/10.1016/j.cjph.2019.04.002>

Received 7 December 2018; Received in revised form 20 March 2019; Accepted 1 April 2019

Available online 10 April 2019

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