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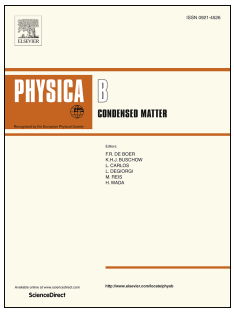

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Marah J. Alrahamneh, Ahmad A. Mousa, Jamil M. Khalifeh

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First Principles Study of the Structural, Electronic,Magnetic and Thermoelectric Properties of Zr_2RhAl

Marah J. Alrahamneh[a], Ahmad A. Mousa[b,*], Jamil M. Khalifeh[a]

[a] *Department of Physics, The University of Jordan, Amman 11942, Jordan*
[b] *Middle East University, Amman 11831, Jordan*

Abstract

The inverse Heusler alloy Zr_2RhAl is investigated using first-principles calculations. The calculations are carried out using the full-potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method that is employed in the WIEN2k package. The structural, electronic, magnetic, and thermoelectric properties are studied. It is found that the ferromagnetic phase of Zr_2RhAl is the most stable with lattice parameter 6.6328 Å. The calculations showed that there is an energy gap in the spin down channel whereas the spin up channel is metallic, resulting in a 100 % spin polarization at Fermi level. This is an obvious characteristic of half-metallic materials. The calculated total magnetic moment of Zr_2RhAl is found to be 2 μ_B which follows the generalized Slater-Pauling rule. The Curie temperature is estimated to be 607 K using the mean field approximation. Transport properties are studied using the Boltzmann theory with constant relaxation time approximation. The variation of transport properties with temperature is investigated using the two current model.

Keywords: Heusler alloys; Electronic properties; Magnetic properties; Thermoelectric properties

*Corresponding author
Email address: amousa@meu.edu.jo (Ahmad A. Mousa)