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Investigation of Structural Stability, Elastic Properties, Electronic Structure and Ferrimagnetic Behavior of Mn_2RhGe Full-Heusler Alloy

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Abstract

The first-principle calculations of density functional theory have been used to study the structural, elastic, electronic and magnetic properties of Mn_2RhGe full-Heusler alloy. The present study reveals that the Mn_2RhGe is stable in X_a-type structure and exhibits a half-metallic ferrimagnetic feature at equilibrium lattice constant. In the Mn_2RhGe, the ferrimagnetic behavior results from antiparallel coupling between Mn (1) and Mn (2) spin moments. The total magnetic moment of Mn_2RhGe is $3\mu_B$, which obeys to the Slater-Pauling rule. The Mn_2RhGe keeps the half-metallic character for the lattice parameters (a) in the range of 5.73 to 5.95 Å, but at a = 6.05 Å this behavior destroyed and the compound becomes metallic in nature. Therefore, the Mn_2RhGe is predicted to be better candidate to explore ferrimagnetic property for possible spintronics applications.

Keywords

Mn_2RhGe full-Heusler alloy; Half-metal; Ferrimagnetism; Slater-Pauling rule