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Investigation of Structural, Half-Metallic and Elastic Properties of a New full-Heusler Compound - Ir_2MnSi

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Highlights

- Ir_2MnSi full-Heusler compound has been studied by using GGA calculation.
- Cu_2MnAl and Hg_2CuTi prototype structures are compared and Cu_2MnAl structure is more stable energetically.
- The magnetic moment of Ir_2MnSi full-Heusler compound is $5 \mu_{\text{B}}/\text{f.u.}$
- Ir_2MnSi compound is a HM and it has $a=6.03 \text{ \AA}$ at GGA method.

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