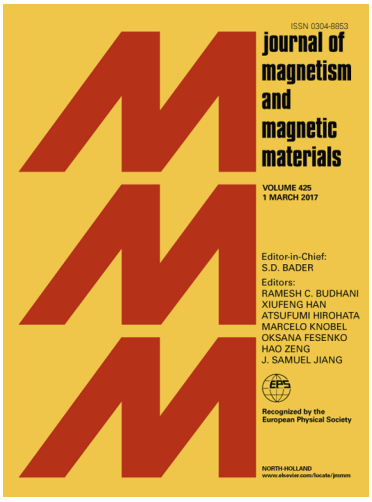


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PII: S0304-8853(17)33583-7
DOI: https://doi.org/10.1016/j.jmmm.2018.03.036
Reference: MAGMA 63807

To appear in: *Journal of Magnetism and Magnetic Materials*

Please cite this article as: D. Jiang, Y. Ye, Q. Gou, D. Wu, Y. Wen, First-principles predictions on structural, elastic and half-metallic properties of $Fe_2LiAs$ Heusler compound, *Journal of Magnetism and Magnetic Materials* (2018), doi: https://doi.org/10.1016/j.jmmm.2018.03.036

# First-principles predictions on structural, elastic and half-metallic properties of $Fe_2LiAs$ Heusler compound

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**Abstract**

The structural, elastic and half-metallic properties of $Fe_2LiAs$ Heusler compound have been investigated by using first-principles calculations. Both $Cu_2MnAl$-type and $Hg_2CuTi$-type structures have been considered for both nonmagnetic and ferromagnetic states. It is found that the ferromagnetic state is more stable than the nonmagnetic one for both structures, and the ferromagnetic $Hg_2CuTi$-type structure is the most energetically preferable. For the $Hg_2CuTi$-type ferromagnetic $Fe_2LiAs$, the elastic properties have been studied and the Debye temperature has been estimated from from the average sound velocity. It is found that the compound is mechanically stable at ground state, exhibits ductile and anisotropic behaviors, and has a Debye temperature of 413.52 K. From the calculated electronic and magnetic properties, the compound is also found to be a half-metallic ferromagnet with a total magnetic moment of 4.0 $\mu_B$ within the relatively wide range of lattice constant. These results suggest that $Fe_2LiAs$ is a promising material for spintronic applications.

*Keywords:* $Fe_2LiAs$ Heusler compound, Structural property, elastic property, Half-metallic property, first-principles

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