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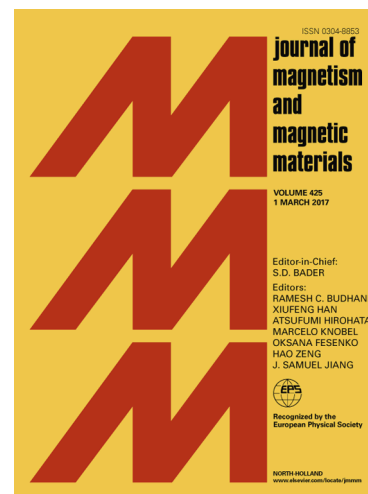
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First-principles predictions on structural, elastic and half-metallic properties of Fe₂LiAs Heusler compound

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Abstract

The structural, elastic and half-metallic properties of Fe₂LiAs Heusler compound have been investigated by using first-principles calculations. Both Cu₂MnAl-type and Hg₂CuTi-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 Hg₂CuTi-type structure is the most energetically preferable. For the Hg₂CuTi-type ferromagnetic Fe₂LiAs, the elastic properties have been studied and the Debye temperature has been estimated 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 μ_B within the relatively wide range of lattice constant. These results suggest that Fe₂LiAs is a promising material for spintronic applications.

Keywords: Fe₂LiAs Heusler compound, Structural property, elastic property, Half-metallic property, first-principles

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