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Research articles

Novel half-metallic $L2_1$ structured full-Heusler compound for promising spintronic applications: A DFT-based computer simulation

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ABSTRACT

In search for novel magnetic materials, we discuss the computer estimation of structural, electronic, mechanical, thermodynamic and magnetic properties of yet-to-be synthesized but stable Fe_2TaGe alloy. We make use of density functional theory and mechanical aspects for this resolution. The scrutiny of structural and mechanical stability outlines the $L2_1$ structure as the stable phase. Interestingly, while the Fe_2TaX (X = Al,Ga,In) compounds are reported to be non-magnetic semiconductors, the Fe-Ge compound comes out to be a ferromagnetic half-metal. The computed electronic structure reveals a half-metallic gap E_{HM} = 0.05 eV for the PBE functional; while as for the mBJ potential, E_{HM} = 0.21 eV in spin-down channel. From the elastic studies, the present system falls out to be a ductile material along with a Debye temperature of 590.14 K. The magnetic evolution predicted from Slater-Pauling rule (Mt-24) manifests the total integral magnetic moment to be one Bohr magneton, and the same is reflected from *ab-intio* simulations. The predictions of thermodynamic and ground-state properties from extensive first-principles calculations could be useful for its future experimental realization with intriguing applications.

1. Introduction

First-principles calculations certainly accelerated the expansion rate in the field of research of single-phase alloys. Heusler alloys due to their multi-dimensional properties are central to a spectrum of applications ranging from energy/information storage to spintronics or thermoelectrics, superconductors, topological insulators [1–3]. Rigorous theoretical investigations, based on machine learning models and density functional theory (DFT) [4,5], aimed at finding new and better single phase Heuslers have been performed in recent years. It was Groot et al. [6] who used to study half metallic Heusler alloys long back ago. With the passage of time, Heuslers emerge out to be a novel collection of materials for spintronic, magnetoresistive and thermoelectric applications [7]. Systemically, numerous Heusler compounds have been put under stimulating experiments as well as theoretical investigations for future devices and technologically efficient applications [8,9]. In conventional electronics, the charge carriers (electrons or holes) offered less operations for tailoring the specific properties; but the simultaneous manipulation of spin states alongside the electronic states lead to the discovery of spin ordering at the Fermi level in such half-metallic systems. At ambient conditions, half-metallic materials display 100% spin polarization and ensure the metallic character of band structure in one spin channel and semiconducting behavior in another spin configuration [10].

Till date, various Fe-based Heusler alloys from unembellished trials have been metered for spin polarization, martensitic transformation and shape memory effect, half-metallic or semiconducting behavior, Slater-Pauling rule and many more other physical properties to count here [11,12]. Fe-based Heusler structures with semiconducting or half-metallic electronic structures constitute a vast family. Among them, the experimentally synthesized Fe_2YSi (Y = Cr, Mn, Fe, Co, Ni) alloys in a recent report were reported to be half-metals [13]. Similarly, FeVRuSi, Fe_2NiZ (Z = Al, Ga, Si, Ge), FeMnSi [14–16] and other such compounds have been investigated for their various physical properties. Bilc et al. carried out a systemic investigation on Fe_2YZ (Y = V, Ti, Nb, Zr, Ta, Hf and Z = Al, Ga, In, Sn, Ge, Si) Heusler compounds and presented their power factors much larger than classical thermoelectrics [17]. In our previous works, we reported the electronic structure, lattice dynamics and transport properties of Fe_2TaZ (Z = Al, Ga, In) alloys along with their electronic properties [18,19]. Fe_2TaGe alloy has been reported to be a stable material via phase diagram analysis and quantum molecular dynamics [20]. To the best of our knowledge, no literature/data is available on its electronic structure, elastic or any other physical properties. Henceforth, we first time report the detailed study of its

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