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Research articles

Robust stability, half-metallic ferrimagnetism and thermoelectric properties of new quaternary Heusler material: A first principles approach

Shakeel Ahmad Khandy[a], Jeng-Da Chai[a,b,*]

[a] Department of Physics, National Taiwan University, Taipei 10617, Taiwan
[b] Center for Theoretical Physics and Center for Quantum Science and Engineering, National Taiwan University, Taipei 10617, Taiwan

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ABSTRACT

Like full or half-heusler materials, equiatomic quaternary Heuslers (EQH) also display various intriguing physical properties. We carried out the strict and rigorous density functional theory calculations to estimate the stability of novel ferrimagnetic FeMnTaAl alloy. In this work, we considered the thermodynamic, energetic, dynamic and mechanical stability criteria, by evaluating the formation energy, phonon dispersion and elastic constants, respectively, which thereby suggest that the synthesis of FeMnTaAl as bulk phase is likely. Later, the electronic structure, magnetic and transport properties are determined from the ground state parameters. After the structural optimizations, the half-metallic character from spin resolved band structures and local spin moments (1 μB) potentially felicitate its spintronic applications. Conservative estimates of Seebeck coefficient (~85 μV/K at 900 K), lattice thermal conductivity (2.8 W/mK at 300 K) and figure of merit (0.03 at 900 K) have also been put forward in this report. The overall structural stability, ferrimagnetism with large T_C accompanied by transport properties will possibly enact the experimental realization for magnetic, thermoelectric or spintronic impressions of this material in future.

1. Introduction

Accelerated discovery of new Heusler magnets or preferable band gap materials in this family usually proceeds by hit and trial method, where mostly the state of the art first principles simulation has established its grounds to be effective in terms of time and cost. At the same time, this route of predicting new compounds may contain surprises or distresses. The vast family of Heusler compounds consist of binary, ternary and quaternary alloys which are fundamentally important due to the exhibition of wide range of properties and potential technological considerations [1,2]. These materials are easy to be altered through structural variants and chemical substitutions and this tunability makes them an interesting family to be studied. Their evolution traces back to a century before and currently these materials flourished from conventional spintronic half-metals or semiconductors to the latest topological Weyl and Dirac materials [3,4]. Intermetallic or Heusler alloys with substantial band gaps are thus attractive for their unusual properties but rare also. Very recent observations of room temperature skyrmions, superconducting and giant anomalous Hall effects have added to the fascinating research adventures in Heuslers systems [5,6].

In the recent past, extensive theoretical studies in search of new equiatomic quaternary Heusler (EQH) alloys have been carried out for spin gapless (SGS), halfmetallic (HM), semimetallic or semiconducting properties [7,8]. EQH alloys are nowadays realized experimentally but theoretical predictions are also perceived rigorously. Keeping in view the onset of their peculiar properties, we present a simplified review of the EQH compounds as much as possible; the materials like, CoFeMnZ (Z = Al, Ga, Si, Ge) [9], FeVRuSi [10], CoFeCrZ (Z = Al, Ga, Ge) [11], FeMnTiAl [12], FeMnCrSb [13] and FeCrRuSi [14] have been predicted as novel HMMs either experimentally or theoretically. CoMnFeSi was recently synthesized experimentally and studied intensively via theory for spin gapless semiconducting (SGS) features as well [15,16]. Later, the scope extended to the rare-earth based compounds e.g, YCoTiZ (Z = Si, Ge) [17], LaCoTiZ (Z = Ge,Sn,) [18] ScCoTiZ (Z = Si,Ge) [18], YCoCrZ (Z = Si, Ge, Ga, Al) [19] and Pd_2YZ (Y = Co, Fe, Mn; Z = B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As, Sb) [20]. Recently, Heusler (EQH) semiconductors with the formula MCoVZ (M = Lu, Y; Z = Si, Ge) [21] are reported to become new spin-filter materials. In such systems the band gap is different in spin down and spin up states. Thus, the number is quite large to count here, and we tried to add one more member to this vast family of magnetic materials. While searching for new materials, we carried out a thorough investigation by changing the X and X′ atoms sequentially keeping the Ta and Al atoms in place, but the above said compound only came out to be the stable. Thus, a first detailed

* Corresponding author.
E-mail address: jdchai@phys.ntu.edu.tw (J.-D. Chai).

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