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Electronic structure, thermoelectric, mechanical and phonon properties of full-Heusler alloy (Fe_2CrSb): a first-principles study

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Abstract. We hereby discuss the structural stability of Fe_2CrSb via energetic considerations, phonon dynamics and mechanical aspects. Later, the electronic, magnetic and thermoelectric properties are discussed in order to reach out the possible explanations of the observed half-metallic bandgap and other physical properties. Phonon dispersion of Fe_2CrSb with positive-only frequencies accompanied by the observed elastic parameters indicate the dynamic stability and mechaneablity of this alloy. The relaxed and optimized structural calculations predict the ferromagnetic Cu_2MnAl-type L_{21} phase as the stable one. This compound has a half-metallic ferromagnetic character with an integer magnetic moment of 3 μB, which is in good agreement with the Slater–Pauling (SP) rule. Finally, we have pronounced the thermoelectric performance against the temperature range of 50–800 K using Boltzman transport theory. The room temperature Figure of merit (0.54) reaches to maximum of 0.67 at 800 K, indicating that Fe_2CrSb can work at low as well as high temperature thermoelectric devices operations.

Keywords. DFT study; full Heuslers; half-metallicity; electronic and magnetic properties; thermoelectric properties; dynamical and thermo-mechanical stability.

1. Introduction

Full-Heusler compounds are transition metal (TM) and p-group based ternary materials (X_2YZ) with 2:1:1 atomic sequence discovered in 1903 by Friedrich Heusler [1]. The first two elements of this ternary structure (X and Y) are TM atoms and the last one is the III-VIA group atom [2]. If the valence electron count of X atom is higher than Y atom, full-Heusler alloys crystallize in the Cu_2MnAl structure (225-space group); otherwise, they form the Hg_2CuTi phase (216-spacegroup). The four Wyckoff-positions: A (0, 0, 0), B (0.25, 0.25, 0.25), C (0.5, 0.5, 0.5) and D (0.75, 0.75, 0.75) in Cu_2MnAl structure are filled as: X occupies the B and D positions, Y at C and Z at A. In the Hg_2CuTi type, C and D are reserved for X atoms, Y occupies the A position and Z occupies the B position [3–7]. Since their discovery, these materials are intensively investigated for their fascinating applications as topological insulators, superconductive and spintronic materials, thermoelectrics, etc. [8]. De Groot *et al* [9] in 1983 were the first to discover the half-metallicity in NiMnSb. In view of the band structure, this property is described as the semiconducting or insulating character of a material in either of the two spin directions and the metallicity is exhibited in the corresponding spin channel. This makes such kind of compounds as the pronounced candidates for technical applications in spin-injection devices [10], spin-filters [11], tunnel junctions [12] or GMR devices [13]. Among, Fe-based Heuslers, the semiconducting properties of Fe_2TaAl, Fe_2TaGa, Fe_2Val, Fe_2HfSn, Fe_2ZrSi, etc. along with their mechanical and dynamical stability have been probed to achieve large Seebeck coefficients as well as display good thermoelectric performance [14,15]. Yabuuchi *et al* [16] found the power of Fe_2TiSi and Fe_2TiSn to reach 160 μV K^{-1} and the Figure of merit to 0.6. Seebeck coefficients of Fe_2ScP, Fe_2ScAs and Fe_2ScSb compounds are observed to be 770, 386 and 192 μV K^{-1}, respectively, and are recommended to have the possible thermoelectric applicability in wide temperature range [17].

In this study, the physical (e.g., structure, mechanical and phonon stability, electronic, magnetic and transport) properties of Fe_2CrSb alloy are keenly examined using the full-potential linearized augmented plane wave method (FP-LAPW) [18,19], within the generalized gradient

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