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First principles understanding of structural electronic and magnetic properties of new quaternary Heusler alloy: FeVRuSi

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Abstract

In this article, we present the electronic structure and magnetic properties of half-metallic FeVRuSi quaternary Heusler alloy using first–principles calculations. Structural optimizations in all the three possible prototypes lead to the Y-III type as its stable ground state structure in *F*-43*m* phase. Spin-polarized electronic structure shows that the material is a semiconductor in the spin down channel while as the metallic character is displayed in spin up channel. It is established that the shape and size of spin down gap is mainly determined by *d*–*d* hybridization between the *d*-states of transition metal atoms Fe and V. The observed total ferromagnetic spin moment of 0.99 μB is contributed mainly by the Fe atom in its unit cell. Covalent type bonding among the constituent atoms is reflected from the electron density plot. This work is liable to inspire the functionalization of transition metal-based alloys for future magneto-electronic and spintronic device applications.

1. Introduction

Holocene predictions/simulations or investigations of new materials of smart class which are very sensitive to the external upshots, like temperature, stress, magnetic and electric fields have placed them in the priority of researchers worldwide. The quaternary intermetallic Heusler alloys fit into this category of smart materials due to the exhibition of numerous interesting phenomena like, high spin-polarization [1, 2], half-metallicity [3–6], thermoelectric properties [7, 8], high Curie temperature [9] and spin gapless semi-conducting properties [10, 11], etc. Till date, ample attention has been dedicated to the half-metallic ferromagnetic Heuslers, either full (X_2YZ-type) or half (XYZ-type); while as the quaternary alloys (XX′YZ-type) are not studied at length. Here, X, X′ and Y′ represents the transition metal atoms and Z is a main group element. The apparent cause behind the existing novel magnetic behavior is attributed to the partially filled *d*-orbitals present in one or more transition metal components in their lattices. There is an intricate relationship between the occupancies of constituent magnetic atoms in their sub-lattices with unlike symmetries. These associated magnetic configurations thereby elucidate the electronic structures of such compounds. The aforesaid reasons are combinedly proposed to be responsible for the emergent novel phenomena in these materials. Owing to the sub-lattice occupancies of four magnetic elements of XX′YZ structures, the quaternary Heusler compounds have offered greater flexibilities with the choices of the constituent atoms and their arrangements on lattice sites resulting in the discovery of newer materials with desirable properties [12]. Following this idea, researchers have geared up the research on quaternary Heusler compounds in recent times. Till date, a lot more XX′YZ compounds have been predicted either experimentally or theoretically to be half-metals or ferromagnets, such as CoFeCrZ (Z = Al, Ga, Ge) [13], CoMnCrAl [14] and CoFeMnZ (Z = Al, Ga, Si, Ge) [15]. The room has now been extended to compounds including rare earths/4d transition metals, such as ZrFeVZ (Z = Al, Ga, In) [16], YCoTiZ (Z = Si, Ge) [17]. The width of the half-metallic band gap of these compounds is normally larger than that of equiatomic quaternary compounds that only contain 3d transition metals, which benefits the constancy of the half-metallic character in practical applications [18]. FeCrRuSi, an equiatomic quaternary Heusler alloy has been reported experimentally to crystallize in F4-3m phase, which is a ferrimagnetic half-metal [19].