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Preserving the half-metallicity at the full Heusler alloy Sc_2CrSi surfaces as well as Sc_2CrSi/HgTe (1 1 1) interface

Jabbar M. Khalaf Al-zyadi *, Hassan I. Asker

Department of Physics, College of Education For Pure Sciences, University of Basrah, Basrah 6100, Iraq

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A B S T R A C T

Using the first principle study within the density functional theory, the electronic and magnetic properties of the bulk on (1 1 1), (1 1 0) and (0 0 1) surfaces of the full-Heusler alloy and the Sc_2CrSi/HgTe (1 1 1) interfaces were verified. In this article, our calculations showed that the compound exhibits half-metallic ferromagnetism with an energy gap of 0.544 eV and a spin-flip gap of 0.1 eV in the majority spin channel at an equilibrium lattice constant of 6.39 Å. The total magnetic moment of the studied compound was calculated according to the Slater rule to be 2 μ_B. The results confirm that the half-metallicity of bulk is completely conserved at the Sc(2)Si-terminated (0 0 1) surface, Sc(1)-, and Si-terminated (1 1 1) surfaces, but destroyed at Cr- and Sc(2)-terminated (1 1 1) surface, the Sc(1)Cr- terminated (0 0 1) surface, and Sc(1)Sc(2)CrSi-terminated (1 1 0) Surface. From the above-mentioned characteristics of Sc_2CrSi exhibit that this alloy is an adequate promising candidate for spin electronics implementations. Moreover, during the calculation of the interfacial adhesion energies, it is found it that Sc(1)-Te and Si-Te configurations are more stable among the others. Regrettably, interfacial configurations show that the half-metallicity of bulk Sc_2CrSi is destroyed for all four possible configurations.

1. Introduction

Microelectronics is based on the treatment of charge carriers in the semiconductors. In these applications, neither spin carriers nor their magnetic moment are used [1]. In contrast, spintronics depends on the spin of the electron, instead of the charge, to store and transfer information [2]. Modern technology has made the connection between these two domains possible by merging spintronics with microelectronics, which means the presence of semiconducting materials near those used in microelectronics with a magnetic behavior controlled by spin carriers. These new applications lead to make electronic features more efficient and smaller, thus facilitate obtaining devices of high capacity and speed of execution [3].

All spintronic devices need a spin source; typically, this source is of ferromagnetic materials. Half-metallic (HM) materials play a major role in the industry of spintronics [4]. HM are materials have two different spin channels; one of the spin channels has the metal behavior, while the other channel has semiconducting behavior (or dielectric) and thus has a full spin polarization at the Fermi level [5,6]. The HM Materials have wide applications in different fields such as spin valves, magnetic sensors, and the primary materials in electrodes [7–9].

In 1983 s, De Groot et al. were the first group discovered the HM when they were studying half-Heusler alloys of NiMnSb and PtMnSb [10,11]. After that, many materials that have an HM property were discovered, such as full-Heusler compounds, zinc blende, and rocksalt [12–14]. There are two types of Heusler compounds: the first type includes the half-Heusler compounds that have the formula of XYZ and the second type comprises the full-Heusler compounds that have the formula of X_2YZ where X and Y are the elements of transition metals, while the Z is the element of the third to the fifth groups [15–17].

In the full-Heusler compounds, when the atomic number of X is smaller than Y over the same period, they are called inverse Heusler compounds [18,19]. Heusler alloys are distinguished from other half-metallic materials because they have high Curie temperatures and they are similar to semiconductors that are crystallized in the ZB structure [20]. There is plenty of research that studied Heusler compounds theoretically and experimentally, such as Zr_2TiAl [21], Zr_2VIn [22], Co_2FeSn [23], Ti_2FeSn [24] and Fe_2CoSn [25], etc, but Sc_2-based full-Heusler compounds have not been extensively studied. Among these compounds, an Sc_2CrSi Heusler alloy has a ferromagnetic property and a total magnetic moment of 2.0 μ_B that corresponds to the Slater Pauling rule [26,27].

* Corresponding author.
E-mail addresses: Jabbar_alzyadi@yahoo.com, gabbar_alzyadi@yahoo.com (J.M. Khalaf Al-zyadi).

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