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ORIGINAL PAPER

Electronic Structure and Magnetic Properties of the (111), (110), and (001) Surfaces for the Full Heusler Alloy Zr_2VGa

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Abstract
In this paper, the electronic and magnetic properties of the Zr_2VGa (111), (001), and (110) surfaces are studied via the first-principles calculations based on the density-functional theory. The calculations indicate that the Zr_2VGa full-Heusler alloy displays a half-metallic behavior with a total spin magnetic moment of 2.0 μ_B at the equilibrium lattice parameter of 6.657 Å. The energy band gap is 0.28 eV at the Fermi level. A weak relaxation at the terminations of the (111) and (001) surfaces is obtained which means that the terminations are stable. However, the stronger relaxations are at the terminations of the (110) surface. Examining the electronic density of states, the half-metallicity is determined which was verified in the bulk Zr_2VGa and it is destroyed at the (111), (001) and (110) surfaces. Furthermore, it is discovered that the atomic spin magnetic moments at the Zr(2)Ga-terminated (001) surface is decreased compared to those of the bulk Zr_2VGa, while the magnetic moments are increased at the Zr(1) and V-terminated (111) surfaces.

Keywords Full-Heusler alloy · Half-metallic ferromagnet · Surface properties · Density of states

1 Introduction

Half-metallic (HM) materials displaying a full spin polarization (100%) are still capturing the attention of the researchers due to their fabulous physical properties, a situation that established these materials as suitable building blocks for spintronic devices [1, 2]. The HM materials can be effectively used as spin injectors for many spin-dependent devices including the magnetic memories [3, 4]. Since the discovery of the first HM material in 1983 by de Groot and his collaborators [5] when the half-Heusler NiMnSb and PtMnSb alloys were investigated, researchers have been continuously digging for other alloys which predict the HM properties. Many novel ferromagnetic materials have been introduced to the literature through theoretical first-principles studies. These materials, especially the semi-Heusler structure type, are highly efficient in several magnetic field applications due their significantly small values of spin magnetic moment and low energy losses [6]. The most interesting property of HM materials is the metallic behavior of the one spin channel along with the semiconducting performance of the other channel at the Fermi level. Among the half-metallic materials are the full-Heusler compounds of the chemical structure X_2YZ (where X and Y are transition metals, and Z is a nonmetallic element, i.e., sp. element) [7]. The study and investigation of HM for full-Heusler compounds have a wide research potential due to their high Curie temperature and structural similarity with zinc blende semiconductors compared with other HM materials [8–10]. Recently, many of the new Zr-based Heusler alloys are discovered to be HM materials, for example Zr_2CoZ (Z: Al, Ga, and In) [11], Zr_2NiZ (Z: Al and Ga) [12], Zr_2VSn [13], Zr_2CoAl [14], Zr_2CrZ (Z: Ga, In) [15], and Zr_2PdZ (Z: Al, Ga, and In) [16]. Most of the HM materials are used in spintronic devices in the form of thin films and/or multilayers, so it is necessary to study the electronic surface properties of the bulk in consideration of the fact that the HM property maybe destroyed at the surface despite its presence in the bulk [17–19]. For example, Han et al. [20] studied the Co_2VGa compound, and they noticed that the HM property was

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