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Electronic structure and magnetic properties of the (001), (111) and (110) surfaces of ScC with zinc blende structure

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ABSTRACT

In this paper, the first-principles full-potential linearized augmented plane-wave method (FPLAPW) is implemented to investigate the structural, magnetic, and electronic properties of (001), (111) and (110) surfaces of zinc blende (ZB) structure of ScC. At the equilibrium lattice constant (5.121 Å), the half-metallicity preserved in the bulk ScC, is destroyed at both Sc(C)-terminated (001), Sc(C)-terminated (111) surfaces, as well as the ScC-terminated (110) surfaces and subsurfaces.

In this study, the atomic magnetic moments were calculated, and the findings indicated that the magnetic moments are increased at the C-terminated (001), and (111) surfaces and decreased at both Sc-terminated (001) and (111) surfaces and the ScC-terminated (110) surface. The magnetic moments also increased at the Sc-terminated (001) and (111) subsurfaces, while they decreased at the C-terminated (001) and (111) subsurfaces as well as the ScC-terminated (110) subsurface.

1. Introduction

Recently, low dimensional (LD) nanomaterials have established themselves as suitable materials for many applications related to the spin-electronic devices such as vertical tunnel junctions [1] and magnetic field sensors [2].

Among several LD nanomaterials, the Heusler alloys provide many features of the metal and semiconductor in the spin-up and spin-down channels. This merit has given the name of half-metallic (HM) magnetism and the concept of HM ferromagnet which was introduced to the literature for the first time by de Groot and collaborators in 1983 [3].

Generally, half-metallic ferromagnets (HMFs) are considered to be a particular kind of substances. A gap at the Fermi level presents one spin channel, while the other channel has metallic character which gives these materials a semiconducting feature. In the past years, the applications of these material to spintronics especially as a source of spin-polarized transporters injected into semiconductors devices have attracted the attention of scientists [4]. Furthermore, the half-metallicity has been also found in oxides like Fe_3O_4 [5], CrO_2 [6,7], perovskite compounds $LaSrMnO_3$ [8], and some diluted magnetic semiconductors such as C-doped ZnS [9]. The calculations of the electronic structure of these materials can provide a valuable information which helps to identify the HMFs using existing semiconducting devices, based on electronic structure calculations, some zinc blende (ZB) and wurtzite binary alloys were predicted to act as HMFs. The reported zinc blende HMFs include transition metal pnictides [10] and chalcogenides [11], in addition to the sp half metallic ferromagnetism in the alkali earth metal which has the pnictides [12] and tetrels [13]. The wurtize HMFs are composed of the transition-metal pnictides and chalcogenides [14], as well as the alkali earth metal whose pnictides were investigated [15].

A few decades ago, researchers could detect the half-metallicity in the ZB CrSb [16], MnSb [17], CrAs [18], and MnAs [19] at room temperature. Up to now, there are some compounds that have been suggested to be HMFs and efforts are continuing to find more materials with these interesting features. Among these materials, the specific properties of Scandium including the high melting temperature (1814K) and small density (2.989 g/cm^3), makes it suitable for many applications in electronic devices, and many other areas [20,21]. Furthermore, the electronic structure of NaCl-type ScC have been widely studied [22]. Additionally, some projects have concentrated on the half-metallicity of the wurtzite ScM (M = C, Si, Ge, and Sn) alloys [23].

These materials are prepared with the NaCl-type (ScC) [24] and CrB-type (ScSi and ScGe) [25]. In previous works, the half-metallicity

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