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A study half-metallic surfaces of the full-Heusler Sc_2CrGe compound and the interface of Sc_2CrGe/InSb (111)

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ABSTRACT

Our study showed that full-Heusler Sc_2CrGe displays half metallic ferromagnetism with an energy gap of 0.57 eV and a spin-flip gap of 0.12 eV in the majority spin channel at an optimization equilibrium lattice constant of 6.5 Å. In this study, we investigate extensively the electronic and magnetic features of the (111), (001), and (110) surfaces and the interface with the semiconductor InSb (111) via applying the first-principles computations of the density functional theory. The atomic density of states confirms that the half-metallicity discovered in the bulk Sc_2CrGe is kept at the Sc(2)Ge-terminated (001), Sc(1)-, and Ge-terminated (111) surfaces, but it is lost at the Sc (2)- and Cr-terminated (111), Sc(1)Cr- terminated (001), and Sc_2CrGe (110) surfaces. For the Sc_2CrGe/InSb (111) interface, the bulk half-metallicity is destroyed at the Sc(1)-In, Sc(1)-Sb, and Ge-In configurations while the Ge-Sb configuration exhibits a full spin polarization. Moreover, the computed interfacial adhesion energy shows that the Sc(1)-Sb shape is more stable than the others. The calculated magnetic moments of interface atoms (Sc and Ge) decrease compared to the corresponding bulk values.

1. Introduction

The half-metallic (HM) ferromagnetism is a material that has two spin bands completely different at the same time and in one substance. One of the two bands shows the metal property, while the other one shows a semiconducting or insulating characteristic with an energy gap at the Fermi level E_F. It is noteworthy that the energy separates occupied and unoccupied states [1]. Therefore, these materials may be considered hybrids between metallic and semiconductors or insulating materials. The HM ferromagnetism was discovered by de Groot et al. in 1983 while they were studying half-Heusler alloys NiMnSb and PtMnSb [2]. During the past three decades, the HM materials attracted the attention of many researchers because of their wide applications in the spin electronic devices [3]. Numerous compounds have been discovered to be HM, such as Heusler alloys, zinc-blende (ZB), rocksalt [4], the manganites $La_{0.7}Sr_{0.3}MnO_3$ [5,6], the spinel Fe_3O_4 [7] and the rutile structural CrO_2 [8]. Heusler compounds belong to a large family of binary (when the compound has two types of different elements), ternary (if it has three types of different elements) and quaternary (when it has four types of different elements) alloys; this division is obviously based on the number of types of elements forming the Heusler compounds. They were discovered in 1903s by the chemist Friedrich Heusler while he was studying Cu_2MnAl alloy [9]. One of the advantages of this discovery is that when two or more non-magnetic elements are combined, magnetic properties appear. The electronic and magnetic properties of Heusler alloys depend on the crystal structure because the atomic arrangement is what leads to ferromagnetism. Heusler compounds are distinguished from other HM materials because they have high Curie temperatures (above 600 K) and their similarity with semiconductors that crystallized in the ZB structure. Heusler alloys can be classified into three types: half-Heusler, full-Heusler, and quaternary Heusler; their chemical formulas are XYZ, X_2YZ and XMYZ, respectively, where mostly the X, Y, and M atoms are transitional elements and Z represents elements of the sp group. The full-Heusler compounds X_2YZ, that crystallize either in the Cu_2MnAl-type (L21) structure with the cubic space group Fm-3 m [10–12], or in the $CuHg_2Ti$-type structure, known as the inverse Heusler structure with the F-43 m space group [13]. It is necessary to explore new Heusler alloys for their wide applications in the field of spin-electronics. Recently, a number of new Sc-based Heusler compounds were found to be HM materials, such as Sc_2CoZ (Z=Si, Ge, and Sn) [14], Sc_2CrZ (Z=C, Si, Ge, and Sn) [15], Sc_2MnZ (Z=C, Si, Ge, and Sn) [16] and Sc_2AgZ (Z=In and Sb) [17], a discovery that enriched Heusler's applications. Most HM materials are applied in the form of thin films or multiple layers when used in spin-electronic devices, so it is

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