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Half-metallicity of the (001), (111) and (110) surfaces of CoRuMnSi and interface half-metallicity of CoRuMnSi/CdS

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Recent studies have indicated that the quaternary Heusler alloy CoRuMnSi shows a half-metallic ferromagnetism (Kundu *et al.*, *Sci. Rep.*, 7, (2017), 1803). The (111), (110), and (001) surfaces and the interfaces with CdS (111) substrate of the quaternary Heusler alloy CoRuMnSi were explored by carrying out a first-principles investigation based on a density functional theory. Calculations showed that the half metallicity can be preserved for the Si-terminated (111) surface and subsurface while the half-metallicity approved in the bulk CoRuMnSi is destroyed at Co, Ru, and Mn-terminations (111) surfaces and subsurfaces. Regrettably, the surface states ruin the gap in the spin-down channel at both MnSi- and CoRu-terminated (001) surfaces and subsurfaces. Remarkably, the (110) surfaces and subsurfaces have a nearly half-metallicity property with a high spin polarization. Based on spin magnetic character calculations, the spin magnetic moments of surface and subsurface atoms are larger and smaller than those in the bulk quaternary Heusler alloy CoRuMnSi. For the interface of CoRuMnSi/CdS (111), the bulk half-metallicity is destroyed at Si–Cd and Si–S configurations.

1. Introduction

Half-metals demonstrate complete spin-polarized band structures that fit in with spintronic applications.[1–3] A half-metal is a material in which one of the spin states reveals a metallic behavior while the other that stands for a semiconducting behavior is called a half-metallic ferromagnet. Therefore, such types could create a cause for spin-polarized currents to occur. Theoretically, the half-metallic ferromagnetism was first accepted as a fact in NiMnSb by de Groot *et al.*[4] Half-metallicity can be observed in various classes of materials, like magnetic oxides,[5] diluted magnetic semiconductors,[6] and Heusler alloys.[7] A large number of intermetallic compounds of the type X_2YZ have been discovered since the discovery of the first Heusler compounds, Cu_2Mn (Al, Sn, Zn, Bi, Sb, or B), by Heusler in 1903.[8] Typically, the X and Y are considered transition elements while the Z belongs to Group III–V in the periodic table. Much attention has been directed to the Heusler alloys owing to their high Curie temperatures and tunable electronic structures. However, not all compounds of this stoichiometry contain the original prototype Cu_2MnAl and a space group ($Fm\,3m$) structure. Accordingly, there are practically thousands of such compounds. After their discovery, and for decades, these intermetallics were little more than a scientific curiosity studied generally due to their ferromagnetic properties. But, a growing interest in other functional properties has been observed in the last few years.[9] These involve magnetic shape memory, magneto-caloric effects, thermoelectric properties, and spintronic behavior amongst others.[10–13] In a Heusler compound, the required condition for a half-metallic behavior is that the total magnetic moment per formula unit is an integer and that it follows and adopts the Slater–Pauling rule,[14–16] which links the total magnetic moment to the number of valence electrons. According to Heusler alloys, the magnetization M and the number of valence electrons N_v are linked or connected either by $M = N_v - 18$ or by $M = N_v - 24$.[17] The half-metallic quaternary Heusler compounds were found to obey these rules. It was proved that the cobalt-based Heusler alloys are very interesting because of their theoretically predicted half metallic electronic structures and that they experimentally exhibit a high spin polarization and high Curie temperatures.[18–24] The half-metallic property and structure in a quaternary Heusler alloy CoRhMnSi were theoretically determined by Kundu *et al.*[25] It is very significant to clearly inspect and examine the surface properties and their interface with semiconductors for practical spintronic implementations due to the fact that the surface and interface usually produce an effect and even damage the half-metallicity of the bulk.[26–30]

In this paper, former studies on a HM ferromagnet of the quaternary Heusler compound CoRhMnSi[25] to the CoRuMnSi (111), (001), and (110) surfaces and the CoRuMnSi/CdS (111)

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