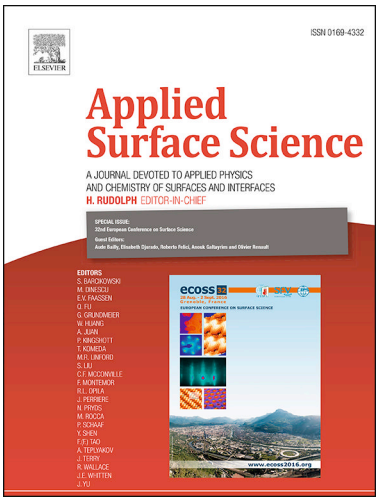

Full Length Article

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Yan Yang, Zhong-Ying Feng, Jian-Min Zhang

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Structural, electronic and magnetic properties in bulk and various (001) surfaces of X_2CoIn (X = Ti, Zr) Heusler alloy

Yan Yang [1, 2], Zhong-Ying Feng [1, 3], Jian-Min Zhang [1,*]

1. *College of Physics and Information Technology, Shaanxi Normal University, Xian 710119, Shaanxi, PR China*

2. *Department of Physics, College of Science, North University of China, Taiyuan 030051, Shanxi, PR China*

3. *Department of Science, Taiyuan Institute of Technology, Taiyuan 030008, Shanxi, PR China*

A B S T R A C T

The structural, electronic and magnetic properties in bulk and various (001) surfaces of X_2CoIn (X = Ti, Zr) Heusler alloy have been investigated by spin-polarized first-principles calculations. The InIn termination is the most stable one and the XIn termination is the second only to InIn termination as the most stable surface, with high spin polarizations 65.2% and 62.3% for X = Ti (80.8% and 69.6% for X = Zr), respectively. The atomic partial density of states (APDOS) and atomic magnetic moments (AMMs) of atoms in the central layer of X_2CoIn (001) surface accord well with those of the corresponding atoms in bulk X_2CoIn structure. The half-metal (HM) feature are destroyed by the surface states for all the five CoCo, XCo, XX, XIn and InIn terminations. The total magnetic moment is contributed by atoms in all layers for Ti_2CoIn (001) surface while is mainly contributed by the atoms in the fourth to central layers (L_4 to L_9) for the ZrIn termination but is mainly contributed by the atoms in the sixth to central layers (L_6 to L_9) for the InIn termination for Zr_2CoIn (001) surface. Further experimental efforts are expected to fabricate the X_2CoIn thin films and investigate the structural, electronic and magnetic properties of them.

***Keywords*:** Heusler alloy; Electronic properties; Magnetic properties; Half-metallicity; Surface

1. Introduction

Nowdays, half-metallic (HM) materials which exhibit a metallic feature in one spin channel while a semiconductor feature in the other spin channel which results in a complete spin-polarization at the Fermi level E_F, have attracted more and more attentions due to the applications for spintronic devices [1]. The magnetic tunnel junctions (MTJs) using two HM layers as electrodes have been widely used for sensing applications, magnetic random access memories (MRAM), the read-heads of modern hard disk drives [2, 3]. Plenty of materials are found to be HM, and Heusler alloys, as ones of HM materials, have been investigated widely [4, 5], since the half-Heusler alloy NiMnSb was predicted to be HM ferromagnet by first-principle calculations in 1983 [6]. An orbital coupling model for cubic full Heusler compounds that provides a *unified* set of rules that account for the chemical ordering, magnetic moment, and composition of the most

*Corresponding author. *E-mail address:* jmzhang@snnu.edu.cn (J.-M. Zhang).