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Current Perspectives

Surface half-metallicity of half-Heusler compound FeCrSe and interface half-metallicity of FeCrSe/GaP

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ABSTRACT

Recent studies showed that half-Heusler FeCrSe exhibits half-metallic ferromagnetism (Huang et al. [20]). In this paper, we investigate extensively the electronic, magnetic, and half-metallic properties of the half-Heusler alloy FeCrSe (111) and (001) surfaces and the interface with GaP (111) substrate by using the first-principles calculations within the density functional theory. The atomic density of states demonstrates that the half-me tallicity verified in the bulk FeCrSe is maintained at the CrSe-terminated (001) and Se-terminated (111) surfaces, but lost at both Cr- and Fe-terminated (111) surfaces and the Fe-terminated (001) surface. Alternatively, for the interface of FeCrSe/GaP (111), the bulk half-metallicity is destroyed at Se–P configuration while Se–Ga interface and subinterface show nearly 100% spin polarization. Moreover, the calculated interfacial adhesion energies exhibit that Se–Ga shape is more stable than the Se–P one. The calculated magnetic moments of Se, Ga at the Se–Ga (111) interface and P at the Se–P (111) interface increase with respect to the corresponding bulk values while the atomic magnetic moment of Se atom at the Se–P (111) interface decreases. We also notice that the magnetic moments of subinterface Fe at both Se–Ga and Se–P (111) interfaces decrease compared to the bulk values.

1. Introduction

Ferromagnetic Heusler and half-Heusler alloys have attracted considerable research attention, because they have high Curie temperatures above the room temperature, and they can be easily prepared as thin films [1,2]. All these make half-metallic (HM) Heusler alloys good candidates for spintronic materials. The $L2_1$ structure of full-Heusler X_2YZ compounds (where X and Y are usually transition metals and Z often is an element from columns III–VI in the Periodic Table) can be regarded as four interpenetrating face-centered cubic (fcc) sublattices. The X atoms are located at A (0, 0, 0) and C (1/2, 1/2, 1/2) while the Y atom is located at B (1/4, 1/4, 1/4) and Z atom occupies D (3/4, 3/4, 3/4). The $L2_1$ structure becomes the $C1_b$-type structure of half-Heusler compounds XYZ when the X position (0.5, 0.5, 0.5) is vacant. The appropriate description of the $C1_b$ structure is a zinc-blende XZ lattice stuffed with Y atoms in an ordered way.

The half-Heusler alloys are a group of ternary intermetallic compounds with an AgAsMg-type $C1_b$ structure. If the number of valence electrons of the half-Heusler alloy XYZ is 18, a gap opens at the Fermi level by the strong D-d hybridization between the X and the Y atoms [3–5]. The third fcc structure shifts by one-fourth of the unit cell from the diagonal body of the rocksalt structure [6]. Key compounds to maximize the efficiency of the devices based on spintronics are the so called HM materials, i.e., there is an energy gap in one spin band at E_F whereas the other spin band overlaps with the Fermi level and shows a metallic character, which results in a complete spin polarization of the conducting electrons at E_F [7, 8].

Research on HM ferromagnets is rapidly growing since its prediction for NiMnSb in 1983 by de Groot and his collaborators [7]. Several new HM ferromagnetic materials have been initially predicted by theoretical first-principles calculations and later verified by experiments, e.g., Heusler alloys [9,10], magnetic oxides and colossal magnetoresistance materials [11], diluted magnetic semiconductors [12–14], transition-metal pnictides and chalcogenides [15–17], and Heusler semiconductors doped with high-valent transition metal atoms [18].

First-principles electronic structure calculations for half-metals showed unusual properties in their spin-resolved band structure [19]. These calculations are very successful in many cases in

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