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Surface and interface half-metallicities of zinc-blende CrAs on GaAs(001)

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1. Introduction

Half-metallic materials attract a great attention due to their important applications in the spintronic devices. Recently, Akinaga *et al.* predicted a half-metallic ferromagnet of CrAs which has a zinc-blende structure(zb) by *ab initio* calculations and synthesized successfully the zb-CrAs on GaAs(001) substrates by molecular-beam epitaxy [1]. They found that the thin film CrAs is ferromagnetic with magnetic moment of 3 μ_B per CrAs unit at room temperature and the critical temperature is higher than 400 K. In this paper, we investigated the surface and interface half-metallicities of zb-CrAs on GaAs(001) by using the highly precise all-electron full-potential linearized augmented plane wave (FLAPW) [2] method within the generalized gradient approximation (GGA) [3].

2. Model and computational method

The system was modeled by Cr-terminated Zb-CrAs(001) slab (with five-layer thickness) attached on each side of seven-layer GaAs(001) single slab (5CrAs/7GaAs(001)/5CrAs). The lattice constants of the 2D unit cell are set to be 7.55 a.u. and the spacing between the layers are chosen to be a quarter of the experimental lattice constant of the bulk GaAs(10.68 a.u.). The Kohn-Sham equation [4] was solved self-consistently in terms of the FLAPW method within the GGA. About 2500 LAPW basis functions per each spin and $\boldsymbol{k}$-point were used to expand the wave functions. The integration was performed by summation over 4 $\boldsymbol{k}$-points inside the irreducible 1/4 wedge of the 2D-Brillouin zone(BZ). All core electrons were treated fully relativistically, while valence states were treated scalar relativistically.

3. Results and discussions

As shown in Fig. 1, we found that the surface and interface of 5CrAs/7GaAs(001)/5CrAs system retains the half-metallic character, i.e., the Fermi level locates in the energy band-gap of the minority-spin states, while the majority-spin states exhibit metallic feature, as in the bulk zb-CrAs [1,5]. The magnetic moment of Cr(S) at the surface is enhanced to 4.03 μ_B with respect to that (3.19 μ_B) of the Cr(S-2), while that of the Cr(S-4) in the interface decreased slightly to be 3.12 μ_B. If we account for the negative magnetic moments ($\sim$-0.18 μ_B) of As(S-1) and As(S-3), the sum of magnetic moments of Cr(S-2) and As(S-3) is about 3 μ_B which is in agreement with the experimental value of 3 μ_B per formular unit.

4. Reference

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Fig. 1 Spin-polarized layer-projected density of states (DOS) of 5CrAs/7GaAs(001)/5CrAs for the Cr, As and Ga atoms in different layers, respectively. The minority-spins are factored by -1 and the DOS of As states were multiplied by 2. The Fermi levels are set to zero.

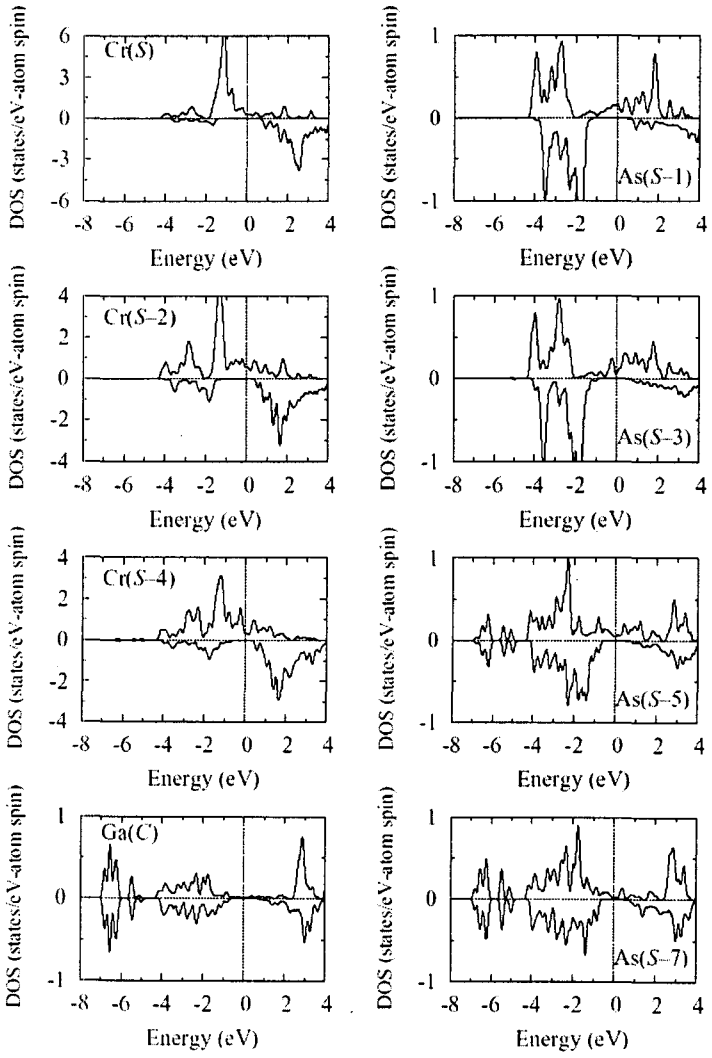

Fig. 1