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Electronic structures and magnetism of zinc-blende CrP(001)

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zinc-blende CrP(001) 표면의 전자구조와 자성

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1. Introduction

In spintronics, we use the electron spin to store and control information. In order to realize spintronic devices, it is needed to inject highly spin-polarized current into semiconductor. Half-metallic materials having complete spin-polarization(100%) at the Fermi level have been attracted much attention for spintronic applications. A first-principles calculation predicted that the artificial zinc-blende(ZB) CrP reveals half-metallicity when the lattice constant is larger than 5.48 Å [1]. In this work, we investigated surface electronic structures and magnetism for CrP(001) by using the all-electron full-potential linearized augmented plane-wave (FLAPW) [2] method within the generalized gradient approximation (GGA) [3].

2. Model and calculational method

Along the [001] direction for the ZB CrP, there are two possible terminations: one is the Cr atom terminated (Cr-Term) and the other is the P atom terminated (P-Term). The CrP(001) surface was modelled by nine- and eleven-layer single slabs for the Cr-term and P-term, respectively. The lattice constant of the two-dimensional (2D) unit cell is set to 3.89 Å and the spacing between the layers are chosen to be 1.38 Å which is one-fourth of the bulk lattice constant, 5.50 Å. Neither surface relaxations nor reconstructions were considered.

The Kohn-Sham equation [4] was solved self-consistently in terms of the FLAPW method within the GGA. About 1600 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

We found that the magnetic moment (3.86 μ_B) of surface Cr atom in the Cr-term is much enhanced with respect to that (3.02 μ_B) of the center layer. This is confirmed from the calculated density of states (DOS) presented in Fig. 1. We also found that the majority d-states of surface Cr atom are much narrowed while the minority d-states of surface Cr are strongly suppressed for the Cr-term. General shape of DOS for the subsurface P atom in Cr-term is similar to those of the inner-layers. For the P-term, there are new states in the band gap for the minority spin states for the surface P layer and the shape of DOS of subsurface Cr is much modified compared to that of the center layer. The magnetic moment of subsurface Cr for P-term is reduced to 2.43 μ_B. The magnetic moments of P atoms are antiferromagnetically coupled with those of the Cr atoms, regardless of the terminations, and the absolute values are approximately 0.16 μ_B. From the calculated DOS, we found that the value of the band gap for the surface Cr atom in Cr-term is

similar to that of the center layer, but the band gap of surface P atom in P-term is much reduced due to the appearance of new states in the band gap.

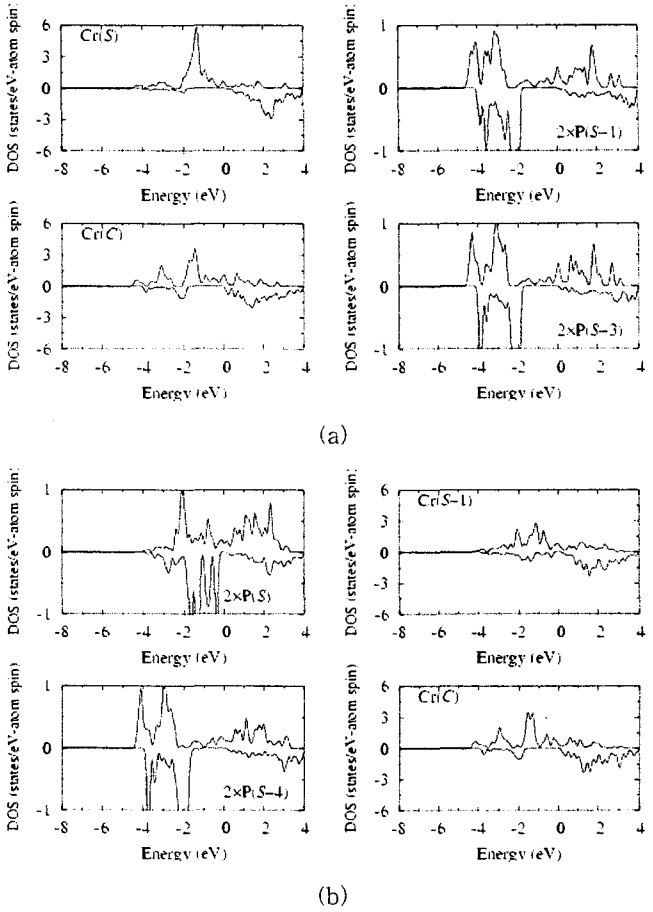

Fig. 1 Spin-polarized layer-projected density of states (in unit of states/eV atom spin) of CrP for (a) the Cr-term and (b) the P-term. The minority spins are factored by - 1, and the values of the P-DOS are multiplied by 2. The Fermi levels are set to zero.

4. Reference

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