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First-principles study on the (111) surface of half-metallic rocksalt VPo

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ABSTRACT

In this work, we have probed the structural, electronic, and magnetic properties of the (111) surface of rocksalt (RS) VPo. The first-principles full-potential linearized augmented plane-wave method is used. Bulk VPo is found to be a half-metallic ferromagnet at equilibrium lattice constant (0.59 nm) with a total spin magnetic moment of 3.0 μ_B per formula unit. At the same equilibrium lattice constant, the V-terminated (111) surface preserves the half-metallic characteristics of the bulk VPo, however, the surface states destroy the gap in the minority spin band of the Po-terminated (111) surface. We also discuss the surface stability.

1. Introduction

Due to the complete spin polarization (100%) at the Fermi level, there have been more and more attentions in half-metallic (HM) ferromagnets for the magnetoelectronics or spintronic devices. Groot et al. [1] first predicted the HM ferromagnetism in the half-Heusler compounds of NiMnSb and PtMnSb. There are some examples verified by the prediction, for example rutile structural CrO_2 [2], spinel Fe_3O_4 [3], and diluted magnetic semiconductors such as V- and Cr-doped zinc-blende (ZB) CdTe [4]. It was found that the V- and Cr-doped ZB CdTe and Cr-doped rutile TiO_2 [5] show HM behavior with total magnetic moments of 3.0 and 4.0 μ_B, respectively, which may be useful in semiconductor spintronics. CrAs with ZB structure was reported to be sprung epitaxially on GaAs (100) and found to be HM practically and theoretically [6]. The ZB CrP and CrS [7] are also HM feromagnets. The half-metallicity of materials could be destroyed at the surfaces. This property is very important in the practical applications. The half-metallicity and electronic structure at the (001) surfaces of ZB CrAs [8] were studied by using FPSKKR method [9]. There are two kinds of surface windup with atoms of anion or the transition metal. Researcher [8] found the As-terminated surface destroys the half-metallicity while the Cr-terminated surface is HM. Rahman et al. [10] found that for ZB CrP the P-terminated (001) surface losses the half-metallicity while the Cr-terminated (001) surface keeps the HM character. There are many theoretical and practical studies for the stability of surfaces [11–17]. For example, Gao et al. [18] presented a theoretical study on the preservation of the half-metallicity at the rocksalt CaN and SrN (111) surfaces and found that the N-terminated (111) surface is more stable than the Ca(Sr)-terminated (111) one in the N-rich environment by analyzing the energy of the surface. Zhang et al. studied the ZB VPo with the lattice constant of 7.02 Å from local density approximation (LDA), and their calculation indicated that the ZB-type VPo is a true HM ferromagnet [19]. The ZB VPo was also found to be HM with the lattice constant of 6.485 Å from generalized gradient approximation (GGA) [20].

Although VPo with ZB phase was predicted to be a HM ferromagnet, it has not been realized experimentally, and thus it is meaningful to search for other possible phase of VPo with half-metallicity. In this paper, we study the HM character for the bulk and the V (Po)-terminated (111) surfaces of rocksalt (RS) VPo. It is found that the V-terminated (111) surface retains the half-metallicity of RS VPo, but the half-metallicity of RS VPo is destroyed at the Po-terminated (111) surface. We also discuss the stability of surface.

2. Computational method

Based on the density functional theory, the structural, electronic and magnetic properties of the bulk and the (111) surfaces of

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