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The half-metallic characteristics of the (001) surface of zinc-blende TiTe

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ABSTRACT

In this paper, we employ the first-principles full-potential linearized augmented plane-wave method, which is based on the density functional theory to investigate the structural, electronic, and magnetic properties of the bulk and (001) surface of zinc-blende (ZB) TiTe. The bulk ZB TiTe is found to be a half-metallic ferromagnet at an equilibrium lattice constant of (6.41 Å). At the similar equilibrium lattice constant, the half-metallicity verified in the bulk TiTe, it is maintained at both Ti(Te)-terminated (001) surfaces and subsurfaces. Furthermore, by calculating the atomic magnetic moment, we find that the magnetic moment increases at the surface, but decreases at the subsurface. In addition, we evaluate the surface stability and found that the Te-terminated (001) surface is energetically more stable than the Ti-terminated (001) surface.

1. Introduction

The $C1_b$-type Heusler alloys, NiMnSb and PtMnSb were the first compounds which explain the expression ((half metal)) discovered by de Groot et al. in 1983 [1]. The half-metallic (HM) ferromagnets [2,3] which is one of the two spin channels is metallic while the other is insulating or semiconducting, leading to 100% spin polarization around the Fermi level. HM ferromagnetism has an ideal characteristic from the standpoint of its application in spintronic devices [4]. Therefore, in recent years, there are many practical and theoretical research works are conducted design and measure pertaining the physical properties of these materials. Especially, transition-metal chalcogenides and pnictides with zinc-blende (ZB) structure, in particular, show fine HM ferromagnetism on the foundation of theoretical calculations [5–14]. In these materials, the main contribution to the total magnetic moment comes from the d electrons in the transition metals of the HM ferromagnets that have a ZB structure. After the detection of HM ferromagnet by de Groot et al., many further systems have been found to be HM ferromagnets, e.g., the full-Heusler alloys [15–17], pyrite structure CoS_2 [18], perovskite $La_{0.7}Sr_{0.3}MnO_3$ [19], and some diluted magnetic semiconductors [20,21]. Kahal et al. [22] studied ZB TiPo and found it is HM at the predicted equilibrium lattice constant of 6.617 Å. Rahman [23] investigated the effect of strain on electronic and magnetic properties. Their calculation showed that ZB CrP/MnP superlattice does not display any half metallicity at its equilibrium lattice constant but shows half-metallic behavior when external strain is applied. Recently, Ahmadian [24] predicted from first-principles calculations that ZB TiTe is a HM ferromagnet. For the practical applications of half-metals in spintronic devices it is very necessary to study the surface and interface with semiconductors of half-metals because, in some materials, the HM is destroyed at the surface and interface. For example, Gao et al. [25] studied the ZB TiSb (001) surface, and found that the half-metallicity is lost at the Sb-terminated (001) surface, while the Ti-terminated (001) surface preserves the bulk half-metallicity. Galanakis studied the half-metallicity and electronic structure at the (001) surfaces of ZB CrAs [26], and found the As-terminated surface destroys the half-metallicity while the Cr-terminated surface is a HM. The half-metallicity of the CrP (001) surfaces was found to be retained for the Cr-terminated surfaces, but to be lost for the P-terminated surfaces [27].

Lee et al. [28] found that the (110) surface of CrP preserves the half-metallicity. Al-zyadi et al. [29] have studied the half-metallicity properties of the (110) and (001) surfaces of the rocksalt VPo, and found that both the (110) and (001) surfaces maintain the bulk half-metallicity.

To the best of our knowledge, there are no theoretical and experimental studies on the TiTe (001) surfaces. In this paper, we

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