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First-principle study of half-metallicity at the TiPo (001) surface and the TiPo/CdTe (001) interface

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ABSTRACT

First-principle calculations for the electronic and magnetic properties of the TiPo (001) surfaces and the interfaces with CdTe (001) substrate are reported here. It is shown that the half-metallicity confirmed in the bulk TiPo is preserved at both Ti- and Po-terminated (001) surfaces, while for the interface of TiPo/CdTe (001) only one interfacial shape shows half-metallicity. We also disclose that the atomic magnetic moments of the (001) surface and subsurface are greatly different from the bulk values. By computing the surface energy, we find that the Po-terminated (001) surface is more stable than the Ti-terminated (111) one. Moreover, by calculating the interface adhesion energies, we evaluate the interfacial adhesive strength for all the possible configurations of the TiPo/CdTe (001) interface.

1. Introduction

Half-metallic (HM) ferromagnetic materials, which are the metallic demeanor in one electron spin channel and semiconducting demeanor in the other, resulting in 100% spin polarization around the Fermi level, have attracted extensive attentions. The half-Heusler alloys NiMnSb and PtMnSb were found to be HM ferromagnets by de Groot et al. [1] in 1983. Until now, several classes of compounds have further been found to be HM ferromagnets, e.g., full-Heusler alloys such as Co_2MnSi [2] and Co_2CrAl [3], rutile-type CrO_2 [4], spinel Fe_3O_4 [5], pyrite structure CoS_2 [6], double perovskite Sr_2FeMoO_6 [7], perovskite $La_{0.7}Sr_{0.3}MnO_3$ [8], and some diluted magnetic semiconductors [9–12]. Recently, some zinc-blende (ZB) transition-metal pnictides and chalcogenides such as CrAs, CrSb and CrTe have attracted more and more research interest, because they have high Curie temperatures and comparable crystal structures with conventional semiconductors [13]. The main contribution to the total magnetic moments of HM ferromagnets with ZB structure aforementioned above comes from the transition metals *d* electrons (we call them *d* HM ferromagnets). Remarkably, some ZB HM ferromagnets without any transition metals have also been found in some alkaline-earth pnictides and carbides [14–16]. The magnetic moments of these HM ferromagnets mainly originate from the anion *p* electrons (we call them *sp* half-metals). The different magnetic mechanisms between *d* and *sp* HM ferromagnets attracted intensive research interest [17–21].

However, for both *d* and *sp* HM ferromagnets, it is very important to study the surface of half-metals and interface with semiconductors for the practical applications of half-metals in spintronic devices, because the surface and interface effects usually destroy the half-metallicity. For example, Galanakis studied ZB CrAs (001) surface for both the InAs and GaAs experimental lattice constants, and found that the Cr-terminated (001) surface preserves the *d* HM features, but due to the surface states in the spin-down band, the As-terminated (001) case loses the bulk *d* half-metallicity [22]. Gao et al. [23] investigated the (001) surface of ZB CaC, which involves two types of surface termination with Ca and C, and revealed that the (001) surface loses the bulk *sp* half-metallicity. Late studies showed that the *d* half-metallicity confirmed in the bulk Co_2FeSi is lost at its surfaces and interfaces with GaAs (001) [17].

Recently, Kahal et al. [24] studied ZB TiPo at the predicted equilibrium lattice constant of 6.617 Å from generalized gradient approximation. Their calculation showed that ZB-type TiPo is a HM ferromagnet, and the spin-orbit coupling has very weak influence on the half-metallicity. To investigate the surface and interface effects, in this paper, employing the first-principle method, we expand the previous studies on the bulk HM TiPo with ZB structure [24] to the (001) surfaces and TiPo/CdTe (001) interface. It is found that the half-metallicity is preserved for both the Ti- and Po-terminated (001) surfaces. We further discuss the difference of atomic magnetic moments between the surfaces, subsurfaces and the bulk system of TiPo. One of the four probable configurations for the TiPo/CdTe (001) interface shows half-metallicity. In addition, we discuss the surface stability and the interfacial adhesive strength.

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