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First-principle study on the surface and interface properties of the half-metallic ferromagnet of rocksalt structural BaC

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ABSTRACT

Recent study showed that rocksalt BaC exhibits half-metallic ferromagnetism (Dong and Zhao, 2011). Here we use the first-principles calculations to investigate the electronic and magnetic properties of the BaC (0 0 1) and (1 1 1) surfaces and the interfaces with the SnSe (1 1 1) substrate. The obtained results reveal that the half-metallicity verified in bulk BaC is preserved at the (0 0 1) and (1 1 1) surfaces. Unfortunately, interfacial configuration shows that the half-metallicity of bulk rocksalt BaC is destroyed for all possible configurations of C–Se, C–Sn, Ba–Se, and Ba–Sn. Moreover, by computing the interface adhesion energies, we evaluate the interfacial adhesive strength for the four possible interfacial structures. We also discuss the changes of the atomic magnetic moments at the (0 0 1) and (1 1 1) surfaces and the interfaces layers with respect to the corresponding bulk values.

1. Introduction

In the past thirty years, a great deal of attention has been paid to the expansion of spin electronic devices because of their potential implementation to the next production of electronic devices. The Heusler alloys exhibit the characteristics of metal and semiconductor in the spin-up and spin-down channels, respectively. This characteristic was given the name of half-metallic (HM) magnetism. The notion of HM ferromagnet was offered by de Groot and collaborators in 1983 [1]. Thereafter, other renowned materials have also been found to be HM ferromagnets [2–12], e.g., the double perovskite, the alkaline-earth pnictides and carbides, the europium chalcogenides, the diluted magnetic semiconductors, the pyrite structure, the transition-metal pnictides and chalcogenides, the rutile and spinel structural compounds. Interestingly, in some alkaline-earth pnictides and carbides [13,14], the magnetic moments are formed mainly by the anion p electrons, and they are named sp HM ferromagnets. Differently, in the zinc-blende (ZB) CrAs, CrSb and CrTe the anion p electrons are completely loaded, therefore the magnetic moments originate from the spin polarization of the 3*d* electrons [15]. Usually, the magnetic moments for ZB HM transition-metal pnictides or chalcogenides are larger than those of ZB sp HM ferromagnets [16,17].

Theoretically, BaC has the structure of rocksalt (RS) with lattice constants of $a = 6.00$ Å [18]. Above room temperature, RS BaC shows a HM ferromagnetism. In addition, it is found that the RS-type structure is energetically most stable among the different four structures: RS, CsCl, ZB, and NiAs [18]. By using first-principles calculations, the bulk compound BaC in zinc blende, RS, and wurtzite structures was predicted to be HM [5,18,19]. In 2011, Dong and Zhao [20] predicted that RS MC (M = Ca, Sr, and Ba) under small pressure belongs to the group of HM ferromagnets.

Because the surface and interface usually affect and even destroy the half-metallicity of the bulk [21–24], it is very important to examine the surface properties and their interface with semiconductors for the practical spintronic implementations. In this paper, by using the first-principles calculations, we extend the previous study on sp HM ferromagnet of RS BaC [20] to the BaC (1 1 1) and (0 0 1) surfaces and the BaC/SnSe (1 1 1) interface. It is found that the bulk HM property is kept at both the (1 1 1) and (0 0 1) surfaces. Unfortunately, the four possible configurations of the BaC/SnSe (1 1 1) interface destroy the HM characteristic.

2. Computational method

To explore the electronic and magnetic properties of the (111) and (110) surfaces of RS BaC and the interfaces with RS semiconductors of SnSe, we employ the first-principle full-potential linearized augmented plane-wave (FPLAPW) method implemented in

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