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Bulk and surfaces half-metallicity of RbSe with zinc-blende structure: first-principles study

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Abstract
In this paper, the electronic, magnetic, and half-metallicity characteristics of the bulk as well as (111) and (001) surfaces of zinc-bland RbSe compound are explained using the first-principles calculations. All of calculations are performed through GGA approximations, and the results reveal that both the bulk and ends of the surfaces preserve the half-metallic property. In addition, the stability of the surfaces is computed. It is discovered that the Rb-terminated (001) is the most stable one compared to other terminates. Based on the magnetic characteristic computations, the spin magnetic moment of bulk is equal to 1 μ_B, while this value has changed at the surfaces due to the effects of surface states. All of the above-mentioned properties mark this compound as a suitable promising candidate for spintronics applications.

Keywords Zinc-blende RbSe · Half-metallic ferromagnetism · Electronic band structure · Cohesive energy · Surface

1 Introduction

The field of spintronics originated from nanotechnology and denoted the role performed by electron spin in solid-state physics as well as promising devices that specifically exploit spin properties and/or charge degrees of freedom [1–4]. The materials with the high electron spin polarization (P) have now become the core of the spintronics devices. These materials which are called the half-metallic materials present both metallic and semiconducting performances. In fact, they have a semiconducting property in the minority band along with a metallic behavior in the majority band with high electron spin polarization, $p = 1$. The half-metallic materials are considered as the most important candidate for many applications. In 1983, de-Groot was able to discover half-metallic ferromagnet of the half-Heusler NiMnSb and PtMnSb materials [5]. Materials such as Heusler alloys are divided into half-Heusler alloys such as NaCrAs [6], full-Heusler alloys such as normal Co_2TiSn, and inverse Zr_2RhGa [7], and quaternary Heusler alloys such as CoZrInSi [8], while another type of half-metallic materials is binary compounds which is separated into zinc-blende (ZB) [9], rock salt (RS) [10], CsCl [11], and wurtzite (WZ) structures [12]. There are many compositions that have been found to have the half-metallic property such as metallic oxides [13] and perovskites [14]. From the above, the half-metallic (HM) and magnetic properties are clearly originated from hybridization and a split exchange of d-electrons of the transition metal, where the materials that have d-electrons of the transition metal have large magnetic moments. Structures that do not contain a transitional metal are known as the sp materials, which are shown to have the HM ferromagnetic property and small magnetic moments such as MC (M = Li, Na, K, Ca, Sr, and Ba) [15–18] and MS (M = Li, Na, and K) [19, 20]. It has been found that this type of material has a high Curie temperature that makes it magnetically stable at room temperature. As the temperature increases, this often affects the width of the energy gap as a result of a lattice constant deformation and a breakdown of the spin polarization of the material [15, 21]. The magnetic properties in 2D or 3D materials have long been investigated, including f, d, or p-electron magnetism. More specially, an interesting half-metal character has been found in some functional materials [22–25].

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