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Electronic structure and optical anisotropy in $Sr_{1-x}Ba_xFBiS_2$ (x = 0, 0.25, 0.5, 0.75, 1) based solar cell materials

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ABSTRACT

We conducted theoretical simulations for exploring the overall physical properties of the pristine $SrFBiS_2$ as well as its derivative alloys ($Sr_{1-x}Ba_xFBiS_2$ (x = 0, 0.25, 0.5, 0.75, 1)) resulting from BiS_2 layers via the compositional effect of substituting strontium with barium. In this respect, we computed the electronic and optical characteristics of $Sr_{1-x}Ba_xFBiS_2$ systems within the concentration limits of x varying from 0 to 1. Based on full-potential linear augmented plane wave scheme, we determined the structural properties of the $Sr_{1-x}Ba_xFBiS_2$ alloys, and the lattice parameter was found to increase with the augmentation of Ba concentration, which in turn agrees well with the available experimental works. The electronic band structures and density of states of $Sr_{1-x}Ba_xFBiS_2$ ($0 \le x \le 1$) alloys were also examined. According to our calculations, the parent compound $SrFBiS_2$ has a semiconducting behavior and its energy gap is about 0.8 eV. The electronic band structures illustrated that the substitution of the divalent Ba^{+2} element instead of Sr^{+2} produces a semiconducting behavior for all $Sr_{1-x}Ba_xFBiS_2$ ($0 \le x \le 1$) alloys. When substituting Ba^{+2} with Sr^{+2}, the acquired optical features, such as the dielectric function, refractive index, reflectivity, absorption coefficient, energy loss functions, and optical conductivity for $Sr_{1-x}Ba_xFBiS_2$ ($0 \le x \le 1$) alloys also exhibited a semiconducting nature. It is easily noticed that the maximum absorption coefficient changes with the variation of Ba concentration. Furthermore, a superior birefringence occurs in the concerned $Sr_{1-x}Ba_xFBiS_2$ alloys when the composition variation undergoes from x = 0 to 1. Intriguingly, the optical spectra for both parent compounds $SrFBiS_2$ and $BaFBiS_2$ and their ultimate $Sr_{1-x}Ba_xFBiS_2$ alloys displayed a high anisotropy. The viable significant role of the spin-orbit coupling in deciding the electronic structures and optical characteristics is due to the presence of heavy bismuth atoms. All our results determined for $Sr_{1-x}Ba_xFBiS_2$ systems are compared with the existing theoretical and experimental reports.

Introduction

In recent years, the layered chalcogenides associated with BiS_2-based superconductors have been proved to be promising functional materials that involve various potential applications in photocatalysis for water splitting, degradation, spintronics and even in solar-cell technologies. In this respect, the discovery of novel layered chalcogenide was revealed and its crystal structure is formed by alternating stacked layers of a typical BiS_2 superconducting and various spacer layers [1–35]. After that, 12 kinds of parent materials based on BiS_2 superconductors have been detected: $REOBiS_2$ (RE = La [8], Ce [9], Pr [10], Nd [11], Sm [12], Yb [8], and Bi [14,15]), $AFBiS_2$ (A = Sr [16,17], Eu [7]), $Bi_6O_8S_5$ [7], $Bi_3O_2S_3$ [29], and $Eu_3F_4Bi_2S_4$ [9]. In addition, the superconducting behavior was inspected in $BiSe_2$-based systems, such as $LaO_{0.5}F_{0.5}BiSe_2$ [21]. A novel crystal structure, such as $SrFBiS_2$ compound [20] was recently reported, which itself has a semiconductor character and persists to be the same even at high pressures [23]. It can undergo to a superconductor phase under the doping effect of the electronic states (i.e. La or Ce substituted at the Sr site) [13,15]. Due to the similarity of Eu^{+2} and Sr^{+2} in the size, the

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