International Journal of Modern Physics B
2150258 (13 pages)

DOI: 10.1142/S0217979221502581

Electronic and magnetic properties of bulk and surfaces half-Heusler alloy KCaB and its bulk thermoelectric properties

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Received 19 June 2021
Revised 21 July 2021
Accepted 22 July 2021
Published 3 September 2021

This paper discusses the structural, electronic, magnetic, and half-metallic properties of half-Heusler alloy KCaB. First-principles calculation based on density functional theory is successfully used to determine properties at bulk and on the (111) and (001) surfaces of KCaB. KCaB is half-metallic ferromagnet with a magnetic moment of 1 μ_B and an energy gap equal to 0.82 eV in the lower spin channel. The *n*-type doped exhibits higher Seebeck coefficient, electrical conductivity, thermal conductivity, and figure of merit than the *p*-type-doped KCaB at room-temperature 300 K. The half-metallic property is preserved in each of the ends Ca and B on the (111) surface and is lost in the ends K (111) and B and KCa (001) slab surface. The relaxation effect on the electronic spin states decreases the magnetic moment of some atoms on the end surface because the relaxation of the atomic sites is affected and the loss of the nearest neighbors affects exchange–correlation interactions. The surface end with Ca is more stable than the surface end with B on the (111) surface and can maintain the property of half metallic under relatively large stress.

Keywords: KCaB half-Heusler compound; half-metallic ferromagnetism; surface property; DFT.

PACS number: 68.35.Ja

1. Introduction

In recent years, spintronic materials have become a research interest due to their applications in various electronic devices.[1] One of the most important candidate materials for these devices is half-metallic materials (HM) with a characteristic spin polarization (SP) of 100% at the Fermi level (E_F).[2] A number of theoretical work

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