

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

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Abstract

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 *[Math Processing Error]* and an energy gap equal to 0.82 eV in the lower spin channel. The *[Math Processing Error]*-type doped exhibits higher Seebeck coefficient, electrical conductivity, thermal conductivity, and figure of merit than the *[Math Processing Error]*-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