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The magnetic and half-metallic properties of the d0-quaternary Heusler alloys KYBX(Y=Ca or Sr, X=S or Se) in ab-initio approach

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Abstract
Heusler alloys have attracted much attention due to their unique electronic structure. Most of the research on the Heusler compounds to date, has involved structures that contain transition elements. Recently, quaternary Heusler compounds without the presence of transition metals have attracted attention both from an experimental and a theoretical point of view. We have applied the first-principle method to investigate the structural, electronic, and magnetic properties of the KYBX(Y=Ca or Sr, X=S or Se) quaternary Heusler compounds. The results of our calculations showed that these compounds are ferromagnetic. After examining the different arrangements of atoms in these compounds, it has been determined that the type I of these structures is the most stable configuration. The electronic properties of these alloys indicate that they have a magnetic moment of 2 μB and are magnetic semi-metals with 100% spin polarization at the Fermi level. Their semi-metallic property primarily originates from the p orbitals of B atoms. These compounds are suitable for spintronic applications.

Keywords: quaternary Heusler compounds, density functional theory, structural properties, electronic properties

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