Half-metallic properties and structural stability of d^0-d half-Heusler compounds *XY*Bi (*X*=K, Rb; *Y*=Sc, Ti, V, Cr)

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Abstract

The electronic, magnetic, and structural stability of novel d^0-d half-Heusler compounds *XY*Bi (*X*=K, Rb; *Y* =Sc, Ti, V, Cr) are investigated using first-principles electronic structure calculations based on density functional theory. The results indicate that six of these compounds, namely, KTiBi, RbTiBi, KVBi, RbVBi, KcrBi, and RbCrBi are half-metallic ferromagnets. The half-metallic energy band-gap of these compounds are calculated in the range of 0.46-0.71 eV. A detailed study of the partial density of states show that the *p*-*d* hybridisation between 3*d* transition metals and Bi 6*p* orbitals is mainly responsible for the half-metallic behavior. The total spin magnetic moments of the compounds under study are in agreement with Slater-Pauling rule $M_{tot}=Z_{tot}-8$, and it is integer valued in a wide range around the equilibrium lattice constant, which indicates that the half-metallic property is not sensitive to the lattice parameter. Employing the structure optimization program USPEX, we have shown that the introduction of d^0 alkali metal atom leads to structural stability of the above novel half-Heusler compounds. In the light of their structural stability, high Curie temperature, and large half-metallic gap, the above compounds are good candidates for spintronic applications.

Keywords: d^0-d half-Heusler, half-metallic ferromagnets, density functional theory, Spintronic

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