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First-Principles study of magnetism and half-metallic properties of the d^0 quaternary heusler alloys BaNYO (Y = K, Rb and Cs)

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First-principles theory was applied to investigate the electronic, elastic, magnetic, and half-metallic behaviors of the newly designed quaternary Heusler compounds BaNYO (Y = K, Rb and Cs) without $3d$ transition metal elements. The elastic properties show that the investigated compounds are ductile and anisotropic. The calculated results show that the compounds are half-metallic with an integer magnetic moment of $2.00\,\mu_B$ at the equilibrium lattice parameter, with 100 % spin polarization around the Fermi level, which follows the famous Slater–Pauling rule, $M_{\text{tot}} = 16 - Z_t$, where M_{tot} is the total magnetic moment and Z_t is the total number of valence electrons. Based on its equilibrium and strained lattice constants, the magnetic and half-metallic behaviors of this compound have been discussed in detail. A large half-metallic gaps of BaNYO (Y = K, Rb and Cs) compounds of 0.95, 0.90 and 0.85 eV respectively have been found in our work, which is nearly larger than in any previous studies. Furthermore, the calculated negative formation energy and cohesive energy indicate that these two alloys have good chemical stability. This theoretical investigation provides further insight into the application of BaNYO compounds as spintronic materials.

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