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## Magnetism and Half-Metallicity of Solids from the Spin Polarization of $P$ Orbitals

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### ABSTRACT

Heusler alloys are of great scientific and technological interest. In addition, devices based on Heusler alloys exhibit a development of new structures with ferromagnetic behavior using transition metals or elements that are inherently non-magnetic. Half-Heusler type XYZ and full-Heusler type  $X_2YZ$  alloys without transition metals, mainly called  $d^0$  ferromagnetic half-metals (FHM) is a recent research field. The particular interest of their ferromagnetic character as well as of the half-metallic (HM) nature with possible applications in spintronic systems does not come from magnetic elements. This series of strongly ferromagnetic materials mentioned above is composed of non-magnetic elements compared to those predicted by Groot *et al.* in 1983. Recently, some studies have also demonstrated the presence of half-metallicity in compounds without partially filled  $d$  atomic orbitals such as alkaline earth carbides and nitrides.

The first-principles electronic structure calculations were applied to predict the ferromagnetism HM in the alkali metals and alkaline earth metals based full Heusler, quaternary Heusler and half Heusler ternary alloys. However, to our best knowledge, there are no experimental or theoretical studies on the various phases of half-Heusler alloys, as well as their phonon dynamics and thermodynamic properties.

In the present work, a comprehensive study was conducted for the  $\alpha$ ,  $\beta$  and  $\gamma$  phases of the half-Heusler alloys using first principles calculations based on the density functional theory (DFT) with and without spin polarization to explore their structural, elastic, dynamic phonon, thermodynamic, electronic and magnetic properties. The alloys studied have been shown to be energetically, elastically and dynamically stable. This implies that the experimental synthesis of these alloys under standard conditions is possible. In addition, the considered half-Heusler alloys are half metals with potential applications in spintronic devices.

