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Stability, electronic and magnetic properties investigations on Zr_2YZ (Y=Co, Cr, V and Z=Al, Ga, In, Pb, Sn, Tl) compounds

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Abstract

Using the full-potential local orbital minimum-basis method, we study the stability, electronic and magnetic properties on Heusler alloys Zr_2YZ (Y=Co, Cr, V and Z=Al, Ga, In, Pb, Sn, Tl). The stabilities of physics and chemistry are estimated, meanwhile the magnetic stability is also evaluated by the Stoner criterion. According to the products of exchange integral and magnetic moment, we deduce the Zr_2Co-based alloys with a higher Curie temperature. Electronic calculations show that these alloys exhibit a half-metallicity except for Zr_2CrPb and Zr_2CrSn, the Zr_2CrPb presents the metallic nature with a ferrimagnetic ground state, while for the Zr_2CrSn, it shows a

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