Regular vs. Inverted structure in Heusler alloys, Burch rule and its applicatibility.

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Many Heusler compounds were considered for spintronic applications, due to possibility of Half Metallic Ferromagnet (HMF) or Spin Gapless Semiconductor (SGS) state. Heusler compounds can crystallize in regular $Fm\bar{3}m$ or inverted structure $F\bar{4}3m$, only in the latter, the mentioned HMF or SGS states are usually possible. Burch rule states that for Heusler X_2YZ compound, the inverted structure is preferred when Y element has higher atomic number than element X. Here, we present effect of high-throughput calculations for $3d$ Heusler compounds, and compare it with the experimental data.