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Novel Occurences of $L1_1$ and $L1_3$ found using the synnergy between High Throughput and Cluster Expansion LANCE NELSON, GUS HART, Brigham Young University, STEFANO CURTAROLO, Duke University — Despite their geometric simplicity, $L1_1$(CuPt) and $L1_3$ ($CdPt_3$) fail to appear as groundstates in experimental systems. ($L1_1$ appears in CuPt only) Are these crystal structures actually energetically unfavorable, or have they simply been overlooked in experimental studies? Here we investigate, using computational methods, the energetic stability of these phases in all binary inter-metallic systems. We combine the results of two techniques,namely High Throughput (HT) and Cluster Expansion (CE), to maximize efficiency and ensure thoroughness. HT results show $L1_1$($L1_3$) to be stable in the following systems: AgPd, AgPt, CuPt, PdPt(CdPt,CuPt,PdPt,LiPd,LiPt). Cluster expansions constructed for these systems verify the HT findings in all cases, with the exception of the HT groundstate PdPt-$L1_1$.(D_4 is found to be energetically more favorable) Monte Carlo simulations, which are used to identify order-disorder transition temperatures, were performed for all occurences of these two phases. While the transition temperatures for some systems are found to be extremely low, others appear to be physically realizable.

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