

Abstract Submitted
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Groundstates in AgPd using cluster expansion methods¹ LANCE NELSON, Brigham Young Universty, GUS HART, Brigham Young University — Palladium alloys have applications in electronics, catalysis, hydrogen storage, and jewelry. The appearance of ordered phases can improve the materials properties for some applications. We present a study of the Ag-Pd system, which is of current interest in electronics and jewelry. We use a model Hamiltonian to quickly search large sets of derivative superstructures for ground states. The model Hamiltonian allows us to perform Monte Carlo simulations to determine transition temperatures. Previous predictions show two unusual ground states: $L1_1$, which has only been observed in Cu-Pt, and a new structure (never observed in any other system) with a 1:3 stoichiometry (dubbed $L1_3$). We find that $L1_3$ is actually unstable. We also predict the ordering temperature for the $L1_1$ phase.

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Lance Nelson
Brigham Young University

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