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Using Machine Learning to Improve Cluster Expansion Predictions[1] WILEY MORGAN, Brigham Young University, KEVIN FRANCIS, University of West Florida, GUS HART, Brigham Young University — Cluster Expansion is used to predict the energies of different configurations and concentrations of a several elements arranged on a fixed lattice. Applications include ground state searches, modeling the energy of solid solutions, and precipitate formation. For materials with a small lattice mismatch, these predictions are generally reliable. However, when the lattice mismatch becomes large, the cluster expansion method often fails. In a number of ternary cases, we have found that the errors in the predictions appear to be connected to the concentration. Partitioning composition space and constructing a cluster expansion model for each partition allows us to make accurate predictions within most of the partitions. We report on atemtps to use machine learning to predict in the partitions where cluster expansion is inaccurate.

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