A Machine Learning Model for Alloy Design

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Developing fast and accurate methods to promote alloy discovery is of practical interest, especially with the vast composition space offered by multi-principal element alloys (MPEAs). While density-functional-theory (DFT)-based methods have accelerated the design of binary and ternary alloys, they are not amenable for rapidly screening the vast combinatorial space of MPEAs. We develop a machine-learning model for predicting the DFT-calculated formation enthalpy of alloys and use it to identify stable alloys. The model uses easily accessible elemental properties as descriptors and has a mean absolute error (MAE) of ∼ 6 meV/atom when compared to the formation enthalpy of binary alloys obtained using DFT. We use the ML model to successfully identify new binary alloys that are subsequently confirmed using DFT and experiments. We further apply it to MPEAs to predict the formation of single-phase solid solutions with bcc and fcc structures.