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How to Predict What to Measure[1] BRAYDEN BEKKER, HAYDEN OLIVER, TYLER WHITAKER, GUS HART, Brigham Young University — Experimentally produced alloys, with useful properties for applications, are often composed of many elements. Computational efforts to study many element systems are inhibited by the vast search space as the number of possible configurations scales dramatically with the number of elements. We present a machine learning approach which allows us to identify a set of configurations in the CoNbV system for training of our model and predicting configurations of interest among the rest of the space. We present the process, for training the potential and identifying structures of interest. We show how the identified ternary configurations can then be extended to higher element models to guide the search for what to measure in the many element systems of experimental interest.

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