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Hands-free thermodynamic alloy modeling of ∼700 binary alloys using a Bayesian approach: Part I GUS HART, LANCE J. NELSON, Brigham Young University, STEFANO CURTAROLO, Duke University, C. SHANE REESE, Brigham Young University — Bayesian approaches have become useful in recent years as increasing computing power has made them practical. Bayes rule itself is nothing more than a simple statement of conditional probability but can be used to make strong inferences. We discuss the general idea behind Bayes rule and how to use it to build physical models. Using a database of about 150,000 first principle calculations, we are building models for ∼700 binary alloys.

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