Hands-free thermodynamic alloy modeling of ~700 binary alloys using a Bayesian approach: Part II LANCE J. NELSON, Brigham Young University, STEFANO CURTAROLO, Duke University, C. SHANE REESE, GUS L.W. HART, Brigham Young University — In recent years, Bayesian statistics has become more popular as a scientific tool. This is mainly due to advances in computing power, which make the Bayesian formalism tractable. Baye's rule, which is a simple statement of conditional probability, is the foundation for Bayesian statistics. When used in conjunction with sampling algorithms, such as Metropolis-Hastings and Gibbs, Baye's rule provides a powerful framework for characterizing important parameters and for making inference. We demonstrate how the Bayesian framework can be applied to alloy modeling, providing the solution to several typical problem areas in this field. Together with our large database of first-principles data this Bayesian framework helps us quickly and accurately characterize hundreds of binary alloys.

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