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Database Optimization for interatomic potential model PINCHAO ZHANG, DALLAS TRINKLE, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign — We develop a new algorithm for database optimization of interatomic potential models with Bayesian statistics. Conventional classical potential fitting schemes generates a best fit parameter set, but do not show inadequacies of the potential model nor give insight into viability of the fitting database. Our algorithm generates an ensemble of potential fits with Markov Chain Monte Carlo and make predictions based on Bayesian error estimation according to the ensemble. We consider a fitting database to be optimal when the sum of relative errors for all entries of the database is minimized. A specific objective function is proposed and an optimized database of the interatomic potential model can be obtained by modifying the relative importance (weights) of different structures in the database. We test the algorithm with a Lennard-Jones potential fitting of Ti, which shows specific limitations of this simple potential model. We also show that the derivative of the objective function with respect to weight determines whether a structure should be added to or removed from the database.

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