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An efficient method to use *ab-initio* calculations to study substitutional order in nanoparticles GERBRAND CEDER, TIM MUELLER, Massachusetts Institute of Technology — To study systems with substitutional disorder researchers commonly use effective Hamiltonians known as cluster expansions. In a cluster expansion the phase space of a system is coarse-grained over a fixed set of crystal sites and the energy is expressed as a linear combination of interactions between these sites. The coefficients of the linear expansion are typically fit to training data generated using *ab-initio* methods. Low-symmetry systems such as nanoparticles require the determination of a large number of distinct coefficients. A large amount of training data must be generated for such problems, and the cost of calculating the energy of each training structure is high due to the low symmetry of the system. For these reasons it has been impractical to use the cluster expansion to study low-symmetry materials with the same level of accuracy as bulk materials. We address this problem by demonstrating new methods that significantly reduce the prediction error of a cluster expansion for a given training set size. Our approach makes it possible to study atomic ordering in nanoparticles at a fraction of the current computational cost.

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