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Effective Hamiltonians to Describe Octahedral Tilt Instabilities in Halide Perovskites JONATHON BECHTEL, JOHN THOMAS, ANTON VAN DER VEN, Univ of California - Santa Barbara — Configurational cluster expansions, based on discrete occupation variables, have proven invaluable for constructing finite-temperature phase diagrams. Here, we develop a cluster expansion method to include continuous degrees of freedom. In this way we capture the effects of anharmonic interactions and high-temperature dynamic instabilities which are needed to describe structural phase transitions as a function of temperature. As a polynomial parameterization of the quantum mechanical zero Kelvin energy surface, the described effective Hamiltonians link *ab initio* calculations to finite-temperature thermodynamics through Monte Carlo simulations. We present the methodology and apply it in a study of phase transitions in perovskite systems where symmetry breaking occurs through octahedral tilts.

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