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Simulating Strongly Anharmonic and Mechanically Unstable Crystals at Finite Temperature JOHN C. THOMAS, ANTON VAN DER VEN, Materials Department, University of California - Santa Barbara — For a wide range of materials, linear elasticity and quasiharmonic models of lattice dynamics are either inaccurate or unphysical. In particular, these methods predict many high-temperature crystal phases to be dynamically unstable, due to their non-convex free energies at low temperature. Unfortunately, the few theoretical methods that go beyond simple harmonic approximations are still inadequate for rigorous and predictive simulation of most strongly anharmonic materials. We describe a simulation framework that enables accurate first-principles prediction of finite-temperature properties of anharmonic and mechanically unstable crystal phases. This framework relies on basis functions, constructed in terms of lattice deformation and atomic displacements, that are invariant to rigid-body translation and rotation, as well as space-group operations of the ideal crystal. This basis set is used to specify order parameters and parameterize highly accurate crystal Hamiltonians, which can be employed within molecular dynamics or Monte Carlo simulation to predict free energies, structural phase transitions, and nonlinear elastic properties. We illustrate the relevance of this approach to thermoelectric semiconductors and metal hydrides.

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