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An efficient ab-initio approach for the anharmonic properties of structurally complex ceramics[1] LIANG-FENG HUANG, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Northwestern University — In the conventional quasiharmonic method for the simulation of crystal anharmonic properties (e.g., thermal expansion and thermomechanics), the phonon spectra of about ten (or more) volumes have to be calculated, which is often computationally prohibitive for complex ceramics with large unit cells. In this work, we describe an efficient alternative method, i.e., a self-consistent quasiharmonic approximation (SC-QHA) method, where the phonon modes of only two or three volumes are necessary. At the same time, it provides a convenient framework to analyze the microscopic origins underlying the anharmonic properties. We successfully apply the SC-QHA method to the hybrid improper ferroelectric Ca3Ti2O7 to explain the recent experimentally measured thermal expansion data [Senn, Phys. Rev. Lett., 114, 0(2015)], and related lattice dynamical properties in an efficient manner.

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