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Interatomic force constants and effective Hamiltonians for structural phase transitions ANIL KUMAR, KARIN M. RABE, Rutgers University — Expansion of the total energy of a crystal around a high-symmetry reference structure provides information about material properties including the phonon dispersion, responses to applied fields, magnetostructural coupling, and structural transitions. For complex oxides, parameterization of the structural energetics by real-space interatomic force constants (IFCs) provides a computationally convenient and physically transparent way of analyzing these properties. By projection into a subspace containing the relevant degrees of freedom, one can construct an effective Hamiltonian to study properties that are not readily accessible with DFT based calculations, including properties at finite temperature or long length scales. It is well known that first-principles density-functional-theory (DFT) based-calculations can be systematically used to determine real-space IFCs of materials; this is part of several first-principles packages including ABINIT and Quantum Espresso. Here, we discuss a simple and efficient approach for construction of first-principles effective Hamiltonians which uses this computational capability to generate and compute the quadratic inter-cell parameters in a single step. We illustrate the method through the application to systems for which effective Hamiltonians have previously been constructed, and show how this approach facilitates the construction of effective Hamiltonians for new classes of crystal structures.

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