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Density Functional Perturbation Theory Parameter Convergence for Phonons RYAN GLUSIC, WILLIAM PARKER, University of Wisconsin - Parkside — Phonons determine material properties such as thermal and electrical conductivity. Allowed modes are solutions to the characteristic equation for the dynamical matrix. One method for constructing the dynamical matrix is density functional perturbation theory (DFPT) in which potential perturbation by atomic displacements is calculated for all unique combinations. The resulting energy second derivatives constitute the dynamical matrix. DFPT contains many parameters, each of which requires convergence to within acceptable numerical error. Using several electronically distinct solid-state structures as test cases, we investigate varying these parameters and the resulting phonon frequencies in terms of their relative and absolute error from a highly converged value. We use also compare the effect of the uncontrolled approximations of DFPT for electronic structure calculations (exchange-correlation functional and pseudopotential) against experimental frequencies. We aim to provide advice on choosing parameters to minimize computation time while producing accurate results in DFPT calculations.

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