

DFPT: Extending the first-order PAW Hamiltonian to GGA+SOC

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The formalism used to generalize calculations of full phonon spectra will be derived in the case of the Generalized Gradient Approximation (GGA) with spinorial wave functions (spin-orbit coupling). This is done in the Density Functional Perturbation Theory (DFPT) formalism within the PAW approach. The main difficulty of the implementation is to correctly take into account the imaginary parts resulting from the phase and from the coupling, as well as to apply the symmetries.

A focus will be made on the on-site exchange and correlation potential implemented as a Taylor development around the spherical contribution to the density.