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Phonons in strongly correlated materials from Hubbard-corrected density-functional-perturbation theory ANDREA FLORIS, Institut für Theoretische Physik, Freie Universität Berlin, Germany and European Theoretical Spectroscopy Facility (ETSF), MATTEO COCOCCIONI, Chemical Engineering and Materials Science Department, University of Minnesota, Minneapolis, MN 55455, USA, E.K.U. GROSS, Institut für Theoretische Physik, Freie Universität Berlin, Germany and European Theoretical Spectroscopy Facility (ETSF), STEFANO DE GIRONCOLI, Scuola Internazionale Superiore di Studi Avanzati (SISSA) and INFM DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy — In this contribution, density functional perturbation theory is generalized to the DFT+U approach. The goal is to compute the vibrational frequencies of strongly correlated systems whose ground-state electronic properties are well reproduced within the DFT+U method. The formalism, extended to both norm-conserving and Vanderbilt ultrasoft pseudo-potentials, allows us to compute phonon frequencies with a computational cost that is independent of the q-vector, thus permitting an efficient exploration of the entire Brillouin zone. The correction to the perturbed self-consistent potential and to the dynamical matrix due to the inclusion of the Hubbard U term, as well as the main features of their implementation will be discussed along with several applications.

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