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First-Principle Perturbative Computation of Phonon Properties of Insulators in Finite Electric Fields XINJIE WANG, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA — The methods of density-functional perturbation theory have been shown to provide a powerful tool for realistic calculations of lattice-vibrational, dielectric, elastic, and other response properties of crystals.[1] Recently, a total-energy method for insulators in nonzero electric fields was proposed.[2] However, the perturbative computation of phonon properties under a dc bias field has not previously been addressed. Here, we start from a variational total-energy functional with a field coupling term that represents the effect of the electric field on the crystal. The linear response of the field-polarized Bloch functions is obtained by minimizing the second-order derivative of the total-energy functional. Due to the presence of the electric field, the field-polarized Bloch functions at each k-point in the Brillouin zone are weakly coupled to those at the neighboring k-points. We implement the method in the `ABINIT` code and perform illustrative calculations of the phonon frequencies for III-V semicondutors.

[1]S. Baroni *et al.*, Rev. Mod. Phys. **73**, 515 (2001).
[2]I. Souza, J. Íñiguez, and D. Vanderbilt, Phys. Rev. Lett. **89**, 117602 (2002).

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