# First-principles calculation of Born effective charges and dielectric constants in finite electric fields via Berry phase approach

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We propose a linear-response approach to the first-principles computation of Born effective charges and dielectric constants of insulators in finite electric field. The total energy of the system in the presence of static, homogeneous electric fields is represented by an electric enthalpy functional[1]

$$F[u^{(\mathcal{E})}_{n\mathbf{k}}, \mathcal{E}] = E_{ks}[u^{(\mathcal{E})}_{n\mathbf{k}}] - \Omega\mathcal{E}\cdot\mathbf{P}_{\rm mac}[u^{(\mathcal{E})}_{n\mathbf{k}}] \ ,$$

where $E_{ks}$ is the Kohn-Sham energy in the absence of electric fields and $\Omega$ is the unit cell volume. We expand the total-energy functional in terms of atomic displacements and electric fields around the equilibrium position at finite fields. The second-order derivatives of the total energy are variational with respect to the first-order responses of wave functions. We show that the Born effective charges and dielectric constants can be determined from the knowledge of the first-order responses of wave functions. We implement the method in the Abinit code.

[1] I. Souza, J. Íñiguez, and D. Vanderbilt, Phys. Rev. Lett. **89**, 117602 (2002).