

First-principles approach to insulators in finite electric fields

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We will describe a recently proposed [1,2] method for computing the response of an insulator to a finite, static, homogeneous electric field, with particular emphasis on its theoretical underpinnings. The method consists of iteratively minimizing a field-dependent energy functional [3] based on the Berry-phase expression for the macroscopic polarization in terms of Bloch states on a uniform grid of k points [4]. We will show that such an approach is justified because (i) the field-polarized electronic manifold is “insulating-like” and lattice periodic, and (ii) the Berry-phase formula of the polarization remains valid in situations in which an homogeneous electric field is applied. The latter assertion will be derived from a more general result, namely, that the Berry-phase expression of the polarization, originally obtained assuming adiabaticity, remains valid under nonadiabatic conditions. That allows us to extend our computational method to dynamical situations in which electric fields of arbitrary time dependence (and strength) are present [5].

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