

Mapping of energy versus polarization in ferroelectric materials

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We present a method for finding the most stable structural configuration of an insulating crystal when its electric polarization is constrained to take on a given value.¹ Our method builds upon an earlier approach² that makes the approximation of including only the lattice response to applied electric fields. By using the recently developed theory of finite electric fields³ to include also the electronic response of the system, we have developed a new approach that is, instead, exact. We illustrate the method by obtaining energy-versus-polarization curves for different kinds of insulating materials, and we show that the method is capable of describing the complexity of the nonlinear structural and dielectric response. In particular, we study the structural behavior of a ferroelectric phase of potassium nitrate under polarization reversal, describing an unusual mechanism in which the reversal is accompanied by a rotation of the NO_3 unit by 60° . We also sketch how our method can be applied in the context of a theory developed to understand the effects of the electrostatic boundary conditions in perovskite superlattices.⁴

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