First-principles simulations at constant electric polarization

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We develop a formalism to perform first-principles calculations for insulators at fixed electric polarization. As shown by Sai, Rabe, and Vanderbilt (SRV),[1] such an approach allows one to map out the energy landscape as a function of polarization, providing a powerful tool for the theoretical investigation of polar materials. While the SRV method is only approximate because the effect of electric fields is described using low-order Taylor expansions, our method is exact because we use the finite-fields approach of Souza, Íñiguez, and Vanderbilt.[2] We apply our method both to systems where the ionic contribution to the polarization dominates, and to systems where this is not the case. We show that the SRV method gives rather accurate results in the former case as expected, while the present exact method provides substantial improvements in the latter case.

[1] N. Sai, K.M. Rabe, and D. Vanderbilt, Phys. Rev. B **66**, 104108 (2002).

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