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A first-principles study of enhancement of polarization with electric field in tetragonal $PbTiO_3$ ANINDYA ROY, Rutgers University, MASSIMILIANO STENGEL, UCSB, DAVID VANDERBILT, Rutgers University — We present first-principles calculations of the electric polarization and c/a ratio of ferroelectric tetragonal $PbTiO_3$ as an external electric field is applied parallel to the polarization direction. The work is motivated in part by experimental observations[1] showing an anomalous enhancement (i.e., nonlinear piezoelectric response) in the c/a ratio for electric fields above $\sim$200 MV/m in $PbZr_{0.2}Ti_{0.8}O_3$. Working here with pure $PbTiO_3$ for reasons of computational convenience, we calculate the strain response to an electric field applied parallel to the spontaneous polarization. We focus mainly on the case of fixed in-plane lattice constants, which appear most suited to the experimental conditions, but we also study the case in which all lattice constants are relaxed. In addition explore the effects of artificial negative pressure, with and without the in-plane epitaxial constraint. Two ab-initio computer codes are used for this purpose, and the results are compared to each other and to the experiment.

[1]A. Grigoviev *et al.*, Phys. Rev. Lett. **100**, 027604, (2008).

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