

Abstract Submitted
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Strain-induced isosymmetric phase transition in multiferroic BiFeO₃ ALISON HATT, NICOLA SPALDIN, UC Santa Barbara, CLAUDE EDERER, Trinity College Dublin — We examine the effect of large epitaxial strain on multiferroic bismuth ferrite, BiFeO₃, using density functional calculations. We investigate a previously unidentified phase transition induced by experimentally accessible values of compressive strain. The transition occurs between phases that are isosymmetric yet have dramatically different structures and properties, the most notable of which is a strong enhancement and rotation of the electric polarization. This presents the opportunity to shift the transition boundary with an applied electric field, similar to a morphotropic phase boundary. Our work contributes to the limited body of knowledge about isosymmetric transitions and explains recent experimental reports of morphotropic phase boundary-like behavior in highly strained films of BiFeO₃ (Zeches *et al.*, to appear Science (2009)).

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