

Abstract Submitted
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First-principles investigation
of phase-change effects in multiferroics¹ OSWALDO DIÉGUEZ, OTTO E.
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Campus de la UAB, 08193 Bellaterra — Using first-principles calculations we have
characterized new phases of bulk multiferroic materials that are close in energy to
the ground state, but that display very different properties. This suggests that the
application of electric fields could induce phase changes that would involve large ef-
fects of different kinds. In particular, (i) we have found stable supertetragonal bulk
phases for the prototype multiferroic bismuth ferrite [Diéguez *et al.*, Phys. Rev. B
83, 094105 (2011)], and (ii) we propose to use a solid solution of bismuth ferrite
and bismuth cobaltite to create a material where it is possible to switch between
two very different phases in a way that involves strong piezoelectric, electric, and
magnetoelectric effects [Diéguez and Íñiguez, Phys. Rev. Lett. **107**, 057601 (2011)].

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