Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles study of magnetoelecric coupling in $TbMnO_3$ ANDREI MALASHEVICH, DAVID VANDERBILT, Rutgers University — At room temperature, the perovskite $TbMnO_3$ forms an orthorhombically distorted lattice with the *Pbnm* space group. Below ∼27 K the magnetic moments on the Mn atoms develop incommensurate cycloidal order, and simultaneously a polarization appears. We present a first-principles study of this low-temperature phase in which the ordering of the Mn^{3+} moments is forced to be commensurate in a 60-atom supercell, approximating the experimental wavevector. The calculations are based on a non-collinear spin treatment of density-functional theory in the local-density approximation, with the polarization computed using the Berry-phase technique. We confirm that the electric polarization appears only when the spin-orbit coupling is turned on. Both electronic and lattice-mediated contributions to the polarization appear, the latter being dominant. We make a normal-mode analysis of the lattice contribution and discuss the ability of a model based on local Dzyaloshinskii-Moriya interactions to reproduce the computed pattern of forces.

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Date submitted: 20 Nov 2007 Electronic form version 1.4