

Abstract for an Invited Paper
for the MAR09 Meeting of
The American Physical Society

First-principles Study of Improper Ferroelectricity in TbMnO₃¹

ANDREI MALASHEVICH, Rutgers University

Perovskite TbMnO₃ at room temperature forms an orthorhombically distorted lattice with the $Pbnm$ space group. Below ~ 27 K the magnetic moments on the Mn atoms adopt an incommensurate cycloidal wave order, and simultaneously a polarization appears along the c direction. We present the results of our first-principles theoretical study of the magnetically induced polarization in TbMnO₃ with a *commensurate* cycloidal wave of Mn³⁺ moments with a wave-vector close to the experimental value.² The calculations are based on density-functional theory in the local-density approximation with the on-site Coulomb correction (LDA+U). The polarization is computed using the Berry-phase technique. We show, in particular, that the spin-orbit interaction is essential for the magnetoelectric coupling. We compute both the electronic and the lattice-mediated contributions to the polarization, and find that the latter is strongly dominant. We analyze the spin-orbit induced forces and lattice displacements from both atomic and mode-decomposition viewpoints, and show that a simple model based on nearest Mn-Mn neighbor Dzyaloshinskii-Moriya interactions is not able to account fully for the results. The direction and magnitude of our computed polarization are in good agreement with experiment. If time permits, calculations on other magnetically induced improper ferroelectrics will be discussed.

¹Work supported by NSF grant DMR-0549198

²A. Malashevich and D. Vanderbilt, Phys. Rev. Lett. **101**, 037210 (2008).