Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-Principles Calculation of the Bulk Photovoltaic Effect in Bismuth Ferrite STEVE YOUNG, FAN ZHENG, ANDREW RAPPE, Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Bismuth ferrite is a multiferroic material with a large bulk polarization and a band gap in the visible spectrum. Significant anomalous photovoltaic effects have been observed in the material; however, the origins of this effect are unclear. While some investigations indicate that observed photovoltages and photocurrents are due to the bulk photovoltaic effect, in striped polydomain samples there is no evidence of this, and the observed response is attributed to a domain-wall-driven mechanism. We have computed the bulk photovoltaic response from first principles using shift current theory and compared it to the available experimental data, finding good agreement. By accounting for the geometry of the polydomain samples, we are able to explain the lack of observed bulk photovoltaic response. Furthermore, we show that these two mechanisms act antagonistically, suggesting that enhanced efficiency may be found in materials where these two effects interact cooperatively.

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Date submitted: 28 Nov 2012 Electronic form version 1.4