Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Multiferroic Aurivillius Phases: the Case of $Bi_5FeTi_3O_{15}$ by *Ab Initio* YAEL BIRENBAUM, CLAUDE EDERER, Materials Theory, ETH Zurich, Switzerland — The Aurivillius phases form a family of naturally layered-perovskites materials with good ferroelectric properties. $Bi_5FeTi_3O_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. However, due to the low concentration of magnetic cations in similar systems, it is unclear how long-range multiferroic behaviour can be achieved. For example, room temperature ferromagnetism has been reported for $Bi_5Co_{0.5}Fe_{0.5}Ti_3O_{15}$, in contrast with no magnetic order found in $Bi_5CrTi_3O_{15}$. To address this question, we establish the ferroelectric and magnetic properties of BFTO, using *ab initio* electronic structure calculations, comparing two commonly used exchange-correlation functionals: PBE and PBEsol. We then discuss a potential site preference for Fe^{3+} and its impact on the polarisation and magnetic couplings. In addition, a brief comparison with $Bi_5MnTi_3O_{15}$ will be made.

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Date submitted: 12 Nov 2013 Electronic form version 1.4