Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Noncollinear magnetism and single-ion anisotropy in multiferroic perovskites** ERIC BOUSQUET, University of Liège, CARLO WEINGART, NICOLA SPALDIN, ETH Zurich — The link between the crystal distortions of the perovskite structure and the magnetic exchange interaction (J), the single-ion anisotropy (SIA), and the Dzyaloshinsky-Moriya (DM) interaction are investigated by means of density-functional calculations in $AFeO_3$ systems. We explore the effect of the crystal distortions (Antiferrodistortive-AFD and Ferroelectric) as well as the effect of the A-cation chemistry on the 3 magnetic properties, J, SIA and DM. Our analysis shows a never explored but possible switching of the weak ferromagnetism in the *R*3*c* phase of $BiFeO_3$ through the competition of the SIA shapes induced by the AFD and the ferroelectric distortions. We also found that-in spite of the $d^5$ electronic configuration of $Fe^{3+}$, the SIA is very large in some structures and is surprisingly strongly sensitive to the chemistry of the A-site cation of the $ABO_3$ perovskite. To clarify the origin of this unexpected effect, we analyze the crystal field splitting by means of Wannier functions.

Eric Bousquet
University of Liege

Date submitted: 04 Dec 2012 Electronic form version 1.4