Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Understanding the spin-driven polarizations in BiMO$_3$ (M =3d transition metals) multiferroics.[1] SANTOSH KC, JUN HEE LEE, VALENTINO R. COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Bismuth ferrite ($BiFeO_3$), a promising multiferroic, stabilizes in a perovskite type rhombohedral crystal structure (space group R3c) at room temperature. Recently, it has been reported that in its ground state it possess a huge spin-driven polarization [1]. To probe the underlying mechanism of this large spin-phonon response, we examine these couplings within other Bi based 3d transition metal oxides BiMO$_3$ (M = Ti, V, Cr, Mn, Fe, Co, Ni) using density functional theory. Our results demonstrate that this large spin-driven polarization is a consequence of symmetry breaking due to competition between ferroelectric distortions and anti-ferrodistortive octahedral rotations. Furthermore, we find a strong dependence of these enhanced spin-driven polarizations on the crystal structure; with the rhombohedral phase having the largest spin-induced atomic distortions along [111]. These results give us significant insights into the magneto-electric coupling in these materials which is essential to the magnetic and electric field control of electric polarization and magnetization in multiferroic based devices. [1] J. H. Lee, and R. S. Fishman, http://arxiv.org/abs/1504.07106

[1]Research is supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and the Office of Science Early Career Research Program (V.R.C) and used computational resources at NERSC.

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Date submitted: 05 Nov 2015 Electronic form version 1.4