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A first principles investigation of a hexagonal ferrite $LuFeO_3$ HENA DAS, Postdoctoral Research Associate, CRAIG J. FENNIE, Assistant Professor — The multiferroic hexagonal manganites $RMnO_3$ (R=Dy-Lu,Y), are a fascinating class of materials that display an unusual, complex interplay between structural, polar and magnetic domains. For example, the electric polarization in these compounds are found to be a by-product of a trimerized (zone-boundary) lattice distortion, arising from the ionic size mismatch between R^{+3} and Mn^{+3} ions. As a direct consequence of this improper ferroelectric transition, the ferroelectric and structural trimer domains are locked; rotation of structural distortion at a structural domain not only flips the polarization, but also rotates the spins. The hexagonal ferrites $RFeO_3$ (R=Lu,Er-Tb) crystallize in the same polar structure as the manganite counterparts. However, unlike the $\mathbf{M}$=0, non-collinear antiferromagnetism in manganites, the ferrites have recently been shown to display week ferromagnetic behaviour[1], the underlying microscopic mechanism of which so far is not understood. In the present study, using first principles density functional calculations, we investigate the structural and magnetic properties of $LuFeO_3$, one of the members of this ferrite series.

[1] A. R. Akbashev, A. S. Semisalova, N. S. Perov and A. R. Kaul, Appl. Phys. Lett **99**, 122502 (2011).

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