Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Distortions in charge-ordered $LuFe_2O_4$ TAKESHI NISHIMATSU, DAVID VANDERBILT, KARIN M. RABE, YOICHI HORIBE, SANG-WOOK CHEONG, Rutgers University, CLAUDE EDERER, Columbia University — Experimental evidence[1] suggests that $LuFe_2O_4$ develops ferroelectricity via a novel charge-ordering mechanism in which the Fe sites (of average valence 2.5) disproportionate into Fe^{2+} and Fe^{3+} sublattices in such a way as to break inversion symmetry. However, the precise nature of the charge and magnetic order, and the structural distortions that accompany them, remain poorly understood. With this motivation, we have undertaken a first-principles study of $LuFe_2O_4$ using DFT-based methods (especially LDA+U). We search for the ground state consistent with a variety of supercell choices and symmetry constraints, and thereby investigate whether the system is unstable to several possible charge and spin orderings. Despite the limitations of a DFT-based approach, it is argued that the results provide useful guidance in the quest to develop an understanding of the novel form of ferroelectricity displayed by this material.

[1]Nature **436**, 1136 (2005)

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Date submitted: 04 Jan 2007 Electronic form version 1.4