Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First Principles Studies of Electronic structure and Lattice Dynamics of Multiferroic $GaFeO_3$ AMRITENDU ROY, Indian Institute of Technology, Kanpur, RAJENDRA PRASAD, SUSHIL AULUCK, ASHISH GARG, ndian Institute of Technology, Kanpur — $GaFeO_3$ (GFO) is a room temperature piezoelectric material with antiferromagnetic ordering in the ground state. However, experimental observation reports ferrimagetic behavior below the magnetic transition temperature, attributed to the site disorder of Fe and Ga sites. This transition occurs at temperatures close to room temperature, depending upon the Fe content of the material. Previous structural characterization studies indicate that the room temperature crystal structure ($Pc2_1n$) is retained at least until 4 K. While there are a few experimental studies on this compound, there is no well established understanding of its electronic structure and lattice dynamics which can give insight into the piezoelectric and magnetic properties of the material. From this perspective, we started our calculations with the experimental lattice parameters of stoichiometric GFO assuming no partial occupancies of the constituent ions. The calculations are carried out using local spin density approximation (LSDA+U). Electronic structure and Born effective charges were calculated based on the ground state structure. First principles density functional theory based calculations using small displacement method was adopted to calculate the phonon dispersion relations for the material. On the basis of the dispersion relations modes were assigned.

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Date submitted: 26 Nov 2010 Electronic form version 1.4