Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Effect of Cation Disorder on Electronic Structures and Optical Properties of Magnetoelectric Gallium Ferrite: A First-principles Study AMRITENDU ROY, IIT Kanpur, SUSHIL AULUCK, NPL Delhi, RAJENDRA PRASAD, ASHISH GARG , IIT Kanpur — Discovery of photovoltaic effects in oxide materials, especially in magnetoelectrics and multiferroics has lead to renewed interests in the optical properties of these materials. Magnetoelectrics with their transition temperature close to room temperature are of particular interest from the perspective of practical applications. Magnetoelectric gallium ferrite (GFO), a material of current interest, exhibits good optical activity and a transition temperature tunable to room temperature and above upon tailoring of cation stoichiometry. Here, we show a detailed first principle study on the electronic structure and optical properties of GFO. We have performed first-principles density functional calculations using GGA+U method to compute the electronic band structure and density of states of the ground state structure of GFO having orthorhombic $Pc2_1n$ symmetry and A-type antiferromagnetic spin configuration. The calculations show that GFO possesses a direct band gap of $\sim$ 2.3 eV, making it a rather low band gap oxide. Subsequent calculations of real and imaginary parts of dielectric constants, refractive index (n), extinction coefficient (k), reflectivity (R), etc demonstrate good agreement with experimental spectra which is further improved upon introduction of cationic site disorder into the ground state structure substantiating the presence of cation site disorder in the material. We also show that major optical transitions in GFO involve transitions from valence band O 2p to conduction band Fe 3d states.

Rajendra Prasad
IIT Kanpur

Date submitted: 11 Nov 2011 Electronic form version 1.4