Supplementary Information

Phase engineered gallium ferrite: a promising narrow bandgap, room-temperature ferroelectric

Somdutta Mukherjee[1,†], Monali Mishra[1,2], Palash Swarnakar[3], Shilpa Sanwlani,[4] Sukalyan Das[2], Amritendu Roy[3,†]

[1] Materials Chemistry Department, CSIR-IMMT Bhubaneswar, Bhubaneswar-751013, Orissa, India
[2] Department of Chemistry, VSSUT Burla, Burla-768018, India
[3] School of Minerals, Metallurgical and Materials Engineering, Indian Institute of Technology Bhubaneswar, Jatni-752050, Orissa, India
[4]Department of Physics, Indian Institute of Science, Education and Research Mohali, Punjab, India

*Corresponding Authors: msomdutta@gmail.com; amritendu@iitbbs.ac.in

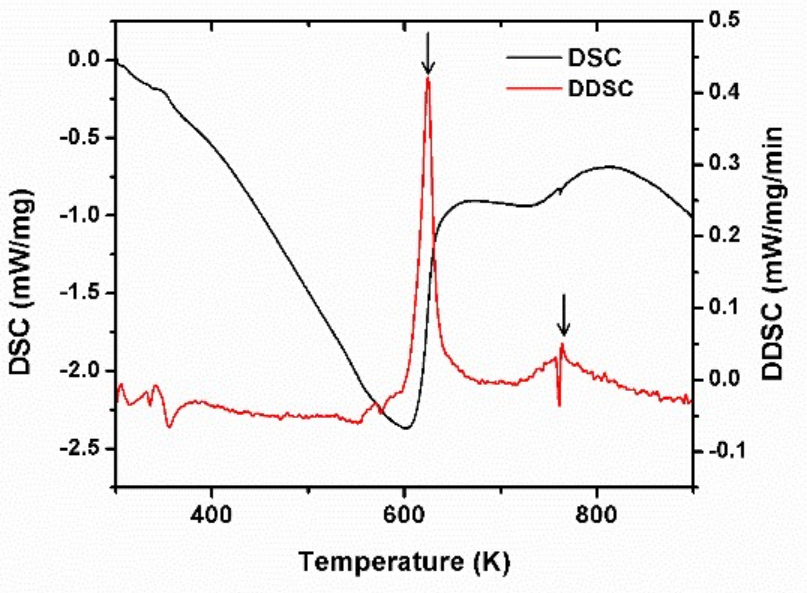

Figure S1: Differential scanning calorimetry of gallium ferrite nanocrystals with $P2_12_12_1$ symmetry produced in our previous study [26]. Presence of a prominent endothermic peak, which is also clear from the differential DSC signal, indicates presence of structural phase transformation across, ~ 620 K.

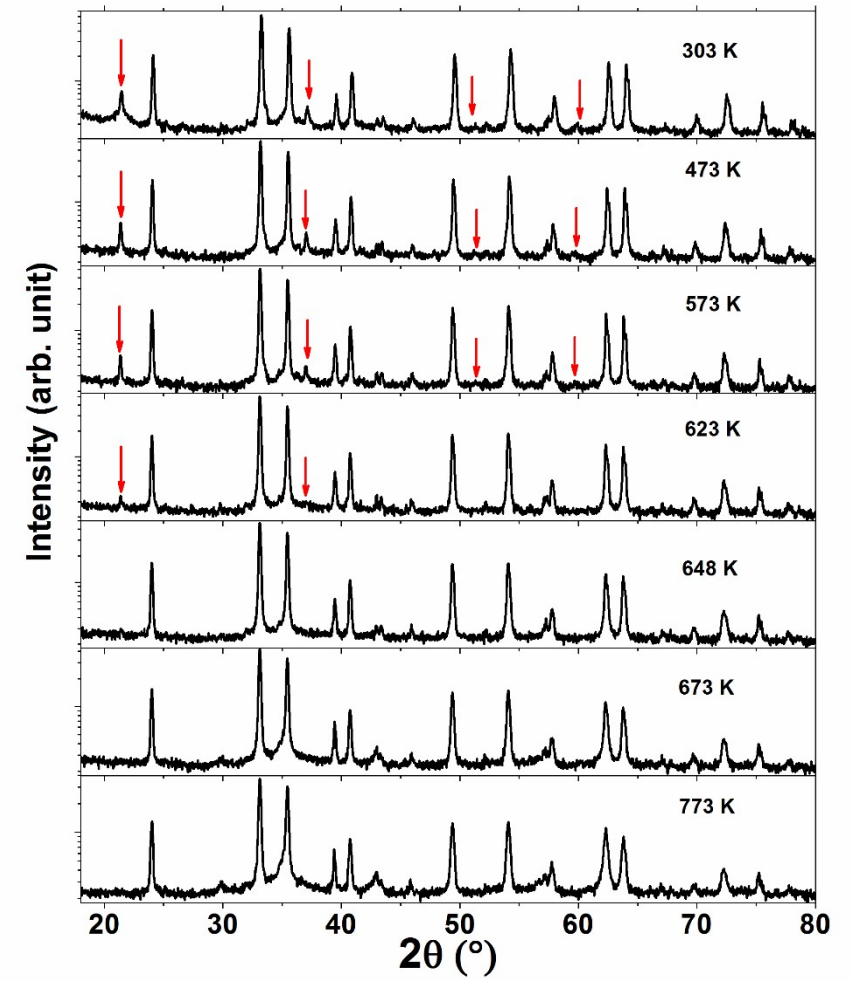

Figure S2: Temperature dependent XRD study of as synthesized GFO nanocrystals with $P2_12_12_1$ symmetry produced in our previous study. [26] With increasing temperature the peaks marked by arrows disappeared beyond 623 K, suggesting symmetry increasing structural phase transition.

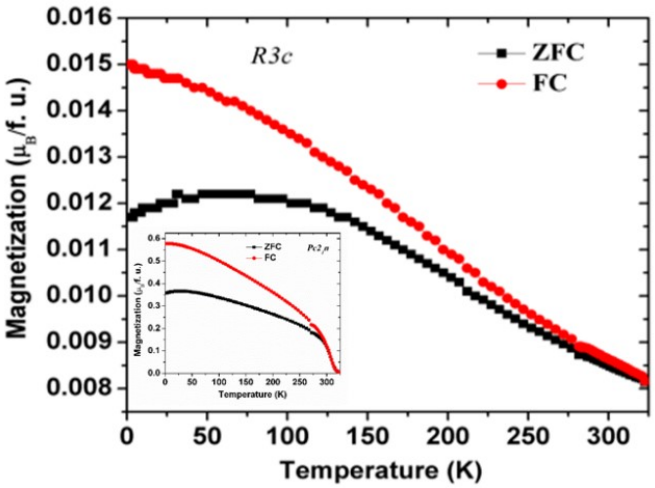

Figure S3: Magnetization plotted as a function of temperature measured on *R3c*-GFO nanocrystals with a probing field of 100 Oe, demonstrating weak magnetic characteristics. Inset shows corresponding magnetization data of sample with bulk symmetry, $Pna2_1$.

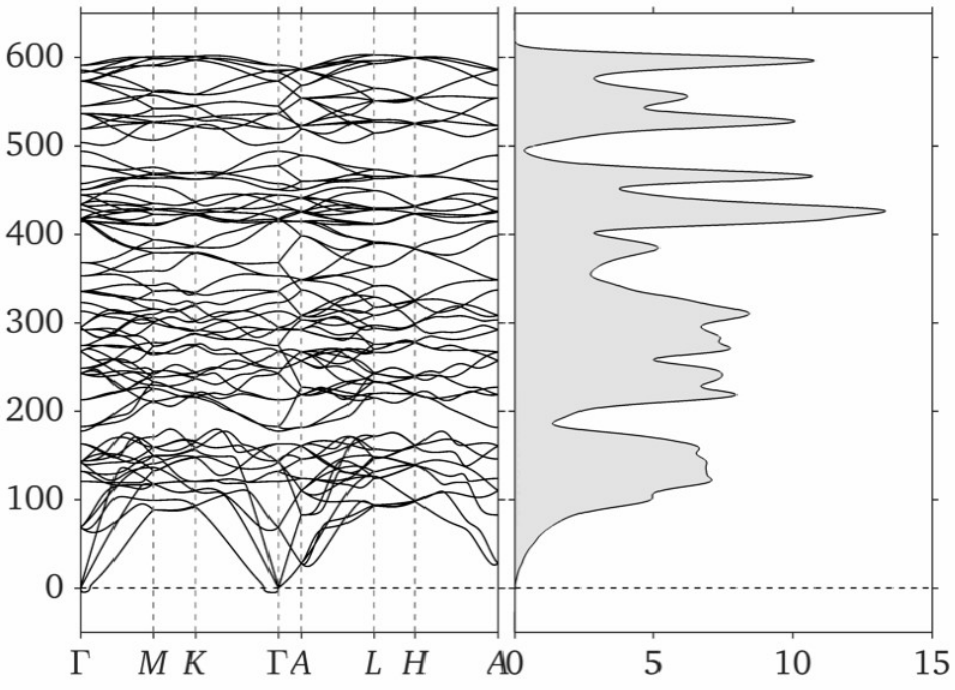

Figure S4: Phonon dispersion curve and phonon density of states of R3c-GFO phase computed using density functional perturbation theory as implemented in Phonopy.[1]

[1] A. Togo and I. Tanaka, Scr. Mater., **2015**, **108**, 1-5.