Electronic Supplementary Information (ESI) for

Influence of Point Defects on the Optical Properties of $La_3Nb_{0.5}Ga_{5.5}O_{14}$ crystals

Jindong Chen [a, *], Hongxu Gu,[b] Shusen Yang [a], Ning Ye [a, *], Kui Wu,[b] Dazhi Lu [b, *]

[a] State Key Laboratory of Crystal Materials, Tianjin Key Laboratory of Functional Crystal Materials, Institute of Functional Crystal, College of Materials Science and Engineering, Tianjin University of Technology, Tianjin 300384, China

[b] State Key Laboratory of Crystal Materials and Institute of Crystal Materials, Shandong University, Jinan250100, China

*E-mail: cjd1225@email.tjut.edu.cn, nye@email.tjut.edu.cn, dazhi.lu@sdu.edu.cn

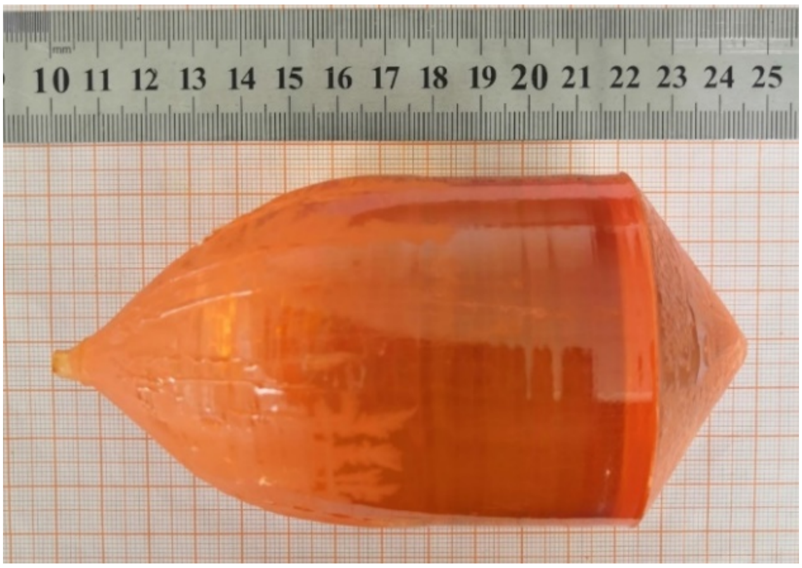

Figure S1. Photograph as-grown LGN single crystal under N_2+ 2%O_2 atmospheres

We used the DFT as implemented in the VienNb Ab initio simulation package (VASP) for defect formation energy calculations. The exchange-correlation potential is described by using the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). The projector augmented-wave (PAW) method is employed to treat interactions between ion cores and valence electrons. The plane-wave cutoff energy was fixed to 400 eV. Given structural models were relaxed until the Hellmann-Feynman forces smaller than -0.01 eV/Å and the change in energy smaller than 10^{-7} eV was attained.

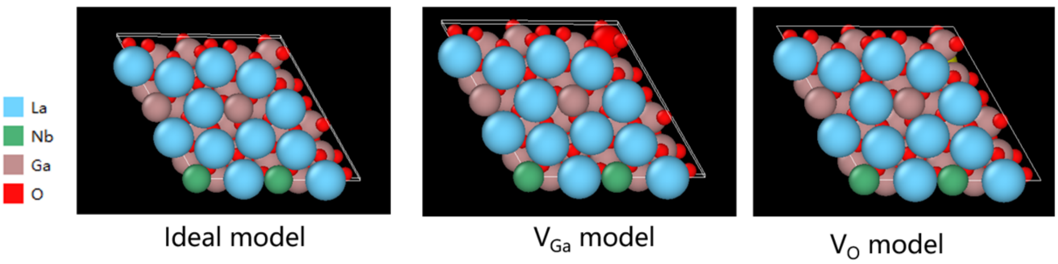

Figure S2. Structure models for defect formation energy calculations.

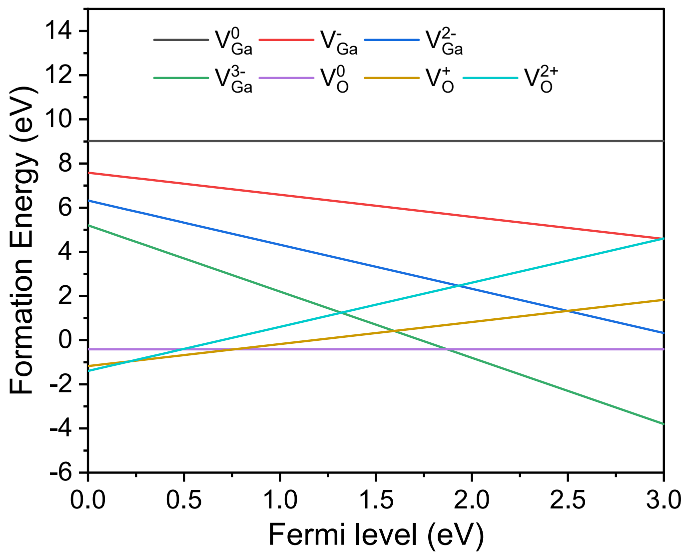

Figure S3. Defect formation energy of oxygen and gallium vacancies