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Supporting Information

Simultaneous tuning of optical and electrical properties in multifunctional $LiNbO_3$ matrix upon doping with Eu^{3+} ion

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1.0. Instrumentation:

All the compounds were characterized with a rotating anode based powder X-ray diffractometer procured from Rigaku, Japan using CuK_α (λ= 1.5406 and 1.5444Å) monochromatic radiation. For FTIR study, a Platinum ATR (by Bruker alpha, Single reflection Diamond crystal, all reflective, gold coated optics, no fragile composite material construction) within the spectral range 5000-500 cm^{-1} was used. Ferroelectric properties were investigated by using aix ACCT's TF analyser 2000. PL study has been carried out using an Edinburgh CD-920 unit equipped with M 300 monochromators and the data acquisition and analysis were carried with the help of F-900 software provided by Edinburgh Analytical Instruments, UK. The lifetime study was carried out based on the well established Time-correlated single-photon counting (TCSPC) technique.

2.0. DFT calculation methodology

Electronic structure calculations of ideal $LiNbO_3$, ferroelectric $LiNbO_3$ structure with oxygen, Li, Nb and antisite defects structures and as well as Eu doping in $LiNbO_3$ (LNO) were performed using a spin-polarized plane wave based density functional theory (DFT) simulations as implemented in Vienna Ab-intio Simulation package (VASP) **[1, 2]**. Projector augmented wave (PAW) potentials **[3]** were used to describe electron-ion interactions which includes the valence states of Li ($2s^2\ 2p^1$ - 3 valence electrons), Nb ($4s^24p^65s^24d^3$ - 13 valence electrons), O ($2s^22p^4$ - 6 valence electrons) and Eu ($5s^2\ 5p^6\ 4f^7\ 6s^2$ - 17 valence electrons). Exchange-correlation potential was described through generalized gradient approximation

(GGA) parameterized by Perdew-Burke-Ernzerhof (PBE) functional **[4]**. A 12x12x4 and 6x6x2 Monkhorst-Pack **[5]** k-space mesh was used for the brillouin zone integration for 30 atom unitcell and 120 atom supercell, respectively. A cutoff energy (E_{cut}) of 500 eV was used for the plane wave basis set throughout the simulation. The optimized E_{cut} and k-point meshes used for the simulations ensure convergence of total energy to within a precision 0.01 meV/atom for ideal and defective unit-cell/supercell. Conjugate gradient algorithm was used to optimized volumes (or lattice parameter) and atomic positions in ideal/defective supercells until the residual forces and stress in the equilibrium geometry were of the order of 0.005 eV/Å and 0.01GPa, respectively. The final calculations of total electronic energy and density of states (DOS) were performed using the tetrahedron method with Blöchl corrections **[6]**.

1. G. Kresse, J. Furthmüller, *Phys. Rev. B*, 1996, 54, 11169.
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3. P.E. Blöchl, *Phys. Rev. B*, 1994, 50, 17953.
4. J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. lett.*, 1996, 77, 3865.
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6. P.E. Blöchl, O. Jepsen, O.K. Andersen, *Physic. Rev. B*, 1994, 49(23), 16223.

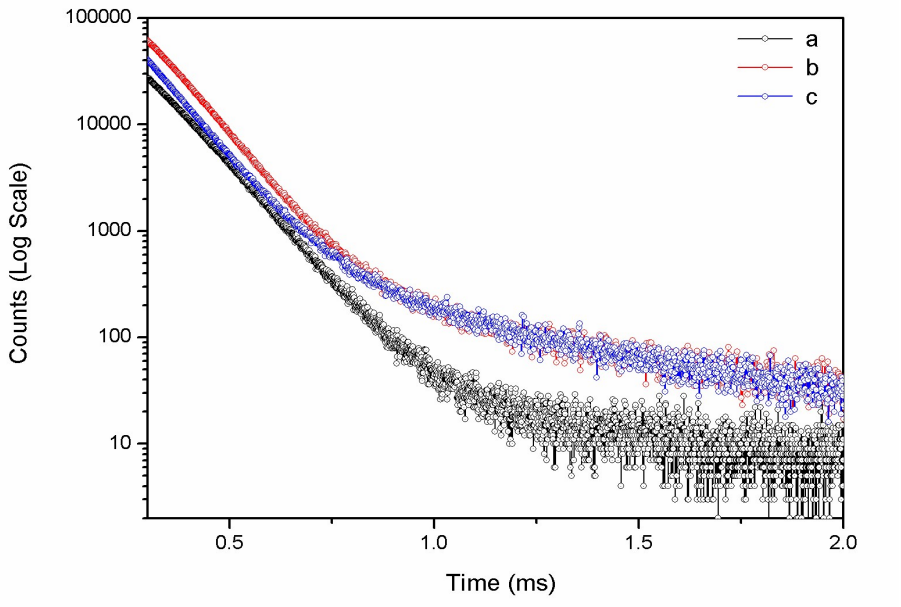

Figure S1: Luminescence decay time profile of undoped LNO: Eu^{3+} at λ_{ex} = 230 nm with (a) λ_{em} = 380 nm , b) λ_{em} = 440 nm and c) λ_{em} = 540 nm

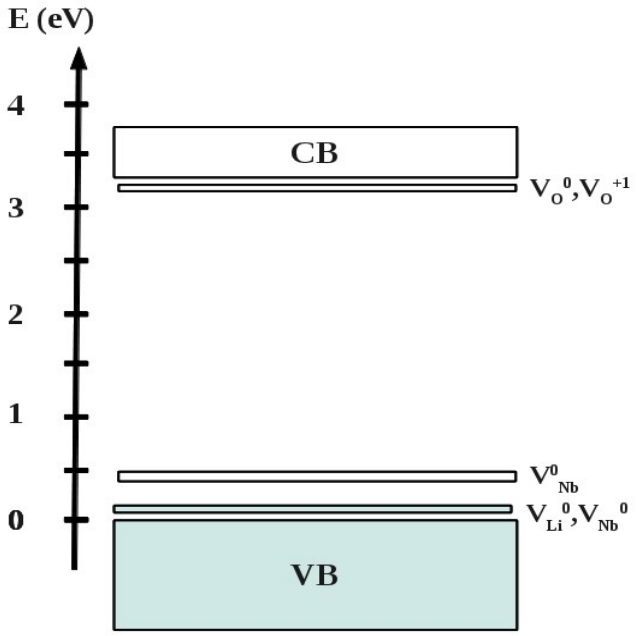

Figure S2. *Defect related impurity states inside the band gap of LNO*