For Supporting Information only

Modulating Light Emission and Electrical Conduction of Oxygen Vacancy Enriched $La_2Ce_2O_7:Sm^{3+}$ Pyrochlore: Role of Dopant Local Structure and Concentration

Santosh K. Gupta,[a,b*] B. Modak[b,c], J. Prakash,[b,d] N.S. Rawat,[b,e] P. Modak,[b,f] K. Sudarshan[a,b*]

[a]*Radiochemistry Division, Bhabha Atomic Research Centre, Mumbai, India–400085*
[b]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, India - 400094*
[c]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai, India–400085*
[d]*Glass and Advanced Materials Division, Bhabha Atomic Research Centre, Mumbai, India–400085*
[e]*Radiological Physics and Advisory Division, Bhabha Atomic Research Centre, Mumbai, India–400085*
[f]*Radiological Safety Division, Atomic Energy Regulatory Board, Anushaktinagar, Mumbai – 400094, India*

***To whom correspondence should be addressed. santoshg@barc.gov.in (SKG)/ kathis@barc.gov.in (KS)**

Information S1:

LCO and LCOS (Sm^{3+}= 1, 5, 7.5 and 10 %) was synthesized using high temperature solid state synthesis method which involved repetitive heating and grinding to get the phase pure product. More details about synthesis can be found out in our recently published work.[1] XRD measurement was carried out on Proto manufacturing (Canada) AXRD benchtop powder diffraction system. TRPLS were carried out using Edinburgh Instruments CD-920 (Scotland) and the data acquisition is done F-900 software. PALS measurements were done with spectrometer having time resolution of 265 ps using Na-22 (positron source) and the data analysis was carried using PALSFit software.[2] Raman analysis was carried out using Raman spectrometer, WITec alpha-300R, GmbH equipped with a 532nm laser and the EIS measurements were performed using an electrochemical work station (CHI 760E, USA). TL readouts were performed at a heating rate of 2^{o}C/s on RISO reader system. The electrochemical impedance spectroscopy measurement was performed in a frequency range of 100 mHz to 100 kHz in an open circuit condition. EC-Lab v11.20 software was used for numerical data fitting to develop equivalent circuits and corresponding circuit parameters.

Vienna ab initio simulation package (VASP) with projector augmented wave (PAW) potential has been used for the Density functional theory (DFT) calculations.[3,4] The set of valence states considered for the pseudo potentials are La (9 electrons:$5p^6$, $5d^1$, $6s^2$), Ce (11 electrons $5s^2$, $5p^6$, $5d^1$, $6s^2$), Sm (11 electrons: $5s^2$, $5p^6$, $5d^1$, $6s^2$), and O ($2s^22p^4$) during geometry optimization. However, during electronic structure calculations for doped systems, we have chosen these

valence states; La (11 electrons: $5s^2$, $5p^6$, $5d^1$, $6s^2$), Ce (12 electrons: $5s^2$, $5p^6$, $5d^1$, $6s^2$, $4f^1$), and Sm (16 electrons $5s^2$, $5p^6$, $5d^1$, $4f^5$, $6s^2$). Exchange correlation functional has been described by generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional. [5,6] Here, we have imposed spin polarized condition throughout the DFT calculations. Total relaxation of ionic positions and cell volume has been considered during the geometry optimization of all the structures. The optimized geometries have been employed for calculations of electronic structure. Energy cut off value of 500 eV and self-consistent energy convergence criteria of 10^{-6} eV have been chosen. For Brillouin zone integration has been carried out by Γ-centered k-point mesh using Monkhorst and Pack scheme.[7] All the figures for structure have been generated using VESTA graphical software package. [8]

Information S2.

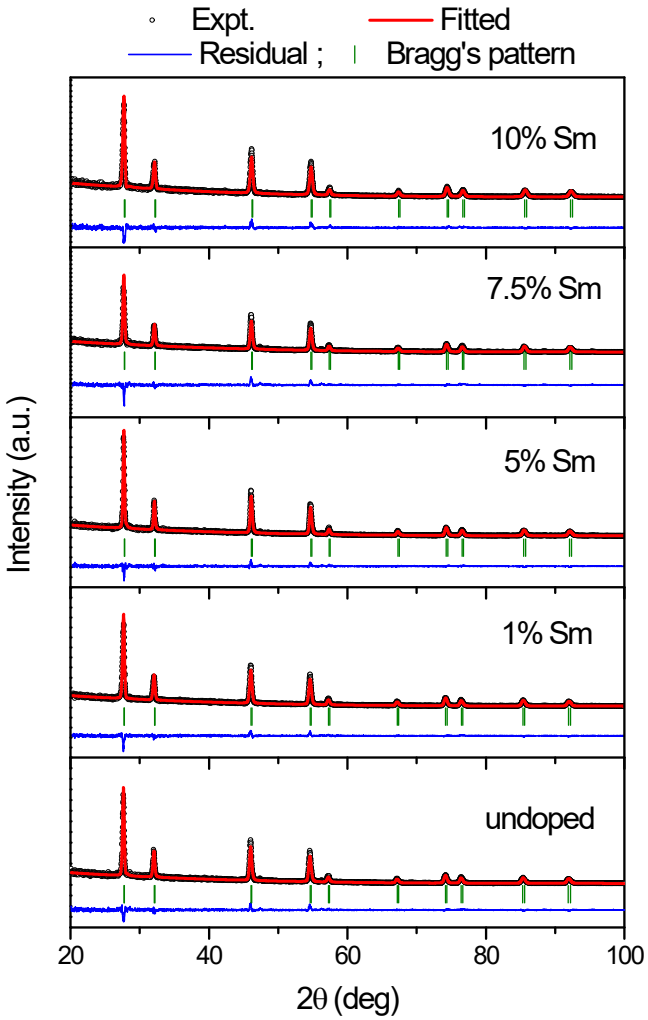

Figure S1: Rietveld refinement of the powder XRD pattern of LCO and LCOS (Sm^{3+}= 1, 5, 7.5 and 10 %)

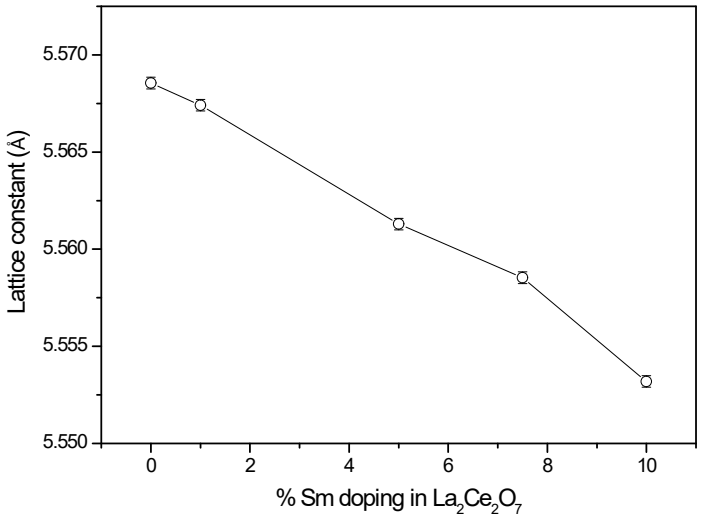

Figure S2: Variation of lattice parameter in LCOS (Sm^{3+}= 0, 1, 5, 7.5 and 10 %)

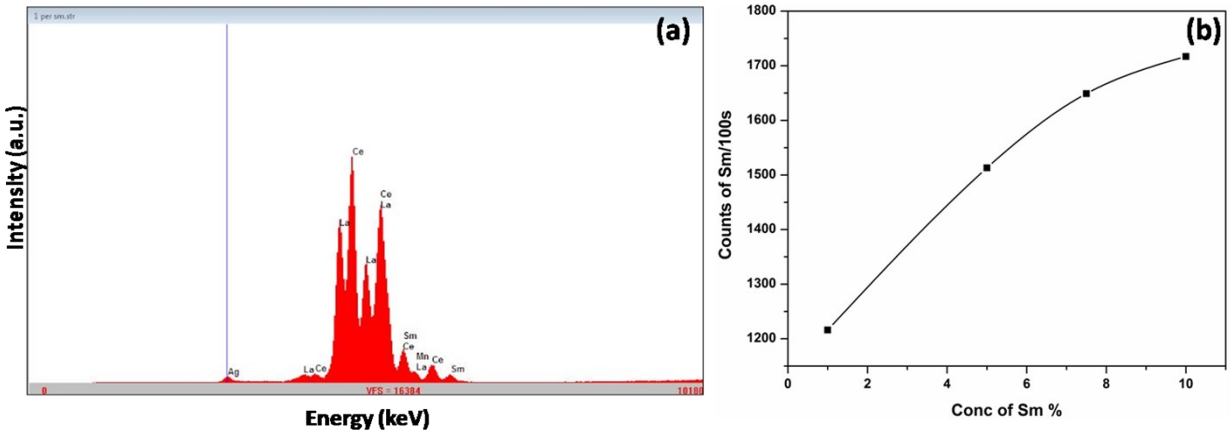

Figure S3: (a) EDXRF spectrum of LCOS (Sm^{3+}= 1.0 mol %) and (b) Sm^{3+} x-ray counts as a function of its concentration

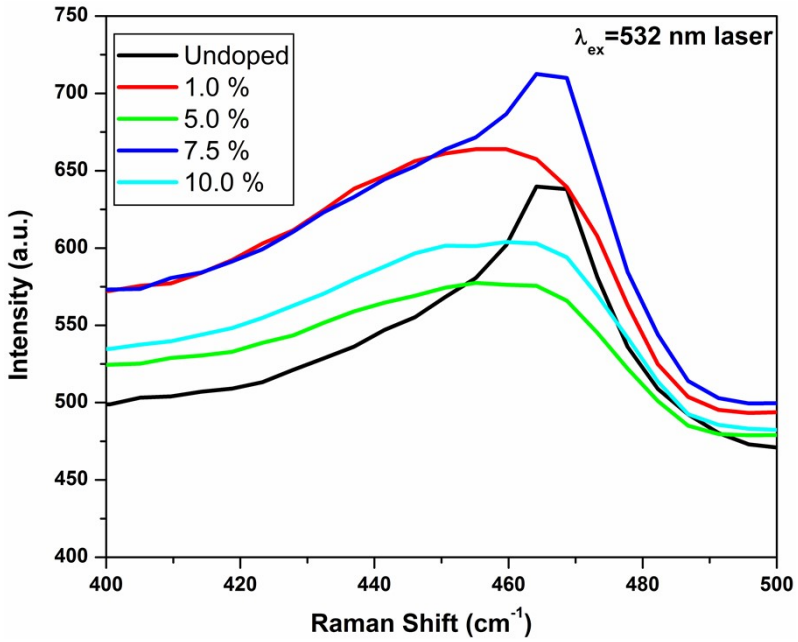

Figure S4: Raman spectra of 400-500 cm^{-1} region of LCO and LCOS pyrochlore

Table S1: Photoluminescence emission lifetime data of LCOS at different doping concentrations

	λ_{ex} = 254 nm and λ_{em} = 616 nm					λ_{ex} = 413 nm and λ_{em} = 616 nm				
Sm^{3+} %	τ_1 (μs)	I_1 (%)	τ_2 (μs)	I_2 (%)	τ_{av} (μs)	τ_1 (μs)	I_1 (%)	τ_2 (μs)	I_2 (%)	τ_{av} (μs)
1%	385 ± 13	48.3 ± 1.8	1563 ± 81	51.7 ± 2.7	993 ± 68	715± 6	100 ± 1			715 ± 6
5%	243 ± 5	44.1± 1.0	894 ± 13	55.8 ± 1.8	606 ± 21	209± 3	35.3± 0.7	741 ± 6	64.7 ± 1	554 ± 12
7.5%	219 ± 3	47.5 ± 0.9	838 ± 10	52.4 ± 1.4	544 ± 16	198± 2	39.1 ± 0.5	685 ± 4	60.9± 0.7	495 ± 7
10%	183 ± 2	46.7 ± 0.8	660 ± 6	53.3 ± 1.0	437 ± 10	168± 2	40.5 ± 0.6	614 ± 3	59.5 ± 0.7	433 ± 6

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