# Effect of Co doping in tuning the band gap of $LaFeO_3$

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## INTRODUCTION

•Band gap engineering has been an important research topic not only in semiconductor but also in perovskite oxides for various purposes such as using in electronic and optical devices, photo-catalysts for water splitting and solar cells.

• Recent studies have shown that the physical properties of $LaFeO_3$ (LFO) can be modified via doping with rare earth, alkali earths, and transition metals.
• Co is one of the transition metals which could produce some perturbation on the physical properties in ferroelectric materials via doping.

• In our present study we aimed to study the crystal structure, surface morphology properties of $LaFe_{1-x}Co_xO_3$ via Co doping with 40, 50 & 60 mol%.
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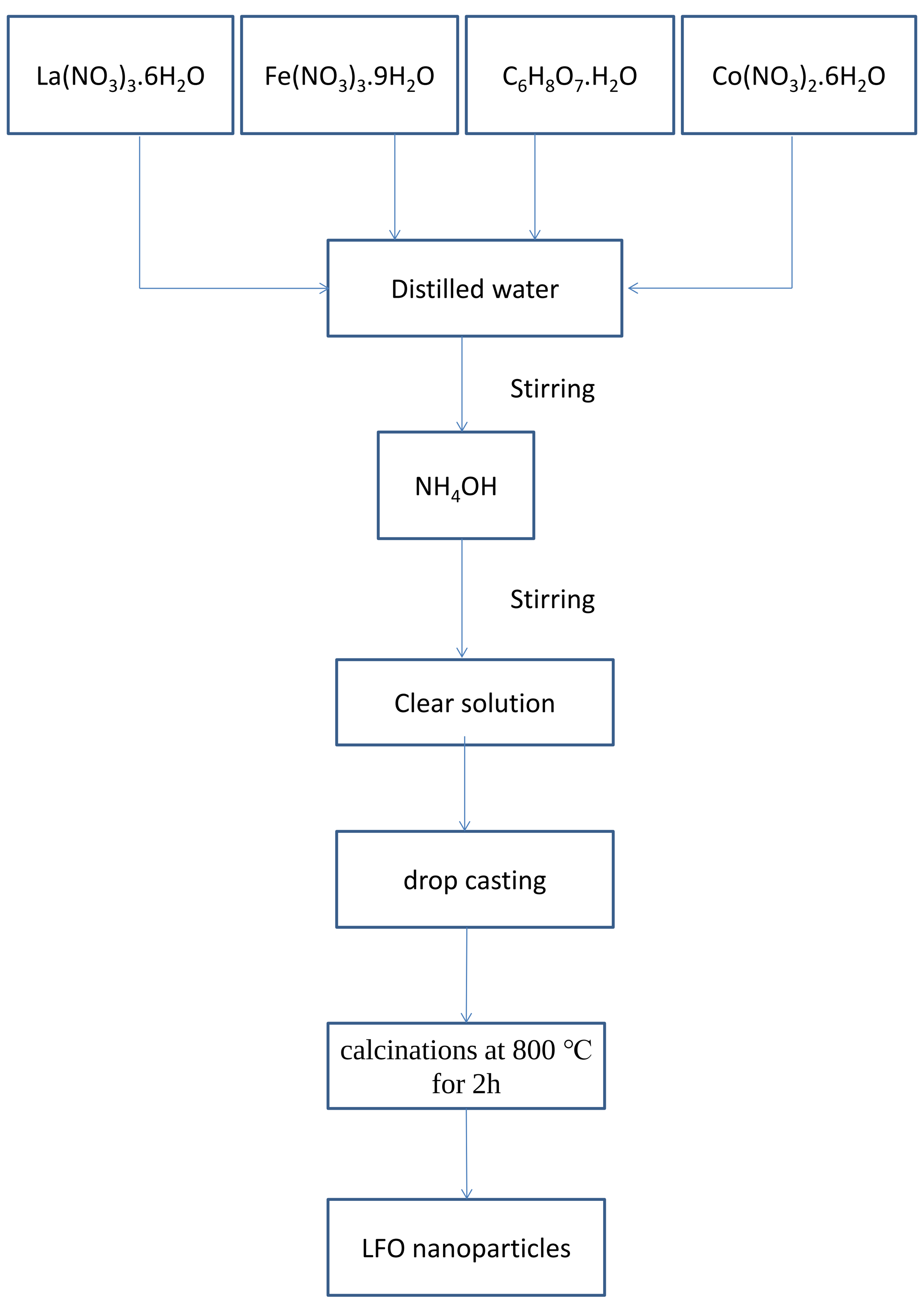
• The sol-gel process is one of the techniques among several reported techniques for preparation of dense nanomaterials with homogeneous texture and uniform morphology.

• In this work we examined the synthesis of LaFeO3 nanocrystals via sol-gel method after calcinations at 800 °C and used for further analysis.

## EXPERIMENTAL METHOD




## RESULTS

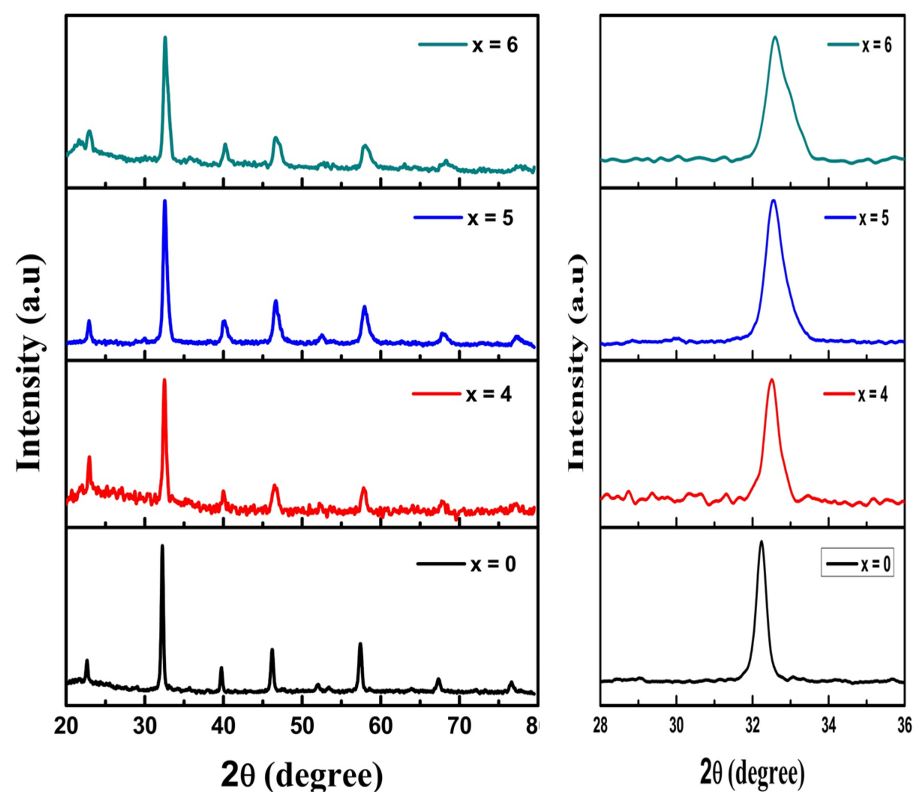



**Fig. 1.** XRD patterns of Co doped LFO films on quartz substrate annealed at 800 °C

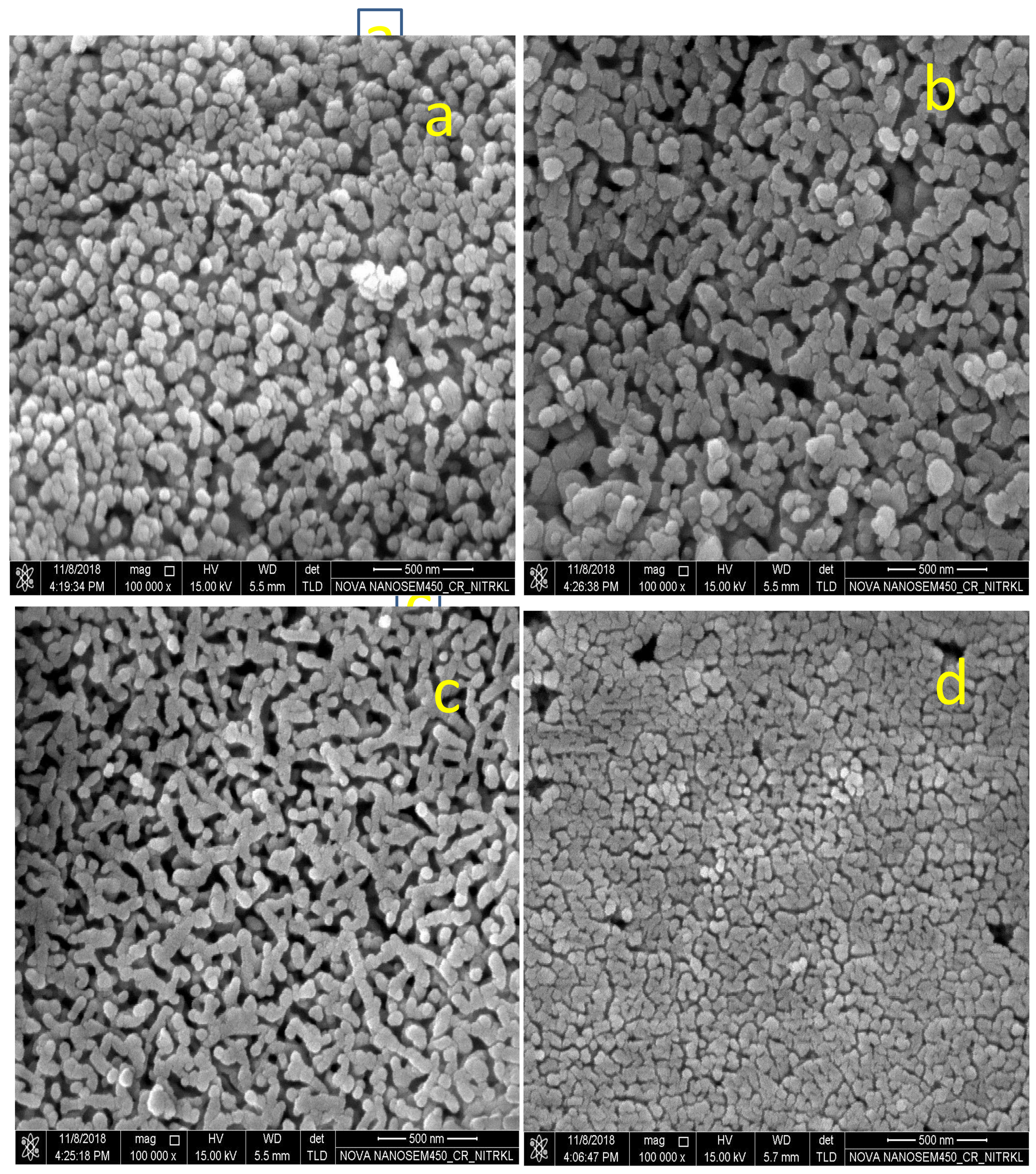



Fig. 2. SEM surface morphologies of (a) $LaFeO_3$, (b) $LaFe_{0.6}Co_{0.4}O_3$, (c) $LaFe_{0.5}Co_{0.5}O_3$ and (d) $LaFe_{0.4}Co_{0.5}O_3$.

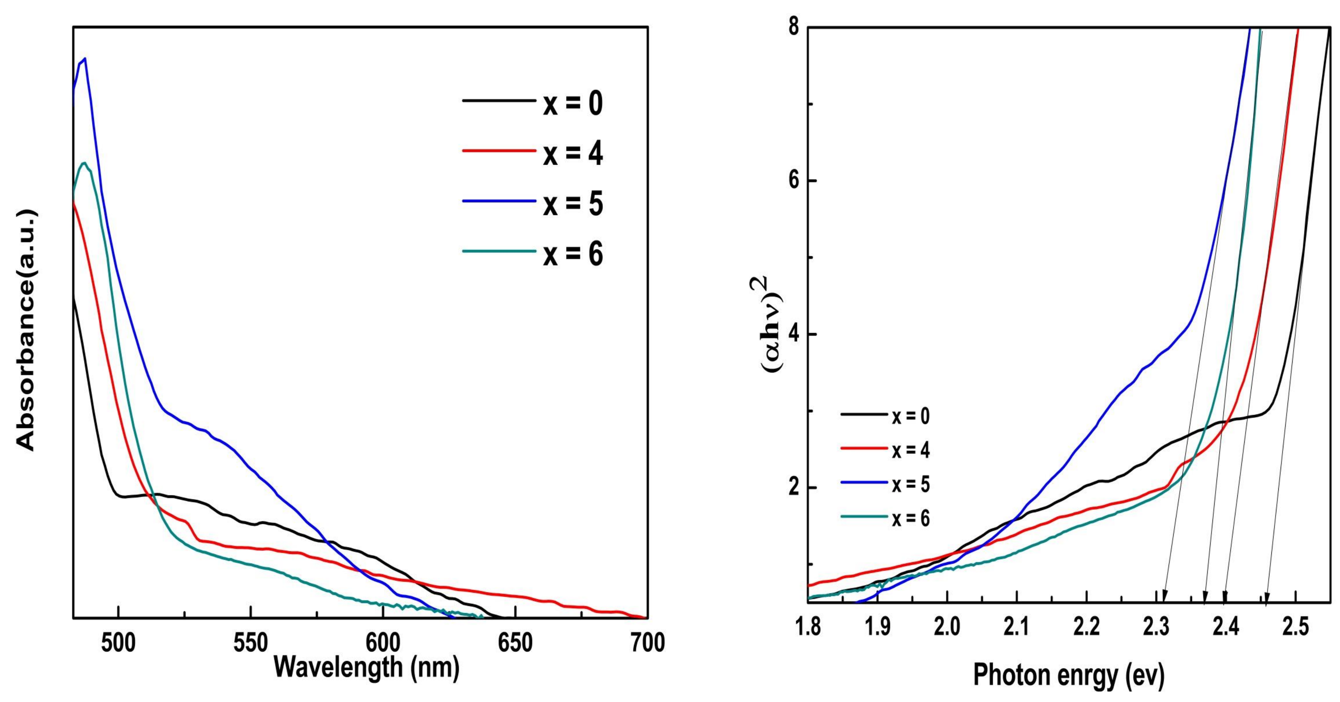



Fig.3 .The characterization of light absorption of pure and Co doped $LaFe_{1-x}Co_xO_3$.

## DISCUSSIONS

•Fig.1 demonstrates the XRD patterns of $LaFe_{1-x}Co_x$ and the prominent diffraction peaks are (002), (200), (202), (004), (312), (400) and (420) located at 2θ equal to 22.7°, 32.6°, 40.03°, 46.7°, 57.33°, 67.06°and 76.5° respectively. The peak shifting is due to the decrease in unit cell parameter of $LaFe_{1-x}Co_x$ with increase in mol% of Co ions since the ionic radius of $Co^{3+}$ ion is less than that of $Fe^{3+}$ ion.

• The surface morphologies of $LaFe_{1-x}Co_x$ nanoparticles can be well recognized from Fig 2 and the grain size ranges from 25nm to 37nm.

•Fig.3 shows the characterization of light absorption of pure and Co doped LFO by UV-Vissible absorption spectrum.

•The band gaps of all synthesized sample were estimated by employing Tauc's equation and found to be 2.44 ev , 2.39, 2.37 and 2.31 ev for $LaFe_{1-x}Co_xO_3$ (x = 0, 0.4, 0.6 & 0.5 )respectively.

•This band gap widening at 10% mol doping might be attributed to two reasons: (i) band gap tailing, which is consequence of the impurity distribution in the material, and (ii) Moss–Burstein effect ,which occurs when the carrier concentration exceeds the conduction band edge density of states.

## CONCLUSIONS

•Combining drop casting and high temperature annealing, we have investigated the structural and optical properties of $LaFe_{1-x}Co_xO_3$ (x=0, 4, 5 & 6 ) nano-particles which were fabricated on quartz substrates by sol-gel method.

• The crystal structures of the obtained LaFeO3 and $LaFe_{1-x}Co_xO$ were carried out by XRD patterns which illuminates that Co atoms were successfully constituted into the host lattice.

• This was further confirmed the formation of NPs by morphological observations via SEM images.

• Absorption studies justify that the band gap of LaFeO3 can be tuned from 2.44 to 2.31 ev via transition metal doping.

• Our work highlights a general approach to perovskite-type NPs with controlled narrow band gap for utilizing in different research areas such as in electronic and optical devices, photo-catalysts for water splitting, as well as solar cells.

**Reference:** 1. Rajashree C, Balu AR, Nagarethinam, Properties of Cd doped PbS thin films: doping concentration effect. Surf Eng 31:316–321 VS (2015).
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