







Short communication

# Synthesis and investigation of structural behaviour and optical properties of BiFeO<sub>3</sub>, YMnO<sub>3</sub> and BiFeO<sub>3</sub>-YMnO<sub>3</sub> nanostructures

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## Highlights

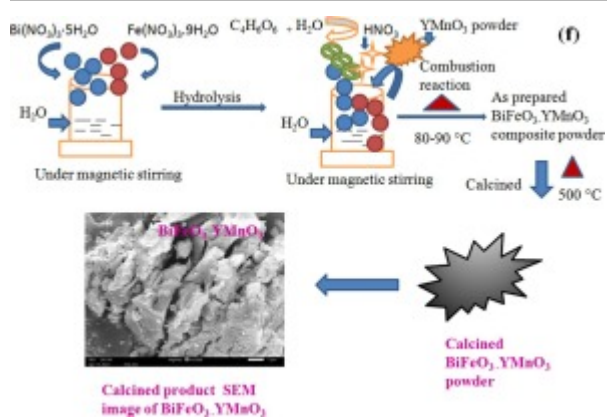
- For the first time, the crystallite size, structural, morphological, and optical properties of BiFeO<sub>3</sub>, YMnO<sub>3</sub>, and BiFeO<sub>3</sub>-YMnO<sub>3</sub> nanostructures were compared via the sol-gel combustion method.
- Powder XRD patterns confirmed the formation of rhombohedral, hexagonal, and rhombohedral-hexagonal crystal structures for BiFeO<sub>3</sub>, YMnO<sub>3</sub>, and BiFeO<sub>3</sub>-YMnO<sub>3</sub>.
- The possible mechanism of formation of the prepared BiFeO<sub>3</sub>, YMnO<sub>3</sub>, and BiFeO<sub>3</sub>-YMnO<sub>3</sub> nanostructures has been investigated.

- Optical band gap ( $E_g$ ) values were measured to be 1.95, 1.35 and 1.28 eV for the  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{BiFeO}_3\text{-YMnO}_3$  samples, respectively using Tauc plots.

## Abstract

In this paper,  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{BiFeO}_3\text{-YMnO}_3$  compounds were synthesized and compared their structural, morphological and light absorption characteristics for the first time. The XRD analysis of the synthesized samples revealed that the crystal structures of  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{BiFeO}_3\text{-YMnO}_3$  are rhombohedral, hexagonal and rhombohedral-hexagonal. SEM images were used to examine the particle shape of all the synthesized compounds. The optical band gap values were measured to be 1.95, 1.35 and 1.28 eV for the  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{BiFeO}_3\text{-YMnO}_3$  samples, using Tauc plots.

## Graphical abstract



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## Introduction

When compared to a single compound, developing composite materials by mixing bi or tri compounds with nanostructure formation has significantly changed the structural, optical and catalytic properties, and magnetic and electrical features [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22]. With the above properties, we can test potential applications such as photocatalysts for waste water treatment, spintronics in magnetic based sensors and

mixing a opto-electronic devices. Based on previous and recent reports on the developed composite compounds, any one multiferroic material with other materials like metal oxide or metal sulphide compounds or co-dopants produces unique features due to these materials' multifunctional behaviour (ie. ferromagnetism, ferroelectricity, improved dielectric properties, enhanced light absorption in the visible portions, reduced optical band gap, and better catalytic properties) [6], [9], [15], [1], [2], [3]. BiFeO<sub>3</sub> and composites based on it, in particular, have been extensively investigated for their multifunctional properties in previous and recent reports, using various chemical routes [1], [2], [3], [4], [5], [6], [7], [8], [13], [14], [15], [16], [17], [18]. In addition, YMnO<sub>3</sub> based material is also multiferroic; however, there have been fewer reports published about its optical, ferroelectric, magnetic and electrical properties, synthesized using different physico-chemical methods [9], [10], [23], [24], [25].

In this work, two multiferroic compounds (BiFeO<sub>3</sub> and YMnO<sub>3</sub>) were chosen and a mixed compound was synthesized using the sol-gel method. The sol-gel synthesized above BiFeO<sub>3</sub>/YMnO<sub>3</sub> compound was found enhanced light absorption in the visible portions, and reduced optical band gap energy using the optical absorption spectroscopy, when compared to the sol-gel synthesized BiFeO<sub>3</sub> and YMnO<sub>3</sub>. The obtained narrow optical band gap value in composite material would be very useful in photocatalytic degradation for catalytic applications. In addition, powder X-ray diffraction (XRD), and scanning electron microscopy (SEM) analysis were used to comparatively investigate the structural behaviour and surface topography for the synthesized BiFeO<sub>3</sub>, YMnO<sub>3</sub> and BiFeO<sub>3</sub>-YMnO<sub>3</sub>. Moreover, the use of the sol-gel combustion synthesis method has some merits like short time reaction synthesis formation (hydrolysis, condensation, gel network particles, combustion reaction occurs at low temperature) followed by sintering to obtain the above composite powders [1].

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## Section snippets

### Experimental

The required chemicals, synthesis method and synthesis reaction step of the formation of bismuth ferrite, yttrium oxide and bismuth ferrite-yttrium oxide material are shown in a flow chart, and can be viewed in supporting information (Fig. S1(a-c)). The resultant products (bismuth ferrite, yttrium oxide and bismuth ferrite-yttrium oxide) were analyzed using powder XRD, SEM and UV-visible spectra. The purpose of the above studies is discussed in detail in the results and discussion section.

## Results and discussion

The diffraction peaks were recorded using powder XRD in the range of the diffraction angle ( $2\theta$ ) from 20 to 70° for the synthesized  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{YMnO}_3\text{-BiFeO}_3$  samples and displayed in Fig. 1 (a-c). The scanned XRD pattern of  $\text{BiFeO}_3$  is displayed in Fig. 1 (a). The XRD patterns of the  $\text{BiFeO}_3$  material are marked on the diffraction peaks as (012), (104), (006), (202), (024), (116), (122), (018) and (300), respectively. When the detected diffraction planes and peak positions were compared with

## Conclusion

In this work, the sol-gel reaction followed by the sintering process used to synthesize three different compounds:  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$  and  $\text{BiFeO}_3\text{-YMnO}_3$ . Powder XRD patterns confirmed the formation of rhombohedral, hexagonal, and rhombohedral-hexagonal crystal structures for  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$ , and  $\text{BiFeO}_3\text{-YMnO}_3$ . Using Debye-Scherrer's formula, the average crystallite size was determined from the well defined sharp and high intensity diffraction peaks and was found to be ~30, 35 and 50nm for  $\text{BiFeO}_3$ ,  $\text{YMnO}_3$ .

## CRedit authorship contribution statement

**J. Gajendiran:** Methodology, Investigation, Writing – review & editing. **S. Gnanam:** Investigation, Writing – review & editing, Conceptualization. **C. Parthasaradhi Reddy:** Formal analysis. **G. Ramesh Kumar:** Conceptualization. **V.C. Bharath Sabarish:** Methodology. **S. Gokul Raj:** Writing – review & editing. **K. Ramachandran:** . **V.P. Senthil:** Formal analysis. **V. Gopi:** Methodology.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this

paper.

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