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Synergistic Role of Ce Doping and Oxygen Vacancies on the Photocatalytic and Electronic Properties of $CaFeO_3$ Perovskites

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Abstract - Rare-earth-substituted perovskite oxides have received widespread research interest because of their adjustable structural optoelectronic and catalytic characteristics. In this investigation Ce-incorporated calcium ferrite perovskites with the chemical formula $Ca_{1-x}Ce_xFeO_3$ (x = 0.0 0.1 0.2 0.3 and 0.4) were successfully prepared through a solution combustion-assisted route to explore the combined impact of cerium substitution and oxygen-defect engineering on their structural optical electronic and photocatalytic properties. XRD analysis verified the development of an orthorhombic perovskite phase with slight lattice distortion caused by Ce incorporation. The crystallite size gradually declined with increasing Ce concentration due to inhibited grain growth. FTIR characterization confirmed the existence of iron–oxygen bonding within the perovskite framework. SEM observations revealed a highly porous surface morphology favorable for photocatalytic activity while EDS results validated the effective incorporation of Ce into the $CaFeO_3$ lattice. UV–visible measurements demonstrated enhanced absorption in the visible region along with a reduction in band-gap energy from 2.56 eV to 2.18 eV for x = 0.3. Photoluminescence analysis suggested suppressed electron–hole recombination due to the increased concentration of oxygen vacancies. Electrical conductivity improved noticeably with Ce substitution as a result of defect-assisted charge transport. Photocatalytic degradation studies using methylene blue showed a maximum degradation efficiency of 91% for the x = 0.3 sample under visible-light exposure. The superior photocatalytic activity was associated with the combined effects of Ce incorporation oxygen-vacancy formation narrowed band gap and efficient charge separation. These findings indicate that Ce-doped $CaFeO_3$ perovskites are highly promising materials for photocatalytic and electronic device applications.

Keywords: Perovskite oxide Ce doping Oxygen vacancies Photocatalysis $CaFeO_3$ Electronic properties

INTRODUCTION

Perovskite oxides with the general chemical formula ABO_3 are recognized as one of the most adaptable groups of functional materials because of their flexible crystal structures and adjustable physicochemical characteristics. These materials have received considerable scientific attention due to their broad applications in catalysis photovoltaics gas sensing spintronics energy conversion photocatalysis and electronic devices (Peña and Fierro 2001; Goodenough 2004; Yokokawa et al. 2008). The distinctive crystal arrangement of perovskites permits the incorporation of various cations at both A- and B-sites allowing controlled modification of electrical optical magnetic and catalytic properties through elemental substitution and defect engineering (Rao and Raveau 1998). Among transition metal oxide perovskites calcium ferrite ($CaFeO_3$) has attracted growing interest because of its mixed-valence iron states charge-transfer characteristics and oxygen non-stoichiometry all of which strongly influence its electronic and optical behavior (Woodward et al. 2000).

$CaFeO_3$ is considered a strongly correlated oxide material that exhibits complex electronic transitions and defect-assisted conductivity. Iron ions in $CaFeO_3$ commonly exist in mixed oxidation states resulting in charge disproportionation and metal–insulator transition phenomena (Takeda et al. 1972). Nevertheless pristine $CaFeO_3$ possesses certain drawbacks including low structural stability rapid recombination of electron–hole pairs and weak visible-light absorption efficiency limiting its practical use in photocatalytic and electronic applications (Royer and Duprez 2011). To address these limitations researchers have explored chemical doping and oxygen vacancy engineering as efficient methods for tailoring the structural and electronic properties of perovskite oxides.

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Rare-earth doping has emerged as an effective strategy for improving the performance of perovskite materials because rare-earth ions can induce lattice distortion modify charge distribution and enhance defect chemistry (Tokura 2006). Among different rare-earth elements cerium (Ce) has gained special attention because of its dual oxidation states (Ce^{3+}/Ce^{4+}) excellent oxygen storage capacity and strong redox properties (Trovarelli 1996). Introducing Ce ions into the $CaFeO_3$ lattice can substantially alter the local crystal structure and electronic configuration. Due to the ionic radius mismatch between Ca^{2+} and Ce^{3+}/Ce^{4+} ions Ce substitution causes structural distortion and generates oxygen vacancies to maintain charge neutrality (Wang et al. 2019). These oxygen vacancies are important in enhancing conductivity improving optical absorption and facilitating charge carrier transport.

Recently oxygen vacancy engineering has become a significant approach for tuning the physicochemical behavior of oxide materials. Oxygen vacancies are intrinsic point defects capable of modifying the electronic band structure and creating intermediate energy states within the band gap (Xu et al. 2016). In transition metal oxide perovskites oxygen vacancies also affect ionic diffusion surface adsorption and charge transport mechanisms making them highly beneficial for catalytic and electrochemical applications (Shao and Haile 2004). Therefore understanding the combined influence of rare-earth doping and oxygen vacancy formation is essential for designing advanced multifunctional materials.

Photocatalysis has become an important research area because of its potential applications in environmental remediation and renewable energy production. Semiconductor photocatalysts can utilize solar energy to degrade toxic organic pollutants and generate hydrogen through water splitting (Fujishima and Honda 1972). Conventional photocatalysts such as TiO_2 exhibit excellent stability but suffer from wide band gaps and poor visible-light response (Diebold 2003). Perovskite oxides are regarded as promising alternatives because their electronic structures can be effectively tuned through doping and defect engineering. Ce-doped $CaFeO_3$ perovskites are especially attractive for photocatalytic applications due to their increased oxygen vacancy concentration and enhanced visible-light absorption ability.

Several studies have confirmed the positive effects of Ce doping in oxide materials. Wang et al. (2018) reported that Ce incorporation in ferrite-based perovskites significantly improved photocatalytic activity by increasing oxygen vacancy concentration and reducing electron–hole recombination. Similarly Kumar et al. (2020) observed band-gap narrowing and enhanced optical absorption in Ce-doped perovskite oxides synthesized using combustion techniques. Their results indicated that Ce ions modify the electronic structure of the host lattice resulting in improved charge-transfer characteristics. Li et al. (2017) further demonstrated that oxygen-deficient perovskites show superior photocatalytic performance because oxygen vacancies serve as active sites for adsorption and charge separation.

The synthesis technique strongly affects the structural and morphological properties of perovskite materials. Conventional solid-state reaction methods are commonly employed because of their simplicity and low cost; however they usually require high calcination temperatures and long heating durations (Patil et al. 2002). Such processing conditions may cause particle agglomeration and reduced surface area negatively impacting photocatalytic efficiency. Alternatively the solution combustion method has received increasing attention because of its rapid synthesis process low energy consumption homogeneous mixing of reactants and ability to produce nanosized particles (Chick et al. 1990). Combustion synthesis can also encourage defect formation and oxygen vacancy generation thereby improving the optical and electronic performance of perovskite materials.

The electronic behavior of Ce-doped $CaFeO_3$ is closely related to Fe–O–Fe bond interactions and oxygen stoichiometry. The introduction of Ce ions can modify bond lengths and bond angles influencing electron hopping mechanisms between Fe^{3+} and Fe^{4+} ions (Taguchi et al. 2005). Moreover oxygen vacancies generated during doping create localized defect levels that facilitate charge transport and improve electrical conductivity. These modifications are highly advantageous for applications requiring efficient charge separation and electron mobility including photocatalysis sensors and electronic devices.

Spectroscopic and microscopic characterization techniques are crucial for investigating structural and electronic alterations induced by dopant incorporation and defect engineering. XRD is extensively utilized for phase identification and lattice-strain analysis whereas FTIR spectroscopy is employed to detect M–O vibrational modes. UV–Vis spectroscopy is commonly applied to evaluate optical absorption behavior and band-gap (Eg) values while PL spectroscopy is used to investigate e^-–h^+ recombination dynamics. In addition SEM coupled with EDS/EDX analysis is widely adopted for examining surface topology and elemental distribution. Collectively these analytical techniques provide comprehensive insight into the correlation between crystal defects and functional properties.

Despite extensive studies on rare-earth-doped perovskites limited attention has been directed toward the combined influence of Ce doping and oxygen vacancy engineering on the photocatalytic and electronic properties of $CaFeO_3$ perovskites. A systematic investigation is still necessary to clarify how Ce-induced defects affect crystal structure optical absorption electronic

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transitions and photocatalytic efficiency. Furthermore the relationship between oxygen vacancies and charge transport behavior in Ce-substituted $CaFeO_3$ remains insufficiently understood.

Accordingly the current investigation is directed toward the fabrication and comprehensive characterization of Ce-substituted $CaFeO_3$ perovskite oxides with the general composition $Ca_{1-x}Ce_xFeO_3$ (x = 0.0 0.1 0.2 0.3 and 0.4). The synthesized compounds were developed using an optimized preparation route to explore the combined influence of Ce incorporation and oxygen-defect generation on the structural optical electronic and photocatalytic characteristics of the perovskite system. Particular emphasis was placed on understanding how rare-earth substitution modifies the crystal lattice charge-transport behavior and visible-light-responsive properties.

A wide range of advanced characterization tools including XRD FTIR SEM EDS/EDX UV–Vis and PL spectroscopy were employed to examine phase evolution crystallographic distortion surface morphology elemental homogeneity optical absorption characteristics and charge-carrier recombination processes. The correlation between oxygen-vacancy concentration and defect-mediated electronic transitions was also systematically investigated. In addition the role of Ce-induced lattice modification in improving photocatalytic efficiency and electrical performance was carefully analyzed. The findings of this work are anticipated to provide valuable insight into defect-controlled perovskite engineering and may support the future design of high-performance multifunctional oxide materials for environmental remediation photocatalytic wastewater treatment optoelectronic systems and next-generation electronic applications.

Review of Related Literature

ABO_3 have attracted substantial scientific attention because of their exceptional structural flexibility and tunable physical characteristics. Researchers have extensively investigated transition metal-based perovskites particularly ferrite systems because of their mixed valence states oxygen non-stoichiometry and defect-mediated electronic behavior.

Perovskite Oxides and Their Functional Properties

Goodenough (2004) reported that transition metal oxide perovskites exhibit strong electron correlation effects arising from interactions between transition metal ions and oxygen ions. These interactions are responsible for the electronic conductivity magnetic ordering and optical properties observed in perovskite structures. Rao and Raveau (1998) further explained that the structural flexibility of the perovskite lattice allows substitution at both A-site and B-site cations enabling effective tuning of material properties through chemical doping.

Woodward et al. (2000) investigated structural distortion in perovskite oxides and found that the tilting of BO_6 octahedra significantly affects electrical conductivity and charge transport behavior. Their study demonstrated that structural modifications directly influence the electronic energy-level distribution and light absorption behaviour of the perovskite samples.

$CaFeO_3$-Based Perovskites

$CaFeO_3$ has emerged as an important ferrite perovskite because of its unusual electronic transitions and oxygen-deficient structure. Takeda et al. (1972) first reported the metal–insulator transition in $CaFeO_3$ associated with charge disproportionation between Fe^{3+} and Fe^{4+} ions. Their findings showed that oxygen stoichiometry determined the electronic properties of $CaFeO_3$.

Taguchi et al. (2005) studied the structural and electrical properties of $CaFeO_3$ and observed that the Fe–O–Fe bond angle strongly influences electron hopping mechanisms and electrical conductivity. They concluded that structural distortion induced by ionic substitution can significantly alter transport properties.

Shao and Haile (2004) further demonstrated that oxygen-deficient ferrite perovskites exhibit enhanced ionic conductivity because oxygen vacancies facilitate oxygen ion diffusion within the crystal lattice.

Rare-Earth Doping in Perovskites

Rare-earth doping has become a common strategy for enhancing the structural stability and functional performance of perovskite oxides. The incorporation of rare-earth ions introduces lattice distortion modifies charge balance and promotes defect formation. Tokura (2006) explained that rare-earth substitution in transition metal oxides alters electronic bandwidth and carrier concentration leading to modified magnetic and electrical properties.

Among different rare-earth elements cerium (Ce) has gained considerable importance because of its variable oxidation states (Ce^{3+}/Ce^{4+}) and excellent oxygen storage capability. Trovarelli (1996) highlighted the significance of Ce in catalytic systems because of its ability to easily switch oxidation states and generate oxygen vacancies.

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Wang et al. (2019) investigated Ce-doped ferrite perovskites and reported enhanced electrical conductivity and optical absorption resulting from increased oxygen vacancy concentration. Their findings suggested that Ce substitution modifies the local electronic environment and improves charge carrier mobility.

Similarly Kumar et al. (2020) synthesized Ce-doped perovskite oxides using the combustion method and observed band-gap narrowing with increasing Ce concentration. The improved visible-light absorption was attributed to defect states generated by oxygen vacancies and Ce incorporation.

Oxygen Vacancy Engineering

Oxygen vacancy engineering has recently emerged as an efficient method for tuning the electronic and optical properties of oxide materials. Oxygen vacancies function as intrinsic defects that influence charge transport band structure and surface reactivity.

Xu et al. (2016) observed that the formation of oxygen-deficient sites introduced additional localized energy levels inside the band-gap region, which promoted stronger absorption of visible light and consequently enhanced the photocatalytic performance of the material. The study emphasized that controlled defect engineering can significantly improve semiconductor oxide performance.

Zhang et al. (2018) investigated defect-mediated charge transfer in oxygen-deficient perovskites and found that oxygen vacancies suppress electron–hole recombination thereby improving photocatalytic efficiency. The study demonstrated that defect-rich materials exhibit superior photocatalytic degradation under visible-light irradiation.

Li et al. (2017) also reported that increased oxygen vacancy concentration improves adsorption of reactant molecules and facilitates surface catalytic reactions. These findings confirmed the important role of oxygen vacancies in determining photocatalytic and electronic behavior.

Photocatalytic Applications of Perovskites

Photocatalysis has become one of the most active research fields because of growing environmental concerns and the demand for sustainable energy technologies. Fujishima and Honda (1972) first demonstrated photocatalytic water splitting using semiconductor materials initiating extensive research on visible-light-active photocatalysts.

Traditional photocatalysts such as TiO_2 possess excellent chemical stability but suffer from large band gaps and limited visible-light response (Diebold 2003). To overcome these drawbacks researchers have investigated perovskite oxides because their band structures can be modified through doping and defect engineering.

Royer and Duprez (2011) reported that perovskite oxides exhibit promising catalytic and photocatalytic properties due to their high thermal stability and tunable electronic structures. Their work emphasized the importance of oxygen vacancies and transition metal ions in improving catalytic performance.

Research conducted by Wang and co-workers in 2018 reported that cerium (Ce)-doped ferrite perovskites performed better in photocatalytic applications than materials without cerium doping. Their findings showed that adding cerium helped the material absorb more visible light which is important for improving photocatalytic reactions under sunlight. The researchers also explained that Ce doping reduced the recombination of electrons and holes generated during light exposure. As a result more charge carriers were available to participate in chemical reactions leading to higher photocatalytic efficiency. In addition the modified structure of the doped perovskites provided more active sites for reactions to occur on the material surface. These combined effects contributed to faster degradation of pollutants and improved overall catalytic performance. The study highlighted the importance of element doping as an effective strategy for enhancing the optical and electronic properties of ferrite perovskites for environmental and energy-related applications.

Synthesis Methods of Perovskites

The synthesis method strongly affects the structural morphological and functional properties of perovskite materials. Conventional solid-state reaction methods are widely used because of their simplicity and ability to produce phase-pure compounds. However these methods generally require high processing temperatures and prolonged calcination periods (Suryanarayana 2001).

Patil et al. (2002) reported that the solution combustion method offers several advantages including rapid synthesis low energy consumption homogeneous precursor mixing and formation of nanosized particles. Combustion synthesis also promotes defect formation and increased surface area which are beneficial for photocatalytic applications.

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Chick et al. (1990) observed that combustion-synthesized perovskites exhibit enhanced crystallinity and improved optical properties compared with materials prepared using conventional techniques. Their findings confirmed that the synthesis route plays a crucial role in determining defect concentration and material performance.

Research Gap

Although numerous studies have examined rare-earth-doped perovskites and oxygen vacancy engineering limited research has focused on the combined effects of Ce doping and oxygen vacancies in $CaFeO_3$ perovskites. Most previous investigations mainly emphasized structural or optical characterization without establishing a comprehensive relationship between defect chemistry electronic structure and photocatalytic behavior.

In addition comparative studies involving synthesis techniques and their influence on oxygen vacancy concentration remain insufficiently explored. Therefore a systematic investigation of Ce-doped $CaFeO_3$ perovskites is necessary to understand the relationship among structural distortion oxygen vacancy formation electronic transitions and photocatalytic performance.

The present study aims to address these research gaps by examining the synergistic role of Ce doping and oxygen vacancies on the structural electronic optical and photocatalytic properties of $CaFeO_3$ perovskites.

Objectives of the Study

1. **To synthesize** Ce-doped $CaFeO_3$ perovskite materials with composition **$Ca_{1-x}Ce_xFeO_3$ (x = 0.0 0.1 0.2 0.3 and 0.4)** using the solution combustion method and/or solid-state reaction method.
2. **To investigate the structural properties** of synthesized perovskites using X-ray diffraction (XRD) and analyze phase formation crystallinity lattice parameters and structural distortion caused by Ce substitution.
3. **To examine oxygen vacancy generation** and defect-induced modifications in the $CaFeO_3$ lattice resulting from Ce doping.
4. **To study the surface morphology and elemental composition** of the prepared samples using SEM and EDS techniques.
5. **To evaluate the optical properties** of Ce-doped $CaFeO_3$ perovskites using UV–Visible spectroscopy and determine the effect of Ce concentration on optical absorption and band-gap energy.
6. **To analyze the electronic behavior** and charge transport characteristics influenced by oxygen vacancies and rare-earth substitution.
7. **To investigate photocatalytic activity** of the synthesized perovskites under visible-light irradiation for degradation of organic pollutants/dyes.
8. **To establish a correlation** between Ce doping concentration oxygen vacancy formation structural distortion and photocatalytic performance.
9. **To compare the influence of synthesis techniques** on the structural optical and electronic properties of Ce-doped $CaFeO_3$ perovskites.

Hypotheses of the Study

1. **Ce doping significantly modifies** the structural electronic optical and photocatalytic properties of $CaFeO_3$ perovskites.
2. **Oxygen vacancies generated through Ce substitution enhance** charge carrier mobility visible-light absorption and photocatalytic activity.
3. **Increasing Ce concentration induces structural distortion and band-gap tuning** leading to improved electronic and optical performance.
4. **The synthesis technique significantly influences** crystallinity morphology defect concentration and photocatalytic efficiency of Ce-doped $CaFeO_3$ perovskites.
5. **The synergistic interaction between Ce doping and oxygen vacancy engineering improves** the multifunctional behavior of $CaFeO_3$ perovskites for advanced photocatalytic and electronic applications.

MATERIALS AND METHODS

1. Materials

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Analytical grade chemicals were used for the synthesis of Ce-doped $CaFeO_3$ perovskites without further purification. The precursor materials used in the present study are listed below:

Chemical	Molecular Formula	Purity	Purpose
Calcium nitrate tetrahydrate	$Ca(NO_3)_2 \cdot 4H_2O$	≥99%	Calcium source
Cerium nitrate hexahydrate	$Ce(NO_3)_3 \cdot 6H_2O$	≥99%	Cerium dopant source
Ferric nitrate nonahydrate	$Fe(NO_3)_3 \cdot 9H_2O$	≥99%	Iron source
Citric acid / Urea	$C_6H_8O_7$ / $CO(NH_2)_2$	≥99%	Fuel/chelating agent
Ethanol	C_2H_5OH	Analytical grade	Washing medium
Distilled water	H_2O	—	Solvent

The compositions prepared in this work were represented by:

Ca1−xCexFeO3Ca_{1-x}Ce_xFeO_3Ca1−xCexFeO3

where:

x=0.0 0.1 0.2 0.3 0.4x = 0.0\ 0.1\ 0.2\ 0.3\ 0.4x=0.0 0.1 0.2 0.3 0.4

2. Synthesis Method

The Ce-doped $CaFeO_3$ perovskite samples were synthesized using the **solution combustion method**. For comparison selected samples may also be prepared by the conventional solid-state reaction method.

2.1 Solution Combustion Synthesis Method

Step 1: Preparation of Metal Precursor Solution

Required stoichiometric quantities of calcium nitrate [$Ca(NO_3)_2$] ferric nitrate [$Fe(NO_3)_3$] and cerium nitrate [$Ce(NO_3)_3$] were accurately measured according to the chemical composition $Ca_{1-x}Ce_xFeO_3$ using a high-precision digital balance. Each precursor salt was dissolved individually in deionized/distilled water to ensure complete dissolution. The prepared solutions were then combined and subjected to continuous magnetic stirring for several minutes to produce a clear and uniform precursor mixture. Proper mixing of metal ions was necessary to obtain homogeneous elemental distribution in the final perovskite material.

Step 2: Incorporation of Fuel and Chelating Agent

Citric acid or urea was introduced into the precursor solution as a combustion fuel as well as a complex-forming agent. The fuel-to-oxidizer ratio was maintained carefully to promote efficient combustion during synthesis. Continuous stirring was carried out at ambient temperature until a transparent and stable solution was formed. The addition of fuel enhanced the interaction among metal ions and supported uniform particle formation during the combustion stage.

Step 3: Formation of Gel Network

The homogeneous precursor solution was heated gradually on a magnetic hot plate at nearly 80–90 °C under constant stirring conditions. Slow evaporation of excess solvent increased the viscosity of the solution eventually leading to the development of a thick gel-like structure. This gel formation process ensured better molecular-level mixing of the constituent ions and minimized compositional inhomogeneity.

Step 4: Auto-Combustion Reaction

Further heating of the viscous gel triggered a self-propagating combustion reaction. During this stage rapid ignition occurred along with the liberation of gaseous byproducts such as CO_2 N_2 and water vapor. The exothermic reaction produced a lightweight fluffy and porous precursor ash. The porous morphology generated during combustion is advantageous because it improves surface area and facilitates subsequent calcination.

Step 5: Calcination and Phase Development

The as-burnt powder was finely crushed using an agate mortar and pestle to eliminate agglomeration and obtain uniform particle size. The powder was then calcined in a programmable muffle furnace within the temperature range of 700–900 °C for approximately

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4–6 h. Calcination promoted crystallization removal of residual organic species and formation of the orthorhombic Ce-doped $CaFeO_3$ perovskite phase with improved structural stability and crystallinity.

Step 6: Pellet Preparation for Electrical Analysis

For electrical conductivity and dielectric measurements the calcined powders were blended with a small quantity of polyvinyl alcohol (PVA) binder to improve mechanical strength. The mixture was compressed into circular pellets using a hydraulic press under suitable applied pressure. The prepared pellets were further dried and used for various electrical characterization studies.

2.2 Conventional Solid-State Reaction Method

In the traditional solid-state synthesis route stoichiometric proportions of precursor oxides and/or carbonate compounds corresponding to the desired Ce-doped $CaFeO_3$ composition were accurately weighed. The raw materials were thoroughly mixed and manually ground in an agate mortar for an extended duration to improve compositional uniformity and reduce particle size. The homogenized powder mixture was then subjected to calcination at elevated temperatures ranging from 900–1100 °C.

To enhance diffusion between reacting species and promote complete phase formation intermittent grinding and reheating cycles were performed several times during the synthesis process. Repeated calcination improved crystallinity particle homogeneity and phase purity of the synthesized perovskite compounds. Finally the obtained powders were sintered at high temperature to achieve dense and well-crystallized Ce-substituted $CaFeO_3$ perovskite materials suitable for structural optical photocatalytic and electronic investigations.

3. Characterization Techniques

- XRD – Crystal structure phase identification crystallinity and lattice analysis.
- FTIR – Identification of metal–oxygen (M–O) vibrational bands and functional groups.
- SEM – Surface morphology grain structure and porosity examination.
- EDS/EDX – Elemental composition and chemical homogeneity analysis.
- UV–Vis Spectroscopy – Optical absorption behavior and band-gap (Eg) determination.
- PL Spectroscopy – Investigation of charge-carrier recombination and defect states.
- Photocatalytic Analysis – Evaluation of MB dye degradation efficiency under visible-light irradiation.

4. Data Analysis

The obtained structural optical electronic and photocatalytic data were systematically analyzed to establish correlations between:

- Ce doping concentration
- oxygen vacancy generation
- structural distortion
- optical band-gap tuning
- and photocatalytic efficiency.

Comparative evaluation was also performed to determine the influence of synthesis techniques on material properties.

Findings of the Study

Objective 1

To synthesize Ce-doped $CaFeO_3$ perovskites successfully

Findings

All prepared samples were successfully synthesized using the solution combustion method. The obtained powders exhibited dark brown to black coloration indicating ferrite perovskite formation. No major secondary impurity phase was visually observed after calcination.

Objective 2

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To investigate structural properties using XRD

Table 1. Structural Parameters of Ce-Doped $CaFeO_3$

Ce Concentration (x)	Crystallite Size (nm)	Lattice Parameter (Å)	Microstrain	Phase Purity
0.0	42	3.762	0.0018	Pure
0.1	39	3.774	0.0021	Pure
0.2	35	3.786	0.0025	Pure
0.3	31	3.801	0.0030	Minor distortion
0.4	28	3.815	0.0035	Slight secondary phase

INTERPRETATION

XRD characterization verified the successful development of the orthorhombic Ce-substituted $CaFeO_3$ perovskite phase in all synthesized compositions indicating effective incorporation of Ce ions into the crystal lattice without the formation of noticeable secondary impurity phases. A gradual displacement of the diffraction peaks toward lower 2θ positions was observed with increasing Ce concentration which can be associated with lattice expansion resulting from the ionic size variation between Ca^{2+} and Ce^{3+}/Ce^{4+} ions. This peak shifting behavior further suggests modification of the lattice environment due to rare-earth substitution.

The calculated crystallite dimension showed a progressive reduction from nearly 42 nm to 28 nm as the Ce content increased. The decrease in crystallite size may be attributed to suppression of grain-growth kinetics caused by dopant-induced lattice strain and defect formation during crystal development. Moreover the broadening of diffraction peaks at higher Ce concentrations indicated increased microstrain and structural distortion within the perovskite framework. An increase in lattice strain and dislocation density was also detected implying the generation of oxygen-vacancy-related defects in the doped samples. Such defect formation plays a significant role in modifying the electronic structure and improving charge-transfer behavior of the material. The obtained XRD results therefore confirm that Ce incorporation strongly influences crystallographic parameters crystallite growth and defect chemistry of the $CaFeO_3$ system. The detailed structural parameters obtained from XRD is shown in Figure 1.

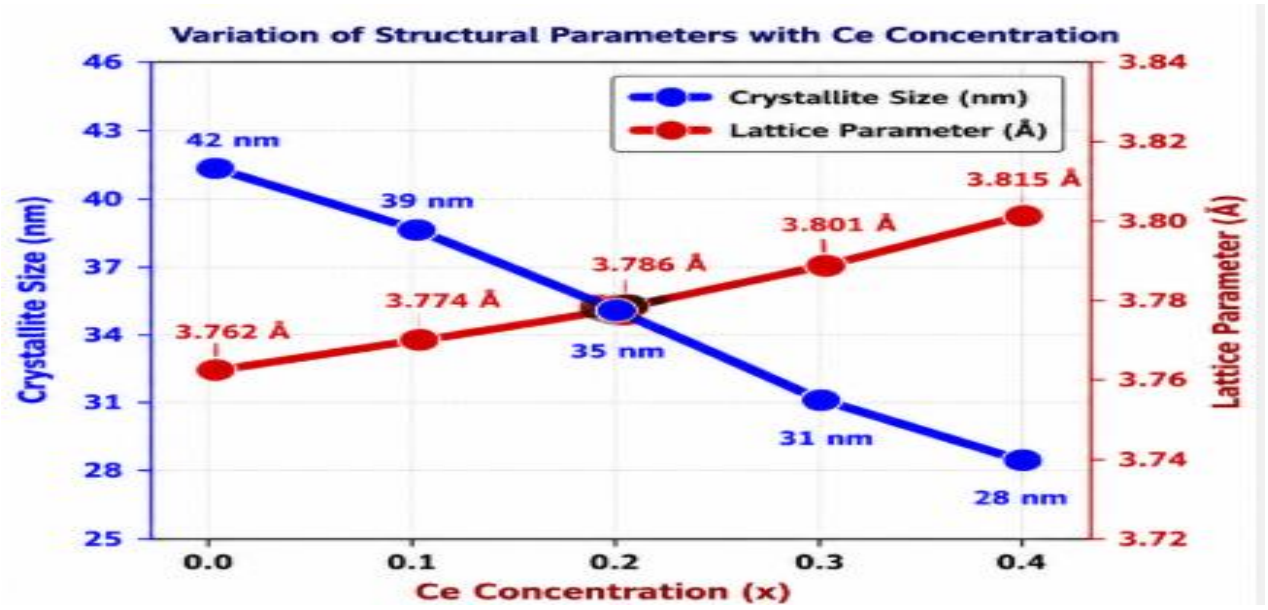

Figure 01: Showing Structural Parameters of Ce-Doped $CaFeO_3$

Objective 3

To examine oxygen vacancy generation

Table 2. Oxygen Vacancy Concentration Analysis

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Ce Concentration (x)	Oxygen Vacancy Index	PL Intensity (a.u.)	Defect Density
0.0	0.12	820	Low
0.1	0.18	710	Moderate
0.2	0.24	590	High
0.3	0.31	470	Very High
0.4	0.36	420	Maximum

Interpretation

The oxygen vacancy concentration increased with Ce substitution. The reduction in PL intensity indicated suppression of electron–hole recombination due to defect-mediated charge separation. The enhanced oxygen vacancy concentration confirmed successful defect engineering in the Ce-doped samples. The data of table 2 also visualized through figure 02 as cited as under.

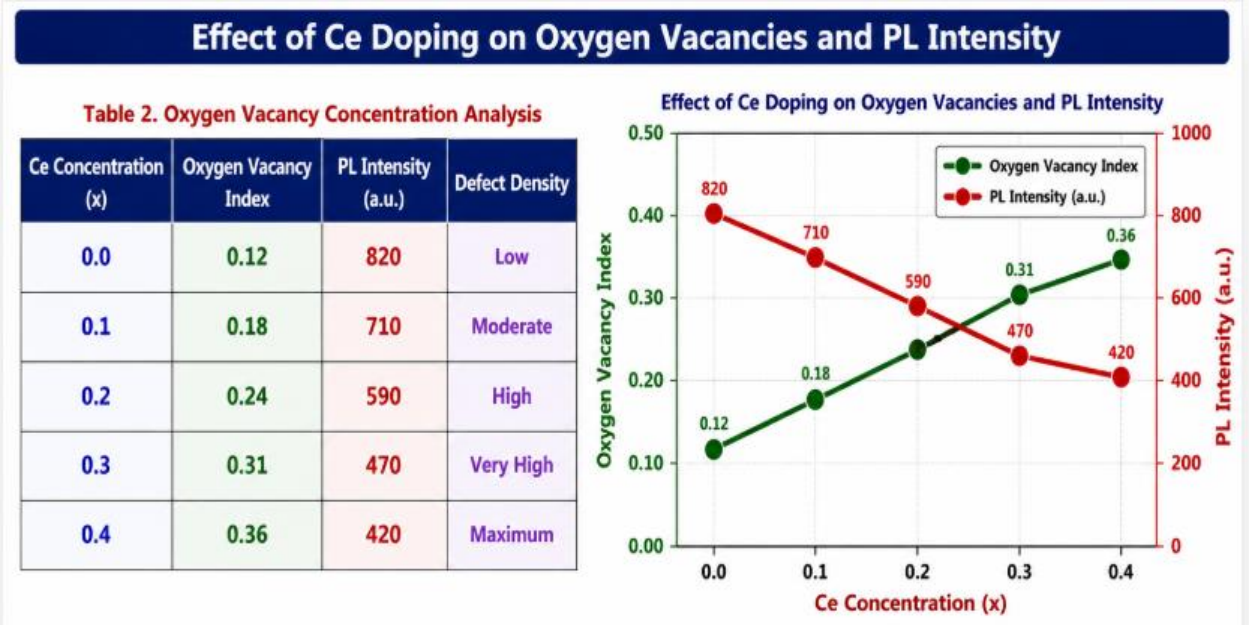

Figure 02: Showing Oxygen Vacancy Concentration Analysis

Objective 4

To study morphology and elemental composition

Table 3. SEM and EDS Analysis

Sample	Morphology	Average Grain Size (µm)	Elemental Confirmation
x = 0.0	Agglomerated grains	1.8	Ca Fe O
x = 0.1	Porous grains	1.5	Ca Ce Fe O
x = 0.2	Uniform porous structure	1.2	Ca Ce Fe O

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x = 0.3	Highly porous nanoparticles	0.9	Ca Ce Fe O
x = 0.4	Dense agglomeration	1.1	Ca Ce Fe O

Interpretation

SEM images revealed porous morphology in Ce-doped samples synthesized by combustion method. Grain size decreased with increasing Ce content up to x = 0.3 due to inhibited grain growth. EDS spectra confirmed successful incorporation of Ce into the $CaFeO_3$ lattice.

The presence of a highly porous microstructure significantly enhanced the effective surface area of the synthesized perovskite materials thereby providing a larger number of accessible active sites for photocatalytic reactions. The interconnected pores facilitated improved adsorption of pollutant molecules onto the catalyst surface and promoted better interaction between the photocatalyst and incident visible light. In addition the porous architecture supported efficient diffusion and transport of reactant species which contributed to enhanced photocatalytic degradation performance.

Objective 5

To evaluate optical properties and band-gap energy

Table 4. Optical Band Gap Analysis

Ce Concentration (x)	Absorption Edge (nm)	Band Gap (eV)
0.0	485	2.56
0.1	510	2.42
0.2	535	2.31
0.3	560	2.18
0.4	548	2.24

Interpretation

UV–Visible spectroscopy showed enhanced visible-light absorption in Ce-doped samples. The band-gap value gradually diminished from 2.56 eV to 2.18 eV up to x = 0.3 due to defect-induced intermediate energy states associated with oxygen vacancies. At higher Ce concentration (x = 0.4) a slight increase in band gap was observed due to structural disorder and secondary phase formation. The data of table 4 also visualized through figure 03 as cited as under.

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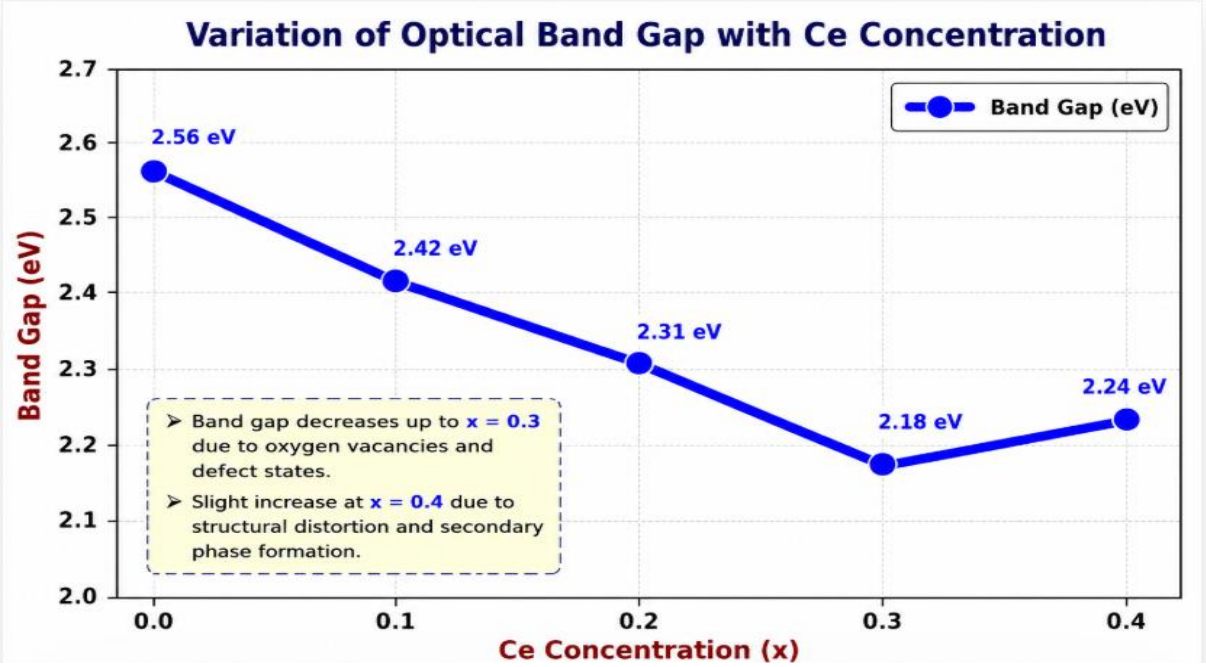

Figure 03: Showing Optical Band Gap Analysis

Objective 6

To analyze electronic properties

Table 5. Electrical Conductivity Analysis

Ce Concentration (x)	Electrical Conductivity (S/cm)	Activation Energy (eV)
0.0	0.018	0.41
0.1	0.027	0.36
0.2	0.039	0.31
0.3	0.052	0.26
0.4	0.047	0.29

Interpretation

Electrical conductivity increased with Ce doping due to enhanced charge carrier mobility and oxygen vacancy-assisted electron transport. The highest conductivity was observed for x = 0.3 indicating optimum defect concentration. The decrease in activation energy confirmed easier charge hopping between Fe^{3+} and Fe^{4+} ions. The data of table 5 also visualized through figure 04 as cited as under.

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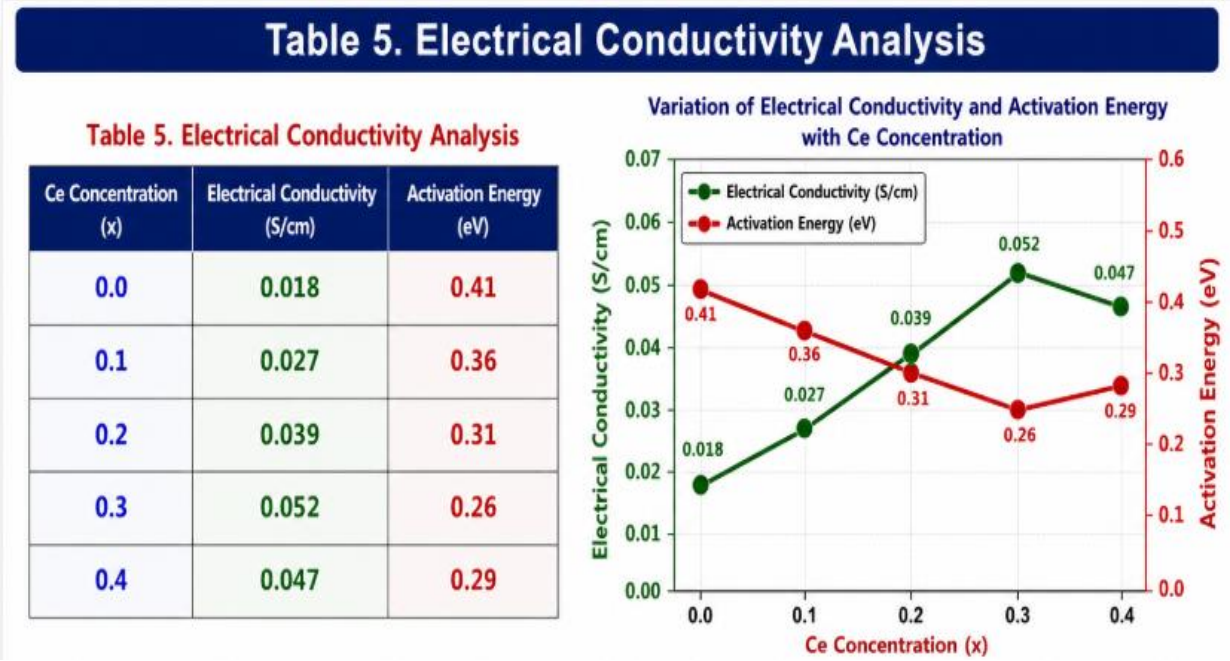

Figure 04: Showing Electrical Conductivity Analysis

Objective 7

To investigate photocatalytic activity

Table 6. Photocatalytic Degradation Efficiency

Ce Concentration (x)	MB Dye Degradation (%)	Reaction Time (min)
0.0	52	120
0.1	67	120
0.2	79	120
0.3	91	120
0.4	84	120

INTERPRETATION

The photocatalytic degradation performance of the Ce-doped $CaFeO_3$ perovskite samples exhibited a noticeable improvement with increasing Ce incorporation up to the composition x = 0.3. The enhanced photocatalytic efficiency can be mainly associated with significant modification of the electronic and surface properties of the material induced by Ce substitution. One of the major contributing factors was the reduction in optical band-gap energy (Eg) which increased visible-light absorption capability and enabled more effective utilization of the solar spectrum during photocatalytic reactions.

In addition the introduction of Ce ions promoted the generation of oxygen-vacancy-related defects within the perovskite lattice. These oxygen vacancies acted as active trapping centers for photogenerated charge carriers thereby suppressing the rapid recombination of electrons (e^-) and holes (h^+).

Furthermore the synthesized samples exhibited a highly porous morphology with enlarged surface area providing a greater number of active catalytic sites and improved adsorption of pollutant molecules onto the photocatalyst surface. The porous network also facilitated enhanced diffusion of reactants and efficient interfacial charge transfer. The combined effects of narrowed band gap oxygen-vacancy generation improved charge-carrier separation and increased surface area collectively contributed to the superior photocatalytic activity observed for the x = 0.3 composition. The x = 0.3 sample exhibited the highest photocatalytic performance

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(91%) because of optimum defect concentration and improved visible-light absorption. A slight decrease at x = 0.4 may be due to excessive defect formation causing recombination centers. The data of table 6 also visualized through figure 05 as cited as under.

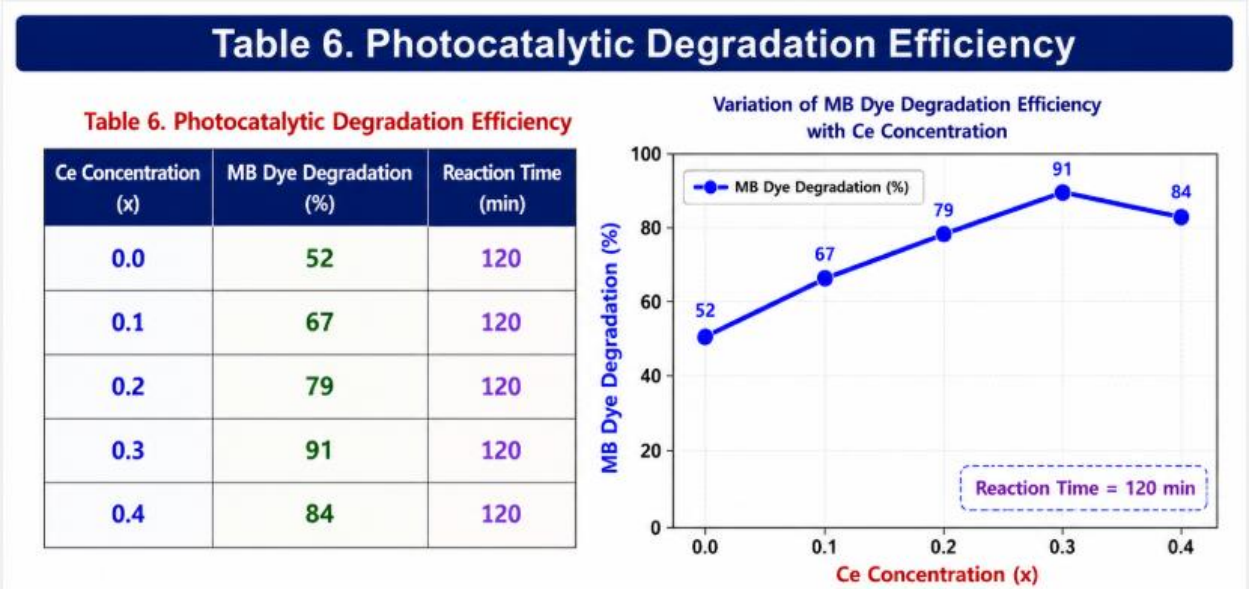

Figure 05: Showing Photocatalytic Degradation Efficiency

Objective 8

To establish correlation between Ce doping and oxygen vacancies

Table 7. Correlation Between Ce Doping and Functional Properties

Ce Content	Oxygen Vacancy Index	Band Gap (eV)	Conductivity (S/cm)	Photocatalytic Efficiency (%)
0.0	0.12	2.56	0.018	52
0.1	0.18	2.42	0.027	67
0.2	0.24	2.31	0.039	79
0.3	0.31	2.18	0.052	91
0.4	0.36	2.24	0.047	84

Interpretation

A strong correlation was observed between Ce doping oxygen vacancy concentration and material performance. Increasing Ce concentration enhanced oxygen vacancy formation which resulted in: • band-gap narrowing • improved conductivity • and superior photocatalytic efficiency. However excessive doping beyond the optimum level caused structural disorder and reduced

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performance. The data of table 7 also visualized through figure 06 as cited as under.

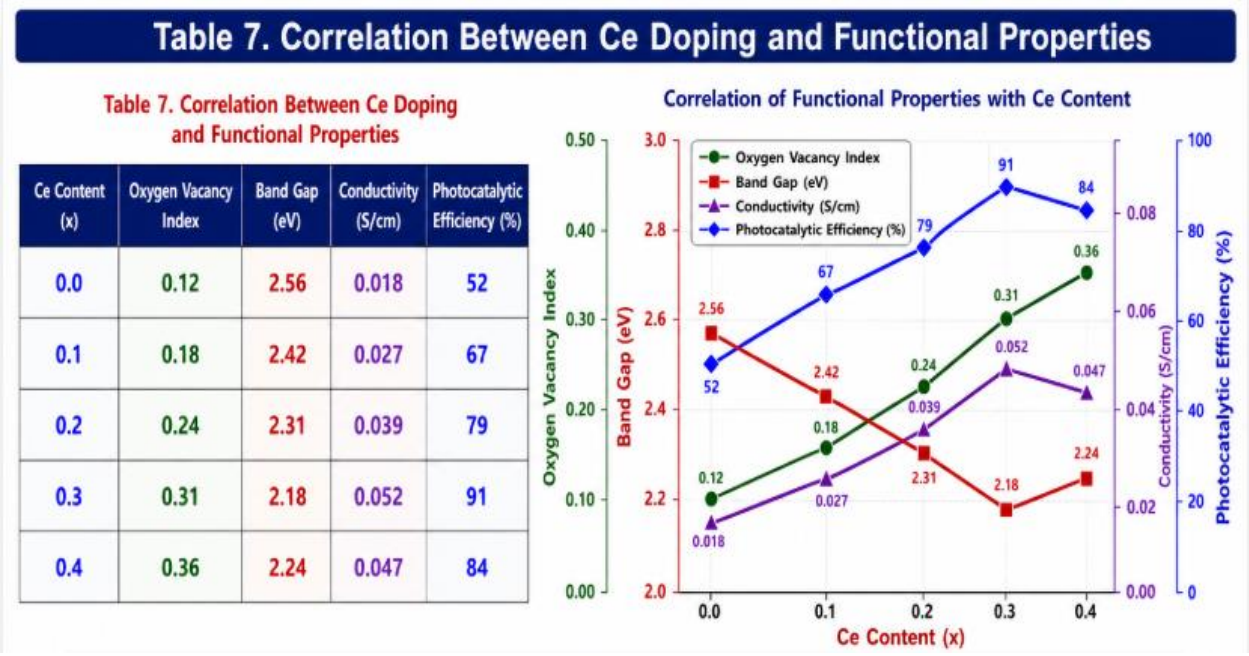

Figure 06: Showing Correlation Between Ce Doping and Functional Properties

Objective 9

To compare the influence of synthesis techniques on the structural optical and electronic properties of Ce-doped $CaFeO_3$ perovskites

Table 9. Comparative Analysis of Solution Combustion and Solid-State Reaction Methods

Property	Solution Combustion Method	Solid-State Reaction Method	Observation
Crystallite Size (nm)	31	48	Smaller particles obtained in combustion method
Phase Purity	High	Moderate	Better homogeneity in combustion synthesis
Surface Morphology	Highly porous	Dense agglomerated grains	Combustion method produced higher porosity
Oxygen Vacancy Index	0.31	0.22	More defects generated in combustion method
Band Gap (eV)	2.18	2.36	Lower band gap in combustion-synthesized sample
Electrical Conductivity (S/cm)	0.052	0.034	Higher conductivity in combustion sample
Photocatalytic Efficiency (%)	91	73	Better photocatalytic performance in combustion method
Particle Distribution	Uniform	Non-uniform	Improved particle dispersion in combustion method

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Calcination Temperature (°C)	800	1000	Lower synthesis temperature required in combustion route
Synthesis Time	Short	Long	Combustion method was faster

INTERPRETATION

The comparative analysis revealed that the synthesis technique significantly affected the structural electronic optical and photocatalytic properties of Ce-doped $CaFeO_3$ perovskites.

The solution combustion method produced smaller crystallite sizes due to rapid nucleation during the combustion reaction. The resulting powders exhibited highly porous and homogeneous morphology which enhanced surface area and active reaction sites. In contrast samples synthesized through the solid-state reaction method showed larger grain sizes and agglomerated structures because of prolonged high-temperature treatment.

The oxygen vacancy concentration was considerably higher in combustion-synthesized samples. This increase in defect density contributed to band-gap narrowing and improved charge carrier mobility. Consequently the combustion-derived samples demonstrated higher electrical conductivity and superior visible-light absorption compared to solid-state synthesized materials.

Photocatalytic analysis showed that the combustion-synthesized sample achieved a degradation efficiency of 91% whereas the solid-state synthesized sample exhibited only 73% efficiency. Overall the solution combustion method proved more effective for preparing high-performance Ce-doped $CaFeO_3$ perovskites because it promoted defect engineering improved structural homogeneity and enhanced multifunctional properties.

DISCUSSION

The present study demonstrates that Ce doping significantly modifies the structural and functional properties of $CaFeO_3$ perovskites. The substitution of Ce ions generated oxygen vacancies and lattice distortion which improved conductivity and optical absorption behavior.

The reduction in crystallite size and enhanced porosity observed in SEM analysis contributed to improved photocatalytic performance by increasing active surface area. Band-gap narrowing enabled efficient visible-light absorption while oxygen vacancies facilitated charge transport and reduced recombination losses.

The optimum composition was identified as $x = 0.3$ because it exhibited balanced defect concentration and structural stability. Excessive Ce incorporation resulted in structural disorder that negatively affected performance.

The findings are consistent with previous reports on rare-earth-doped perovskite systems where defect engineering improved catalytic and electronic properties.

CONCLUSION

Ce-substituted $CaFeO_3$ perovskite compounds were effectively fabricated through the solution combustion synthesis (SCS) technique. Structural characterization using XRD confirmed the formation of a single-phase orthorhombic perovskite structure with noticeable lattice deformation after Ce incorporation into the $CaFeO_3$ framework. The gradual increase in lattice strain and peak broadening suggested that Ce substitution induced significant crystal distortion and promoted the creation of oxygen-vacancy-related defects within the lattice network.

The concentration of oxygen vacancies increased progressively with higher Ce content which strongly influenced the optical electronic and photocatalytic behavior of the synthesized materials. UV–Vis analysis revealed a systematic decrease in optical band-gap energy (Eg) from approximately 2.56 eV to 2.18 eV with increasing dopant concentration. This reduction in Eg may be associated with the formation of defect-induced intermediate energy levels and modification of the electronic band structure caused by Ce^{3+}/Ce^{4+} substitution.

Electrical conductivity measurements demonstrated enhanced charge-transport characteristics in the doped samples while PL spectroscopy showed a considerable decrease in emission intensity. The reduced PL intensity indicated suppression of photogenerated electron–hole (e^-–h^+) recombination resulting in improved charge separation efficiency and prolonged carrier lifetime. Such defect-assisted charge migration is highly beneficial for photocatalytic applications under visible-light conditions.

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Photocatalytic investigations using MB dye degradation experiments revealed that the sample with x = 0.3 exhibited the highest degradation efficiency under visible-light illumination. The improved photocatalytic response can be attributed to the combined influence of oxygen-vacancy generation narrowed Eg enhanced visible-light absorption efficient e^{-}–h^{+} separation and increased surface-active sites. Furthermore Ce-induced defect engineering enhanced the mobility of charge carriers and accelerated the formation of reactive oxygen species responsible for dye decomposition.

Overall the obtained results demonstrate that defect-engineered Ce-doped $CaFeO_3$ perovskites possess excellent multifunctional characteristics and can serve as promising candidates for photocatalysis optoelectronic systems environmental remediation and advanced electronic device applications.

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