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STRUCTURE–MORPHOLOGY–DEFECT RELATIONSHIPS IN $CaTiO_3$-BASED PEROVSKITES FOR ENVIRONMENTAL APPLICATIONS

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ABSTRACT

This review provides a comprehensive and critical analysis of the structure–morphology–defect relationships in $CaTiO_3$-based perovskites, with an emphasis on their environmental applications, particularly in water treatment and photocatalytic degradation processes. The paper systematically examines the influence of crystal structure, synthesis routes, microstructural evolution, and defect chemistry on the functional performance of $CaTiO_3$ materials. Special attention is given to the role of crystallographic phase stability, particle size distribution, surface area, porosity, and aggregation phenomena in controlling adsorption capacity and charge carrier dynamics. Different synthesis strategies—including solid-state reaction, sol–gel processing, hydrothermal and microwave-assisted routes, spray pyrolysis, and green mechanochemical methods—are comparatively evaluated with respect to their effects on morphology control and defect formation. Furthermore, the integration of $CaTiO_3$ with carbon-based materials and the development of doped or composite systems are analysed as strategies for enhancing photocatalytic activity and environmental stability.

By correlating structural features with the physicochemical performance indicators reported in the literature, this review identifies current limitations, unresolved challenges, and promising directions for future research. The analysis aims to provide a coherent framework for the rational design and optimization of $CaTiO_3$-based perovskites in environmental remediation technologies.

KEYWORDS: perovskite, $CaTiO_3$, SWOT analysis, environmental applications, ZnO reinforced composites

1. Introduction

Semiconductor oxides represent one of the most intensively investigated material classes for environmental remediation, particularly in photocatalytic water treatment. Among them, binary oxides with the general formula AO_2, such as TiO_2, have traditionally dominated the field due to their chemical stability, well-established synthesis routes, and relatively high photocatalytic efficiency under UV irradiation. However, despite these advantages, AO_2 systems exhibit intrinsic limitations, including restricted compositional flexibility, limited defect tunability, and challenges in band structure engineering without introducing significant recombination centres.

In contrast, ternary perovskite oxides with the general formula ABO_3 offer a structurally versatile alternative. The perovskite framework accommodates two distinct cationic sites (A and B), enabling independent control of lattice distortion, electronic configuration, and defect chemistry. This structural adaptability constitutes a major strength of ABO_3 systems, as it allows for the systematic tuning of

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electronic structure, oxygen vacancy concentration, and interfacial properties through aliovalent doping or compositional substitution. From a SWOT perspective (Figure 1), the principal strengths of ABO_3 materials compared to AO_2 oxides include enhanced chemical flexibility, greater tolerance to lattice distortion, and the ability to stabilize complex defect landscapes without structural collapse. These features are particularly advantageous for photocatalytic processes, where charge separation efficiency and surface reactivity depend critically on controlled defect engineering.

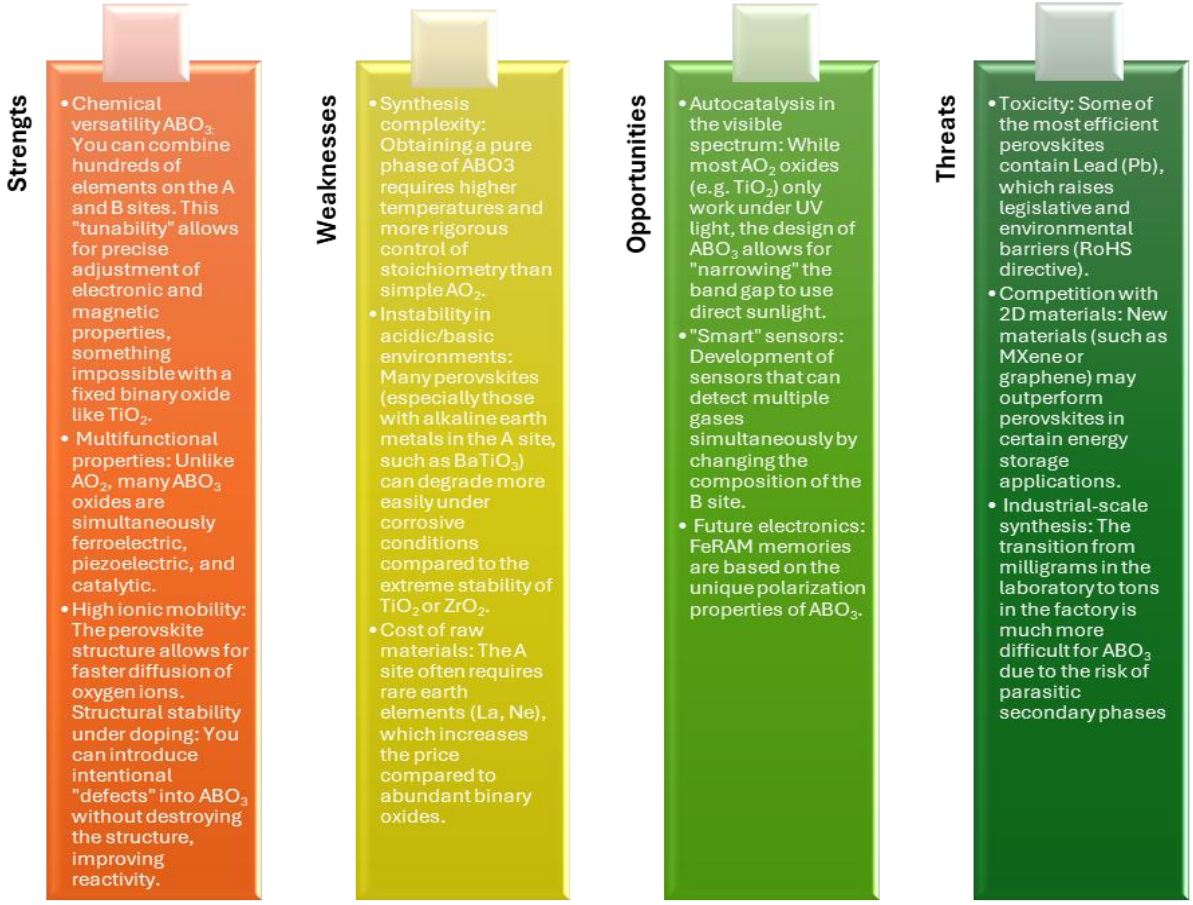

Fig. 1. *SWOT analysis of ABO_3 against AB*

Among oxide perovskites, calcium titanate ($CaTiO_3$) has attracted considerable attention owing to its chemical stability, non-toxicity, and structural robustness under environmental operating conditions [1, 4, 6]. At ambient temperature, $CaTiO_3$ crystallizes in an orthorhombic structure derived from the distorted cubic perovskite lattice, where TiO_6 octahedral tilting governs both band structure and defect accommodation. The electronic configuration of $CaTiO_3$ is characterized by a valence band primarily composed of O 2p states and a conduction band dominated by Ti 3d orbitals, resulting in a wide band gap typically reported in the range of 3.2–3.6 eV [3, 6]. Although this band gap restricts intrinsic activity to the ultraviolet region, the material remains highly attractive for environmental applications. In recent years, $CaTiO_3$-based materials have been extensively investigated for environmental remediation, particularly in photocatalytic water treatment and the degradation of organic pollutants [6, 11, 12, 20, 23]. The environmental relevance of $CaTiO_3$ stems from several key attributes: high chemical stability in aqueous media, resistance to photo corrosion, compatibility with green synthesis routes, and tuneable electronic properties through doping or composite formation. Various synthesis strategies—including solid-state reaction, sol–gel processing, hydrothermal and microwave-assisted methods, spray pyrolysis, and mechanochemical approaches—have been developed to tailor particle size, morphology, and defect concentration [1, 4, 7, 8, 13, 14]. These synthetic variations directly influence surface area, crystallinity, oxygen vacancy formation,

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and charge carrier dynamics, all of which are critical parameters for photocatalytic efficiency.

The environmental performance of $CaTiO_3$-based systems is not determined solely by bulk crystal structure but rather by the interplay between structural distortion, morphological evolution, and defect chemistry. Morphological control through hydrothermal growth or microwave-assisted processing can yield nanocubes, nanorods, or hierarchical architectures that modify surface exposure and reactive facet distribution [14, 15]. Concurrently, intrinsic defects such as oxygen vacancies and extrinsic modifications introduced by rare-earth or transition-metal dopants can alter band structure, promote charge separation, and influence the generation of reactive oxygen species [17, 19-21]. Furthermore, integration with carbon-based materials such as graphene oxide enhances adsorption capacity and facilitates interfacial charge transfer, thereby improving photocatalytic degradation efficiency [12].

Despite the expanding body of literature on $CaTiO_3$-based photocatalysts, a unified framework correlating crystal structure, defect formation, morphological evolution, and environmental performance remain insufficiently consolidated. Many reported improvements are attributed either to increased surface area or to band gap modification, yet the interplay between crystallographic distortion, vacancy stabilization, and morphology-controlled surface reactivity is rarely addressed in an integrated manner. The objective of this review is, therefore, to provide a systematic and critical assessment of the structure–morphology–defect relationships in $CaTiO_3$-based perovskites with a specific focus on environmental remediation. By correlating crystallographic characteristics, synthesis routes, microstructural features, and defect engineering strategies with reported photocatalytic performance, this work aims to identify consistent trends, highlight methodological limitations, and propose future directions for the rational optimization of $CaTiO_3$ materials in water treatment technologies [1-27].

2. Crystallographic characteristics

The geometric stability of the structure is described by the Goldschmidt tolerance factor, which correlates the ionic radii of cations A and B with that of oxygen. For values close to unity, the cubic structure is stable; for significant deviations, structural distortions occur. If the tolerance factor is less than 1, the BO_6 octahedrons undergo rotations and inclinations, leading to orthorhombic or rhombohedral symmetries. If it is greater than 1, tetragonal distortions or structural instabilities may occur.

The stability of the structure is described by the Goldschmidt tolerance factor:

$$t = \frac{r_A + r_O}{\sqrt{2}(r_B + r_O)}$$

where r_A and represent the ionic radii of the A-site and B-site cations, respectively, and r_O is the ionic radius of oxygen. For an ideal cubic perovskite structure, $t \approx 1$, indicating optimal packing of the BO_6 octahedra within the lattice. Deviations from unity result in structural distortions driven by octahedral tilting and lattice strain. For values of $0.8 < t < 1$, the perovskite structure is generally stable, though deviations lead to orthorhombic or rhombohedral distortions.

In $CaTiO_3$, the Goldschmidt tolerance factor is approximately $t \approx 0.97$, indicating a slight geometric mismatch between the A-site Ca^{2+} cation and the TiO_6 octahedral framework. This deviation from the ideal cubic configuration induces cooperative rotations of the TiO_6 octahedra and stabilizes an orthorhombic structure (space group *Pbnm*) at room temperature, as seen in Fig. 2. The associated octahedral tilting, commonly described by the Glazer notation ($a^-a^-c^+$), modifies Ti–O–Ti bond angles and orbital overlap between O 2p and Ti 3d states, thereby influencing band structure, charge transport, and defect energetics.

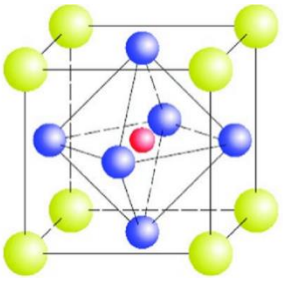

Fig. 2. *Perovskite structure*

A defining characteristic of the ABO_3 perovskite lattice is its chemical flexibility, which allows for partial or complete substitution at both the A and B sites without collapsing the crystal framework. This structural tolerance enables controlled doping and electronic tuning, facilitating the adjustment of optical, dielectric, and catalytic properties. In $CaTiO_3$, the orthorhombic lattice accommodates aliovalent dopants while maintaining structural coherence, making defect engineering and band structure modification viable strategies for performance optimization.

From an electronic perspective, the perovskite architecture promotes metal–oxygen–metal orbital overlap, and the B–O–B bond angle becomes a critical parameter governing conductivity and charge

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mobility. Octahedral distortions alter bandwidth and carrier dynamics, while also influencing the formation of energy and distribution of intrinsic defects such as oxygen vacancies. In $CaTiO_3$, the structural distortion associated with $t < 1$ introduces lattice strain that lowers the energetic barrier for vacancy formation in specific crystallographic environments. These vacancies, in turn, affect crystal growth kinetics during synthesis by modifying surface energy anisotropy and diffusion pathways, ultimately shaping particle morphology and aggregation behavior.

Consequently, morphology cannot be regarded solely as a processing outcome but rather as a manifestation of the underlying structural–defect equilibrium. Nanocubic architectures, hierarchical assemblies, or mesoporous aggregates reflect the interplay between lattice distortion, defect stabilization, and growth dynamics. The resulting surface configuration governs adsorption capacity, active site density, and interfacial charge transfer efficiency. Environmental performance, particularly photocatalytic degradation efficiency, therefore, arises from a coupled mechanism in which crystallographic distortion dictates defect stabilization, defects influence morphological evolution, and morphology controls surface reactivity and charge carrier separation.

$CaTiO_3$ thus represents a structurally adaptable perovskite system in which crystallographic symmetry, defect chemistry, and morphology are intrinsically interconnected. Its orthorhombic lattice undergoes temperature-driven transitions (Pbnm → tetragonal → cubic), further affecting dielectric behavior and defect stability. Various synthesis approaches—including solid-state, sol–gel, coprecipitation, hydrothermal, combustion, spray pyrolysis, and microwave-assisted routes—enable the modulation of phase purity, grain size, and defect concentration. Sol–gel processing offers molecular-level stoichiometric control and stabilization of the orthorhombic phase above 700–800 °C, while microwave-assisted treatments reduce processing time and enhance chemical homogeneity. Hydrothermal methods provide advanced morphological control, and coprecipitation yields monocrystalline nanoparticles with controlled dimensions.

Taken together, the perovskite framework of $CaTiO_3$ provides a robust and versatile platform in which structural parameters, defect formation, and morphological evolution are tightly coupled. This integrated structural–defect–morphology relationship constitutes the basis for the rational optimization of $CaTiO_3$-based materials in environmental remediation and related functional applications.

3. Morphology and specific surface area

Morphology and specific surface area are essential structural parameters in the control of the functional properties of $CaTiO_3$, directly influencing adsorption processes, surface reactivity, photocatalytic behavior, optical properties, and interaction with polymer or biological matrices. The integrated analysis of the studies [1-27] highlights that morphology is predominantly determined by the synthesis method, the ratio of precursors, the heat treatment temperature, and possible dopants.

Aerosol processing (spray-pyrolysis) tends to impose a spherical morphology, related to the formation of particles from atomized droplets. In the spray-pyrolysis study, monophasic $CaTiO_3$ powders with spherical particles and sizes in the nano-submicron range are obtained. In addition, it is explicitly emphasized that the concentration of the precursor solution controls the surface texture (smooth at low concentrations vs. rougher/heterogeneous appearance and stronger agglomeration at high concentrations), as well as the dimensional distribution (e.g., particles around ~0.4 μm at low concentrations, respectively often 0.6–0.8 μm at higher concentrations). From a mechanistic perspective, the explanation proposed in the article (rapid evaporation, internal stresses, formation of saline "crust") is consistent with the physics of droplet drying and the transition from dense/smooth particles to particles with a rough surface or even shell-like defects [4].

In the family of sol-gel "soft chemistry" routes, the primary particle sizes can descend to the fine nanometre regime, but agglomeration remains a recurrent phenomenon [1, 2, 7]. For $CaTiO_3$ sol–gel powders, primary particles with sizes of approximately ~13 nm size and agglomerations on the order of ~30 nm, observed by TEM, are reported, suggesting that drying and densification of the gel lead to particle association, even when nucleation produces nanometric units [7]. In the same logic of obtaining "green"/mechanochemical materials (intense grinding followed by calcination), nanocrystalline $CaTiO_3$ is obtained, with a crystallite size of approximately ~23.5 nm; here, mechanical activation accelerates the solid-solid reaction and lowers the temperature/energy necessary for phase formation, but does not necessarily imply fine morphological control at the level of individual particles. Hydrothermal syntheses (including microwave-assisted variants) most strongly promote anisotropy and particle "architectures", by controlling local supersaturation, ionic transport, and selectivity of crystallographic faces. A relevant example is hydrothermal synthesis at 180 °C for 16 h, where the change in the titanium precursor from solid (TiO_2) to

liquid (titanium isopropoxide) radically alters the $CaTiO_3$ morphology: from cubic morphology to a hollow rectangular morphology, suggesting a different nucleation/growth dynamic and possibly a dissolution–reprecipitation/Kirkendall mechanism under certain conditions [9]. Similarly, microwave-assisted hydrothermal synthesis at 140 °C for 16 min leads to the formation of microcubes (~3.0 μm) in the $CaTiO_3$:Sm system, and the variation of Sm^{3+} doping (within the investigated range) does not significantly change the morphology, indicating that the kinetic regime imposed by microwave irradiation dominates the shape selection (microcubes) more than the subtle effects of doping at low concentrations [14].

At the level of nanoparticles obtained by moderate heat treatments and analysed in detail, a structural hierarchy is often observed: nanometric crystallites, submicron aggregates, and agglomerates. In a study of the $CaTiO_3$ (perovskite) system, average crystallite sizes on the order of ~80 nm (determined by Rietveld refinement) [11] and secondary agglomerations around ~500 nm are reported, evidenced by SEM morphological analysis, confirming that the actual morphology observed in SEM can be governed by the aggregation of primary particles. This is critical for surface-dependent properties (adsorption/photocatalysis) and for sintering, because the specific surface area and effective porosity are controlled not only by the size of the crystallite, but also by the agglomeration mode.

In environmental remediation-oriented work with $CaTiO_3$–carbon composites (e.g. $CaTiO_3$/GO), the morphological rationale is explicitly connected to the specific surface area and the role of the surface in adsorption: it is emphasized that integration with graphene-based materials aims to increase the adsorption of pollutants through a large specific surface area and to facilitate charge transfer (limiting e^-/h^+ recombination). Even though this statement is functional, it anchors morphology (and, implicitly, texture/area) as a critical parameter in the design of $CaTiO_3$ materials for surface processes [12].

In the field of rare earth-doped and rapidly sintered $CaTiO_3$-based phosphors, anisotropic rod-type morphologies are distinguished. For $CaTiO_3:Eu^{3+}$ (combining coprecipitation and sintering), SEM highlights rod-shaped particles. In addition, microwave-assisted sintering produces slightly larger particles with more surface defects than conventional sintering, a difference attributed to the fast-heating regime and short treatment time [18].

Doping and associated phase transformations can change morphology at the level of ceramic particles, sometimes more dramatically than changing the synthesis pathway. For La-doped $CaTiO_3$ ceramics, SEM analysis indicates a morphological evolution directly correlated with the composition and the set of phases: for poorly doped samples, asymmetrical "feather-like/columnar" structures appear (tens to hundreds of nm), while at concentrations of 0.05–0.10 mol %A, small, spherical granules of about 10–20 nm are reported; at concentrations where the $La_{0.3}Ca_{0.7}TiO_3$ phase is formed and becomes dominant, the morphology evolves towards lamellar particles, "diamond-shaped", organized in dendritic structures [20]. In this case, morphology functions as a direct indicator of phase transformations and changes in crystalline growth mechanisms, probably associated with differences in cation diffusion and surface energy between coexisting phases, relevant to both photocatalytic performance and mechanical behavior through densification and particle connectivity.

For $CaTiO_3$ obtained by classical chemistry (coprecipitation), predominantly spherical, crystalline particles with diameters of the order of hundreds of nanometres and with a pronounced tendency to agglomeration are reported. In the coprecipitation-based study, SEM/TEM micrographs indicate agglomerates consisting of spherical particles with an average size of ~200 nm, and confirmation by HRTEM/SAED supports the crystalline character and the formation of the perovskite (orthorhombic) phase [17]. This type of morphology is typical of systems where nucleation is abundant, but growth control is limited by coalescence and capillary forces at drying/calcination, resulting in larger secondary particles than primary crystallites.

In the study on synthesis by the mechanochemical method [25], SEM micrographs highlight particles with predominantly irregular morphology, some crystals presenting pseudo-hexagonal appearance, with dimensions below 90 nm. BET analysis indicates a type IV isotherm with H1 hysteresis, corresponding to mesoporous materials, and the reported specific surface area is 301.1 m^2/g. This value is unusually high for a perovskite oxide obtained by treatment at 1000 °C, suggesting the existence of a highly fragmented and porous aggregate structure. The increase in crystallite size from 17.7 nm (1:1 ratio) to 40.27 nm (1:7 ratio) is highlighted, which confirms the role of the TiO_2 precursor in the nucleation and coalescence of the particles. In PEO/$CaTiO_3$ systems [27], XRD analysis shows a decrease in the intensity of the crystalline peaks of the PEO phase after the introduction of nanoparticles, indicating an increase in the amorphous fraction. Although $CaTiO_3$ is not morphologically analysed by SEM in this study, its effect on the polymer matrix microstructure demonstrates relatively homogeneous dispersion and efficient interfacial interaction.

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4. Photocatalysis and surface engineering

Heterogeneous photocatalysis based on semiconductor oxides is one of the most studied solutions for the degradation of organic pollutants and for advanced oxidation processes in water treatment. In this context, $CaTiO_3$, a perovskite material of the ABO_3 type, has established itself as a promising alternative to TiO_2 due to its high chemical stability, non-toxic character, and structural flexibility through doping and composite formation.

Although the $CaTiO_3$ bandgap (~3.4–3.6 eV) limits activity predominantly to the UV domain, recent literature demonstrates that, through defect engineering and integration into heterostructures, the activity can be extended to the visible domain. Studies dedicated to the synthesis of $CaTiO_3$ at low temperatures for the degradation of methylene blue confirm the photocatalytic potential of this material in the treatment of contaminated water [6].

Visible expansion strategies include boron doping (B–$CaTiO_3$) or integration with graphene oxide (GO). The B–$CaTiO_3$/GO composite exhibits improved methylene blue degradation under visible light with an optimal loading of 5 wt.% GO. The mechanism involves efficient separation of e^-/h^+ pairs and the generation of radicals $\cdot OH$ and $O_2^{\cdot -}$ [12].

Studies on $CaTiO_3$ synthesized at low temperatures for dye degradation [6] indicate the potential of the material in wastewater treatment, especially in combination with doping or carbon supports.

The valence band of $CaTiO_3$ is dominated by O 2p orbitals, and the conduction band by Ti 3d orbitals. The absorption of photons with energy ≥ Eg leads to the generation of electron–hole pairs:

$$CaTiO_3 + h\nu \rightarrow e_{CB}^- + h_{VB}^+$$

Electrons reduce dissolved oxygen to superoxide radicals, and holes oxidize water or hydroxyl groups, generating hydroxyl radicals, responsible for mineralizing organic pollutants [6], Electrons reduce dissolved oxygen:

$$O_2 + e^- \rightarrow O_2^{\bullet -}$$

Holes oxidize water or hydroxyl groups:

$$H_2O + h^+ \rightarrow \bullet OH + H^+$$

The radicals generated are responsible for the mineralization of organic pollutants.

Oxygen vacancies introduce intermediate levels in the band gap and favour the separation of charge carriers. Studies on $CaTiO_3$ synthesized by controlled chemical routes show that heat treatments influence the concentration of defects and, implicitly, the photocatalytic efficiency [1, 7].

Also, low-temperature synthesis for photocatalytic applications [6] confirms that reducing the crystallite size and increasing the number of structural defects lead to improved dye degradation efficiency.

In the study on the green chemistry synthesis of $CaTiO_3$ [23] the nanocrystalline material demonstrated a degradation of up to 93% of methylene blue under sunlight, with a high specific surface area (≈301 m^2/g), favourable to adsorption and surface reactions, being reported. The results indicate a direct correlation between the active surface area and the photodegradation efficiency.

Anionic or cationic doping alters the band structure. The controlled synthesis of $CaTiO_3$ by sol-gel or hydrothermal methods allows the uniform distribution of dopants [2, 11].

B–$CaTiO_3$/GO composites exhibit superior efficiency in dye degradation under visible light due to: GO's electronic conductivity, rapid electron transfer, and reduced e^-/h^+ recombination.

The study on graphene oxide perovskite composites highlights the significant increase in methylene blue degradation compared to pure $CaTiO_3$ [12].

Doping with lanthanide ions (Sm^{3+}, Pr^{3+}, Eu^{3+}, Er^{3+}) is a major vector of functionalization:

- $CaTiO_3:Sm^{3+}$ exhibits intense orange emissions due to $^4G_{5/2} \rightarrow {}^6H_j$ transitions, making it suitable for FED and LED applications [14].
- $CaTiO_3:Pr^{3+}$ demonstrates persistent luminescence properties (afterglow), where oxygen vacancies and local excess Ca act as trap levels [17].
- $CaTiO_3:Eu^{3+}$ exhibits dominant red emission at 617 nm ($^5D_0 \rightarrow {}^7F_2$), optimizable by microwave-assisted sintering [18].
- $CaTiO_3:Er^{3+}$ produces up-conversion emission under excitation 980 nm, with green and red emissions; hydrothermal films exhibit excellent hydrophilicity and demonstrated biocompatibility on BHK cells [19]. The control of the dopant concentration influences the luminescent intensity and quenching phenomena, with an optimal concentration below 3% molar for Er^{3+} being reported.

5. Influence of the synthesis method on performance in water treatment

The sol-gel and coprecipitation methods [1, 2, 7, 11, 13] allow the production of nanoparticles with increased specific surface area, which favours the adsorption of organic molecules and the accessibility

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of the active centres. In nanoparticles obtained by microwave-assisted sol-gel [13] the reduction of processing time and dimensional control contribute to the increase of photocatalytic efficiency.

The spray-pyrolysis method [4] produces submicron spherical particles, and the control of the concentration of precursors influences the surface texture and, implicitly, the kinetics of the degradation reactions. Mechanochemical synthesis [23] highlights the possibility of obtaining an eco-friendly material with high photocatalytic activity and no residual toxic effects on the environment (confirmed by phytotoxicity and antimicrobial activity tests).

The integration of $CaTiO_3$ with graphene oxide [12] is an effective strategy for increasing performance in water treatment. The B–$CaTiO_3$/GO composite exhibits: an increase in specific surface area, improved pollutant adsorption, reduced electron–hole recombination, and efficient charge transfer at the semiconductor–carbon interface.

These effects lead to faster and more efficient degradation of dyes compared to pure $CaTiO_3$.

Doping with lanthanides or transition metals alters the electronic structure and creates intermediate levels in the band gap, facilitating the expansion of absorption into the visible domain. In La-doped $CaTiO_3$ ceramics [20], improved photocatalytic activity correlated with structural and morphological changes in the material is reported.

In the case of $CaTiO_3$ doped with Sm or Eu [14, 18], although the primary objective is optoelectronic, defectological changes can indirectly contribute to photocatalytic activity by increasing trap centres for carriers.

Vanadium doping [21] leads to morphological changes (cuboidal structures) and influences charge transfer, which is relevant for advanced oxidation processes. In the article on $CaTiO_3$ asymmetric membranes [24], the use of the controlled porous structure for separation processes and potential for integrated catalytic systems in water treatment are explored. The control of porosity and microstructure allows the flow and access of reactants to the active surface to be optimized. A major advantage highlighted in the analysed literature is the non-toxic character of $CaTiO_3$. In the mechanochemical study [25], the degradation products of methylene blue showed no significant phytotoxic effects on seed germination, and antimicrobial tests indicated the absence of residual toxicity. This characteristic differentiates $CaTiO_3$ from other semiconductor oxides that can generate problematic byproducts.

6. Critical analysis of structure–morphology–defect relationships in $CaTiO_3$-based perovskites for environmental applications

The existing literature on $CaTiO_3$-based perovskites for environmental remediation demonstrates substantial progress in synthesis optimization, structural tailoring, and defect engineering [1-3]. Nevertheless, a closer examination of the published results reveals conceptual inconsistencies and methodological limitations that necessitate a critical reassessment. Although numerous investigations report enhanced photocatalytic performance through morphological refinement and dopant incorporation [6, 11, 20, 21], the correlations proposed between structural parameters and environmental efficiency are often qualitative rather than quantitatively validated.

A frequently invoked argument in the literature concerns the direct proportionality between specific surface area and photocatalytic efficiency. Nanometric $CaTiO_3$ powders synthesized via sol–gel, mechanochemical, microwave-assisted, or green routes typically exhibit improved degradation of model pollutants such as methylene blue [6, 8, 11, 25]. The enhancement is generally attributed to increased adsorption capacity and a higher density of reactive surface sites. However, comparative analyses indicate that surface area alone cannot fully explain catalytic performance. Materials obtained by spray pyrolysis [4] or combustion routes [5], despite moderate surface areas, may exhibit competitive stability and activity, while hydrothermal products with controlled morphology [14, 15] often demonstrate superior performance even without exceptionally high BET values. These discrepancies suggest that surface area must be interpreted in conjunction with crystallinity, defect concentration, and charge carrier dynamics.

The role of intrinsic defects, particularly oxygen vacancies, is widely emphasized in studies dealing with $CaTiO_3$ photocatalysts [6, 11, 20, 21]. Oxygen vacancies are commonly described as shallow donor states capable of facilitating charge separation and extending light absorption. Nevertheless, direct quantification of defect density remains limited across the literature. In many cases, defect presence is inferred indirectly from band gap shifts or XRD peak variations [3, 18], without systematic confirmation via spectroscopic techniques. Excessive vacancy concentration may increase recombination centres and compromise structural stability, yet such trade-offs are seldom discussed in depth. Therefore, defect–performance relationships often remain suggestive rather than demonstratively causal.

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Doping strategies involving rare-earth or transition-metal ions have been extensively explored as a means of electronic structure engineering [14, 17, 19, 20, 21]. For instance, lanthanum-doped $CaTiO_3$ ceramics exhibit morphological transformations correlated with enhanced photocatalytic response [20], while vanadium incorporation modifies charge transfer behavior and cuboid morphology [21]. Similarly, Sm^{3+} and Pr^{3+} substitutions influence microstructure and luminescent properties [14, 17], indirectly affecting charge carrier recombination pathways. However, the mechanistic interpretation of dopant effects frequently relies on band gap narrowing arguments without detailed verification of band edge positions relative to redox potentials. Moreover, the potential formation of secondary phases is not consistently evaluated [20], and the distinction between structural effects and genuine electronic modifications remains insufficiently clarified.

The synthesis route further complicates the structure–property relationship. Solid-state and conventional ceramic processing methods yield highly crystalline materials but often with limited surface area [1, 2]. In contrast, sol–gel and microwave-assisted techniques enable finer control over particle size and homogeneity [7, 13, 16], while hydrothermal processing promotes anisotropic growth, including nanocubes and hierarchical architectures [14, 15]. Green mechanochemical approaches emphasize sustainability and environmental compatibility [8, 25], aligning well with remediation applications. However, despite the diversity of synthetic methodologies, few studies evaluate scalability or long-term operational stability, particularly under realistic wastewater conditions. Membrane-based $CaTiO_3$ systems [24] and polymer-based nanocomposites [10, 27] illustrate alternative integration strategies, yet comprehensive assessments of durability and recyclability remain limited.

Another critical aspect concerns the experimental evaluation protocols used to assess environmental performance. Most investigations rely on model dye degradation under controlled laboratory illumination [6, 11, 12, 25]. Although such tests provide valuable comparative insight, they do not necessarily represent complex industrial effluents containing mixed organic and inorganic contaminants. Mineralization efficiency, toxicity of degradation intermediates, and catalyst leaching are rarely examined in detail. Composites incorporating graphene oxide [12] demonstrate improved charge separation and adsorption capacity, reinforcing the importance of interfacial engineering; however, systematic long-term cycling studies are often restricted to a few repetitions. The absence of standardized testing conditions—light intensity, catalyst dosage, pH, and pollutant concentration—further complicates direct comparison among studies [6, 11, 20].

From a theoretical standpoint, computational investigations into the structural and electronic properties of $CaTiO_3$ polymorphs provide valuable insight into band structure modifications and defect energetics [3]. Nonetheless, the integration between density functional theory predictions and experimental photocatalytic data remains sporadic. Few works attempt to correlate calculated defect formation energies with measured activity trends. A predictive framework linking crystal symmetry, morphology, defect density, and environmental degradation kinetics is largely absent, despite the growing number of experimental reports [1-27].

Collectively, the literature confirms the promising potential of $CaTiO_3$-based perovskites for environmental applications, including water treatment and photocatalytic degradation [6, 11, 12, 20, 25]. However, the field is still characterized by descriptive correlations rather than mechanistically validated models. Future research must adopt a more rigorous and standardized methodology that integrates defect quantification, band alignment analysis, morphology control, and real-environment performance evaluation. Only through such systematic integration of structural, morphological, and electronic parameters can $CaTiO_3$-based perovskites evolve from laboratory-scale demonstrations to scalable and reliable environmental remediation technologies [1-27].

7. Conclusions and future perspectives

This review has critically examined the structure–morphology–defect relationships in $CaTiO_3$-based perovskites with an emphasis on their environmental applications, particularly photocatalytic water treatment. The analysis of recent literature demonstrates that the environmental performance of $CaTiO_3$ cannot be attributed to a single structural parameter but rather emerges from the complex interplay between crystallographic distortion, microstructural evolution, defect chemistry, and surface engineering. Structural characteristics such as octahedral tilting and orthorhombic symmetry influence the band structure and defect accommodation, while synthesis-controlled morphology governs surface accessibility, porosity, and aggregation behavior. Intrinsic defects, especially oxygen vacancies, play a dual role by promoting charge separation at moderate concentrations while potentially acting as recombination centres when excessive. Extrinsic doping and composite formation further modify the electronic structure and interfacial charge transfer, yet

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their effects remain highly dependent on dopant solubility, phase stability, and defect distribution.

Although $CaTiO_3$-based materials show promising photocatalytic degradation efficiency under laboratory conditions, particularly for model organic dyes, the field remains largely empirical. Reported performance improvements are often interpreted through qualitative correlations rather than mechanistically validated models. The absence of standardized testing protocols limits long-term stability studies, and scarce evaluation under realistic wastewater matrices restricts the translation of laboratory findings into practical environmental technologies. Furthermore, quantitative characterization of defect densities and band edge alignment remains insufficient, and the integration of computational predictions with experimental validation is still sporadic.

Future research should therefore move toward a more rigorous and predictive framework. Systematic defect quantification using advanced spectroscopic techniques, combined with density functional theory calculations of defect formation energies and band alignment, would clarify the true contribution of intrinsic and extrinsic modifications. Morphology control must be addressed not only from a surface-area perspective but also in terms of facet-dependent reactivity and charge transport pathways. In addition, scalable synthesis routes that maintain structural and defect integrity should be prioritized to bridge the gap between laboratory-scale preparation and industrial applicability.

Equally important is the evaluation of environmental performance under realistic operating conditions. Studies should extend beyond model dye degradation to include mineralization efficiency, toxicity of degradation intermediates, catalyst recyclability, and structural stability over extended cycling. The development of standardized photocatalytic testing methodologies would enable meaningful comparison across studies and facilitate the identification of truly optimized compositions.

In conclusion, $CaTiO_3$-based perovskites represent a structurally versatile and environmentally stable class of materials with significant potential for sustainable water treatment technologies. However, advancing from descriptive structure–property correlations toward quantitatively validated design principles is essential. A comprehensive integration of structural analysis, defect engineering, morphology control, and realistic environmental evaluation will be decisive for the rational optimization and practical implementation of $CaTiO_3$-based systems in environmental remediation.

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