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The Impact of Different Doping Strategies on the Performance of Perovskite Materials

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Abstract. Perovskite materials have attracted considerable attention in catalysis, energy storage, and photoelectric conversion owing to their structural stability, low cost, and excellent physicochemical properties. However, their practical applications are still limited by several challenges, including high reaction energy barriers, insufficient active sites, and low photoelectric conversion efficiency. This paper systematically summarizes recent progress in improving the performance of perovskites through element doping. It focuses on the regulatory effects of metal element doping, non-metal element doping and multi-element co-doping on the physicochemical properties and application of perovskites are discussed in detail. Previous studies have shown that targeted doping modification can significantly enhance the performance of perovskites in reactions such as catalytic methane oxidation, low-temperature fuel cell electrolytes, photothermal CO2 methanation, piezoelectric catalytic hydrogen production, and pollutant degradation. In addition, this paper discusses current limitation, including insufficient theoretical calculations, limited long-term stability evaluation, and challenges in large-scale production. Future research directions are proposed, including the integration of density functional theory calculations for rational material design, evaluation of long-term stability, and the development of green and scalable synthesis processes. This review aims to provide theoretical guidance and technical support for promoting the industrial application of perovskite materials in energy and environmental fields.

Keywords: Perovskites, Doping Modification, Catalytic Performance, Energy Conversion

1. Introduction

Perovskite has a very abundant global reserve and is widespread. The perovskites mainly consist of the natural mineral $CaTiO_3$ and various oxides with the same structure but different elements [1]. Among them, perovskite oxides are one of the most representative and widely studied categories. Their general formula is ABO_3, where the A site is usually a base metal or rare earth metal ion, and the B site is a transition metal ion [2]. This crystal structure exhibits excellent stability and provides great potential for applications in electrocatalysis, energy storage, and photoelectric conversion.

Although perovskites have shown great potential as catalysts, they still encounter numerous challenges in practical applications. In catalytic reactions, perovskites often suffer from high

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reaction energy barriers and insufficient active sites, leading to low catalytic performance. In the field of energy conversion, reducing the cost of hydrogen production and increasing the efficiency of photoelectric conversion is the key bottleneck for commercial applications. In addition, the development of persistent luminescent materials that can be activated by near-infrared light remains a significant challenge.

Here, the element doping modification of perovskites is adopted to conduct multi-dimensional performance discussions on perovskite materials. By introducing specific metals (such as Fe, Co, Ni, Tm, etc.) or non-metals (such as S, Br, etc.) at the A or B sites of perovskite materials, or by conducting dual-element co-doping, the electronic structure, lattice distortion degree, and defect concentration of the materials can be systematically adjusted. Through detailed experimental data and mechanism analysis, they revealed the intrinsic influence patterns of different doping types on the physical and chemical properties of perovskite materials. This not only provides a theoretical basis for enhancing the catalytic performance of perovskite in the battery industry, hydrogen production industry, and environmental governance, but also points out the direction for the development of new high-performance photovoltaic functional materials. It also offers practical and feasible modification methods for supporting the technological progress in related industries.

2. Metal doping

2.1. Doping of metallic elements

Doping metal elements into perovskite materials is one of the main methods to enhance the performance of perovskite. By doping metal elements, the catalytic efficiency of perovskite in catalytic reactions can be significantly improved. During the methane catalytic oxidation reaction, Maxime Delporte et al. [3] synthesized Fe-doped perovskite $CaTi_{1-x}Fe_xO_{3-\delta}$ (CTFx) by the Peccini method, and successfully synthesized $CaTiO_3$-Gly (CTFx-Gly) using glycerol as the chelating agent. Modulating the Fe concentration can alter the content of Fe^{3+} in CTFx-Gly. It was concluded that the rate of the catalytic oxidation reaction of methane with respect to the unit iron content was positively correlated with the ratio of Fe^{3+}-6CN. This indicates that by doping with Fe, the content of Fe^{3+}-6CN can be effectively changed, thereby increasing the rate of the methane catalytic oxidation reaction.

In the field of low-temperature ceramic fuel cells, Hong et al. [4] used the sol-gel technique to incorporate cobalt into $CaTiO_3$ to synthesize Co-$CaTiO_3$ as the electrolyte, creating a unique surface charge region that can facilitate the redistribution of ion charges and the ion transport. Through X-ray photoelectron spectroscopy (XPS) and electron paramagnetic resonance (EPR) analysis, it was found that partial substitution of Co_{3+} for Ti^{4+} led to local lattice distortion, increased the concentration of oxygen vacancies (Vo), formed additional ion channels, and thereby enhanced the ionic conductivity. Especially within the temperature range of 420°C to 520°C, the ionic conductivity of $CaTiO_3$ doped with 10% Co is between 0.123 and 0.07 S/cm, surpassing the ionic conductivity of other substances as electrolytes. Therefore, using Co-$CaTiO_3$ as the electrolyte can effectively enhance the ionic conductivity at low temperatures, thereby promoting the electrolysis of low-temperature ceramic fuel cells (420–520°C).

To address global warming, the reduction of carbon dioxide emissions and its rational utilization have attracted the increasing attention of many scientists. Yuan et al. [5] loaded Ni nanoparticles onto $CaTiO_3$ nanosheets by grinding, and thus obtained Ni/$CaTiO_3$. Through EPR measurement and Density functional theory (DFT) calculation, it was found that the introduction of Ni atoms can more effectively promote the generation of Vo in $CaTiO_3$, facilitating the formation of an active interface between the Ni metal and the $CaTiO_3$ carrier, creating a special layer rich in Vo and

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containing Ni doping, which reduces the migration energy barrier of hydrogen atoms and effectively improves the migration efficiency of hydrogen atoms. The SFLPs (Lewis acid sites) formed due to the existence of Vo enable Ni/$CaTiO_{3-X}$ to exhibit a hydrogen desorption region suitable for the photothermal CO_2 methanation reaction. Together with the dynamically generated OH (Lewis base sites), they provide appropriate CO_2 adsorption and activation sites. Therefore, Ni-doped $CaTiO_3$, by simultaneously enhancing the migration efficiency of hydrogen atoms and providing suitable CO_2 adsorption and activation sites, can achieve efficient and highly selective photothermal carbon dioxide methanation reactions, promoting the degradation and reutilization of carbon dioxide in the environment.

In the field of biomedicine, Gulizhabaier Abulipizi et al. [6] synthesized CTT nanoparticles by doping Tm into $CaTiO_3$. In CTT, due to the substitution of Tm^{3+} for Ca^{2+}, to maintain charge balance, Ti^{3+} and Vo were produced in the matrix. This Ti^{3+}-Vo defect is the key "trap" for storing excitation energy. Under deep red light (approximately 688 nm) excitation, low-energy photons gradually pump the electrons of Tm^{3+} through a multiphoton process, causing them to reach the excited state. The excited-state Tm^{3+} transfers energy to the Ti^{3+}-Vo defect pairs in the matrix, and the electrons are trapped, forming a metastable Ti^{4+}-Vo^{-}. Under the thermal disturbance at room temperature, the electrons trapped in the trap slowly release back to Tm^{3+}, thereby exciting Tm^{3+} to generate a near-infrared PersL signal at 803 nm. By doping Tm into $CaTiO_3$, we synthesized CTT nanoparticles, which broke the traditional limitation of persistent luminescent materials that require high-energy light (such as ultraviolet light) for excitation. This enabled charging with deep red light/near-infrared light. Therefore, CTT materials are highly suitable for biomedical luminescence imaging.

2.2. Metal compound doping

Although the doping of metal elements in perovskite materials is quite extensive, the doping of metal compounds is also very important for improving the performance of perovskite materials. In the field of piezoelectric catalytic hydrogen production, Wang et al. [7] synthesized $CaTiO_3$ doped with CoP using the solid-phase method. After loading, the band gap of CoP/$CaTiO_3$ decreased, facilitating the separation of electrons (e^-) and holes (h^+) in the polarization field, thereby enhancing the efficiency of piezoelectric catalysis. The perovskite doped with 5% CoP exhibited the highest piezoelectric catalytic efficiency and excellent stability. The H_2O_2 yield reached as high as 9657.30 μmol $L^{-1}g^{-1}$ within 2 hours, and remained stable even after five cycles. The results of another set of experiments show that as the oxygen content in the gas decreases sharply, the production of H_2O_2 significantly decreases. This indicates that O_2 plays a crucial role in the piezoelectric catalytic process of generating H_2O_2. Subsequently, it was determined that superoxide radicals are the main active substance in the piezoelectric catalytic process of the 5% CoP doped sample. In the reaction mechanism, e^- react with dissolved oxygen to form $^{\bullet}O^{2-}$, and subsequently $^{\bullet}O^{2-}$ reacts with e^- and protons h^+ to produce H_2O_2. Due to the lower conduction band position of CoP compared to $CaTiO_3$, this electric potential difference facilitates the spatial separation of e^- and h^+, thereby significantly enhancing the piezoelectric catalytic performance. This result provides a new environmentally friendly and cost-effective material for hydrogen production through piezoelectric catalysis, and also promotes the industrial application of piezoelectric catalytic hydrogen production technology.

In the photocatalytic system, Tayyebeh Soltani et al. [8] used Ag–MnO x doped $CaTiO_3$, and found that when the Ag–MnO_x/CTO sample, which was simultaneously loaded with Ag nanoparticles and MnO_x species by the synchronous light deposition method, was used for photocatalytic CO_2 and H_2O reactions to generate CO and H_2O_2, its yield significantly increased and

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the selectivity between the two reduction products (CO and H_2O_2) still remained at a high level (S = 76%). This photocatalyst and its photocatalytic reaction system exhibit excellent stability. After a 24-hour reaction test, the selectivity of the catalyst for the reduction products and oxidation products of CO and H_2O_2 remained high, at 73% and 91% respectively; and the R(e/h) value calculated based on the gaseous and liquid products was still close to 1. In the Ag–MnO_x/CTO sample, light excites the photocatalyst, causing the generation of e^- in the conduction band and h^+ in the valence band. On the surface of Ag nanoparticles, e^- will reduce CO_2 and combine with protons to form CO and H_2O; h^+ will transfer to the surface of the MnO_x species, and through $NaHCO_2$, indirectly oxidize H_2O to H_2O_2. Ag–MnOx doped $CaTiO_3$ can significantly enhance the efficiency of photocatalytic reactions of CO_2 and H_2O. It does not require an external bias and can fully utilize renewable solar energy, promoting the further development of photocatalysis and photocatalyst design, and also contributing to the development of green and sustainable chemistry.

In the research on piezoelectricity and multiferroicity, Wu et al. [9] discovered that by doping NiO_x (x = 0–3.0) into the $BiFeO_3$-based solid solution, it exhibited a rhombohedral perovskite structure, being dense and free of inclusions. The NiOx doping inhibited the growth of $BiFeO_3$ grains and enhanced the insulating property, ferroelectricity, piezoelectricity and ferromagnetism of the ceramic. When the applied electric field is 3 kV/mm, as the doping amount x increases, the leakage current monotonically increases, while the resistivity gradually decreases, and the insulation performance has been significantly improved. Compared with the samples without NiO_x doping, the tangent value of the dielectric loss of this system monotonically increases with the increase of doping amount x, and the piezoelectricity is enhanced. When the annealing temperature increased from 50 ℃ to 475 ℃, the piezoelectric constant (d33) gradually decreased from 151 pC/N to 93 pC/N; when the annealing temperature was further raised to 500 ℃, it was observed that d33 dropped sharply to 40 pC/N. However, when the annealing temperature is between 525 ℃ and 575℃, d33 is almost 0 pC/N. At this temperature, the ceramic shows almost no piezoelectricity, thus demonstrating the excellent piezoelectric performance and good temperature stability of BFO-BT-Ni-0.5. The values of its magnetization intensity (Mr) and magnetic field intensity (Hc) also increase first and then decrease as x increases. When x = 2.0, the ceramic achieves the optimal ferromagnetic properties (Mr = 0.117emu/g), and still exhibits enhanced ferromagnetism on a macroscopic scale. Therefore, by doping BiFeO3-based solid solutions with NiO_x, the various properties of the ceramic material have been enhanced, making it a new type of advanced multifunctional material that can be applied in the high-tech field.

3. Non-metallic doping

Non-metallic doping is also an indispensable method for modifying perovskites [10]. In the field of photocatalysis, Guo et al. [11] introduced Br into $Cs_2AgBiCl_6$ perovskite, thereby developing a highly efficient visible light photocatalyst based on $Cs_2AgBiCl_6$. Based on the optical absorption characteristics, it is indicated that the doped sample has a red shift in the absorption edges. By using the Tauc formula, the optical band gap (Eg) of the sample is calculated to be reduced, thereby effectively broadening the visible light absorption range and promoting the generation of more photoelectrons. From the time-resolved photoluminescence spectra (TRPL) and electrochemical impedance spectroscopy (EIS), it can be concluded that the carrier lifetime and transmission efficiency may also be enhanced, thereby leading to an increase in the photocurrent. Furthermore, experiments were conducted to investigate the effect of different Br doping concentrations on the degradation rate of methyl red. It was found that $Cs_2AgBiCl_4Br_2$ exhibited the highest activity. The generated photoelectrons in it have better charge transfer ability and longer carrier lifetime.

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Therefore, more photogenerated electrons can be transferred to the material surface to participate in chemical reactions, thereby achieving higher photocatalytic performance. This also points out a path for the development of highly efficient photocatalysts.

In the research on battery applications, Hang et al. [2] enhanced the catalytic activity by doping $Sr_2FeCo_{0.6}Mo_{0.4}O_{5+\delta}$ (SFCM) with S, B, and P elements respectively. The substitution of oxygen elements in SFCM by S doping not only generates more adsorbed oxygen as the active sites for the oxygen evolution reaction (OER), but also accelerates the migration of adsorbed oxygen, enhances the adsorption of OH- on the catalyst surface, and speeds up the OER reaction rate. This improves the catalytic activity of the catalyst, making the OER reaction more favorable both in terms of kinetics and thermodynamics. The introduction of B has changed the content of lattice oxygen in SFCM perovskite oxides, enabling more lattice oxygen to be activated and stabilizing the lattice oxygen species in SFCM perovskite oxides. This prevents excessive loss of lattice oxygen and enhances the catalytic activity and stability of the electrocatalyst. P replaced the high-valent Mo element in the SFCM electrocatalyst, generating more oxygen vacancies, which changed the specific surface area of the catalyst, fully exposing the active sites of the catalyst, and enhancing the catalytic activity and the intrinsic reaction activity of the catalyst. This provides us with a new design idea for modifying catalyst materials by using non-metallic element doping.

In order to efficiently degrade phenolic pollutants, Yang et al. [12] modified the $LaCoO_3$ perovskite by S doping under an argon atmosphere, significantly enhancing the reaction efficiency of this catalyst in the system of peracetic acid (PAA) for degrading bisphenol A (BPA). The results show that S-$LaCoO_3$-2 (with a mass ratio of S to $LaCoO_3$ of 3:16) has the best catalytic degradation effect. Electrochemical tests revealed that in the catalytic degradation process of BPA by the S-$LaCoO_3$-2/PAA system, there exists a direct electron transfer pathway. The S doping can increase the adsorbed oxygen, Co (II) and Vo ratios on the surface of $LaCoO_3$, reduce the lattice oxygen content, and lead to a decrease in the charge transfer impedance (Rct). According to the EIS test results, S-$LaCoO_3$-2 has the smallest Rct value and the highest redox potential. The electron transfer between the catalyst and PAA is accelerated, which is conducive to the progress of the catalytic reaction. The quenching experiment combined with EPR demonstrated that organic free radicals and singlet oxygen were the main reactive oxygen species responsible for the degradation of BPA in the S-$LaCoO_3$-2/PAA system. The presence of these two substances, combined with the direct electron transfer pathway, enables the S-$LaCoO_3$-2/PAA system to efficiently remove BPA from water.

4. Co-doping

The co-doping of perovskite also plays a significant role in enhancing its performance. In the field of photocatalytic water splitting, Kaori Takagi et al. [13] successfully synthesized $CaTiO_3$ powder doped with Al, Sc and Mg using a fluxing agent method, and formed a single-phase perovskite structure. When Al^{3+} replaces the Ti^{4+} sites, due to its lower valence state, it creates positive charge vacancies, which can reduce the harmful excess electrons generated by Vo, optimize the carrier concentration, and at the same time cause local lattice distortion, forming deep-level defects. The introduction of Sc^{3+} significantly inhibited the grain growth, resulting in smaller particles, which was beneficial for shortening the distance that charge carriers diffuse to the surface. However, it would lead to a decrease in the crystallinity of the crystal. The introduction of Mg^{2+} not only can alleviate the local lattice distortion caused by Al^{3+}, effectively inhibit the formation of deep-level defects, but also can improve the crystallinity of the crystal and compensate for the defects brought by Sc. These findings indicate that the $CaTiO_3$ doped with Al, Sc and Mg can serve as a highly promising material for efficient water splitting and a wide range of photocatalytic applications.

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In terms of denitrification performance, Tang et al. [14] used the sol-gel method to co-dopant Ce and Cu in the $LaMnO_3$ perovskite. Through the study of Ce-doped $LaMnO_3$ perovskite catalysts, it was found that when the proportion of Ce atoms replacing La atoms at the A site was 0.1, the denitrogenation activity of the catalyst was the strongest, and the NO conversion efficiency reached 86.7% at 350℃. Based on this, $La_{0.9}Ce_{0.1}Mn_{1-y}Cu_yO_3$ (with y = 0.05, 0.1, 0.2, 0.4) was prepared by doping Cu. According to the experimental results, when y = 0.2, the denitration efficiency of the catalyst is the highest. The NO conversion efficiency reaches 91.8% at 350°C. Through the characterization experiments, it was found that the partial substitution of Cu for the B sites of Mn affects the size of the tolerance factor and the degree of lattice distortion of the perovskite, thereby changing its unit cell volume and average lattice size. In this state, the $La_{0.9}Ce_{0.1}Mn_{0.8}Cu_{0.2}O_3$ catalyst possesses an appropriate mesoporous structure and the largest number of Cu active sites, resulting in strong intermetallic interactions and a high surface chemical adsorption oxygen concentration. Therefore, the $La_{0.9}Ce_{0.1}Mn_{0.8}Cu_{0.2}O_3$ catalyst exhibits the best denitration efficiency among the catalysts prepared by doping Cu into $La_{0.9}Ce_{0.1}MnO_3$ perovskite, which is conducive to promoting its practical application in the industrial field of denitration.

5. Conclusion

This article systematically reviews the regulatory effects of various doping strategies on the physical and chemical properties of perovskite materials (particularly $CaTiO_3$-based materials). In terms of metal doping, research has confirmed that the introduction of transition metals such as Fe, Co, and Ni can significantly optimize the catalytic activity and ionic conductivity of perovskite materials. In terms of non-metallic doping, the introduction of elements such as Br, S, and P effectively regulated the bandgap structure and surface chemical properties of the material. In the case of co-doping, the synergistic effects [15] of multiple elements such as Al/Sc/Mg and Ce/Cu further optimized the carrier separation efficiency and surface reaction kinetics, enabling the perovskite to exhibit superior activity compared to single-doped materials in the applications of water splitting for hydrogen production and low-temperature denitrification. Although the various doped and modified perovskite materials reviewed in this article have demonstrated promising application prospects, there are still some shortcomings. Most current studies are still limited to laboratory-scale synthesis and testing, with insufficient consideration of cost control. Future research should focus on promoting the transition of perovskite materials from laboratory research to industrial application.

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