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Design of Nanomaterial-Based Catalysts and Their Applications in Green Chemistry

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Abstract. Nanomaterials show great potential in catalysis because of their unique chemical and physical properties. In this paper, the basic principles, advantages and disadvantages of the catalytic design of nanomaterials, their impact on the environment, and their wide application in the fields of energy, environment, and chemical industry are reviewed. First, the definition and disadvantages of nanocatalysts are introduced, the catalytic reaction mechanism of nanocatalysts is discussed, and the comparison with metal nanoparticles and metal oxides is made. Secondly, the molecular structure of nanomaterials is discussed in detail, including the selection of catalytic activity and catalytic stability, and then the application examples of nanomaterials in carbon dioxide emission reduction, water cracking. And biomass conversion is analyzed. Finally, the impact of nanomaterials on the environment and solutions is summarized, as well as the advantages of nanomaterials in enterprises and factories, and the future research direction is prospected. This paper aims to provide comprehensive theoretical guidance for the design and application of nanomaterials catalysis.

Keywords: nanomaterials, catalytic design, sustainability, stability, chemicals

1. Introduction

1.1. Definition of nanomaterial-based catalyst

As a substance that can promote chemical reactions, a catalyst plays an important role in many fields. In recent years, with regard to the rise of nanomaterials, nanomaterial catalysts have been widely studied and applied in different fields. Anomaterials are materials whose structural components have at least one dimension less than 100 nanometers. Materials that are nanoscale in one dimension (and extend in the other two) are layers, such as thin films or surface coatings. Some features of computer chips fall into this category. Materials at the two-dimensional nanoscale (and extending in one dimension) include nanowires and nanotubes. Materials at the three-dimensional nanoscale are particles, such as precipitates, colloids, and quantum dots (tiny particles of semiconductor materials). Nanocrystalline materials composed of nanoscale grains also belong to this class [1]. When we use catalysts in industry, the first thing we have to consider is high catalytic

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efficiency, strong stability and other characteristics. However, nanomaterial catalysts have just such characteristics. Nanocatalysis is considered a productive technology due to the large surface area and extended catalytic efficiency of nanoparticles (NPs) [2]. Therefore, nanomaterial catalysts are often suitable for accelerating chemical reactions in various industrial processes, especially in green chemistry.

1.2. Advantages of nanomaterial-based catalyst

Due to the special structure of nanomaterials, it can remain stable under reaction conditions, ensuring that it can maintain efficient catalytic performance during a long reaction process. Also, the catalysts could be used for the industrial products manufacturing process with high conversion rate. For example, nano-rare earth oxide/zinc oxide can be used as a catalyst for the selective oxidation of ethane to ethylene by carbon dioxide. With this nano-catalyst, the reaction of ethane and carbon dioxide can be highly selectively converted into ethylene, with the conversion rate of ethane up to 60% and the selectivity of ethylene up to 90% [3]. At the same time, the nanomaterial catalyst has strong anti-poisoning ability and activity a complicated environment. The size, shape, and composition of nanomaterials can be precisely regulated, which can further optimize the reaction process, thereby reducing the generation of by-products and improving the reaction efficiency. Some nanomaterial catalysts can react under mild conditions, reduce environmental energy consumption and environmental pollution, and contribute to future sustainable development. Nanomaterials contain the functions of active ingredients and carriers, which can be used to catalyze the reaction, simplify the process flow and reduce the cost. The advantages of nanomaterial catalysts can make it widely used in various fields. Figure 1 shows a schematic representation of nanomaterials and their applications



Figure 1. A schematic representation of nanomaterials and their applications [4]

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1.3. Disadvantages of nanomaterial-based catalyst

Nanomaterial catalysts also have some disadvantages despite so many advantages. In the chemical process, for the selection of catalysts, people usually choose to use low-cost catalysts for chemical reactions. However, the high price and cost of some nanomaterials (platinum, palladium, gold, etc.), low yield and complex synthesis process limit their application in chemical processes. At the same time, the small size of nanomaterial catalysts makes the complexity of separating catalysts from the final product create environmental and economic barriers that limit their scope [5]. Their small size also makes them easy to enter the tissues and cells of living organisms, posing potential health risks and even cancer risk. On the other hand, the disadvantage of traditional heterogeneous catalyst systems is that the available surface area of the reaction molecules is reduced, which inhibits their efficiency and thus affects their use in the process. Most industrial heterogeneous catalysts have a high surface area attached to the active component [5]. Proximity to all active sites is essential to achieve rates and selectivity comparable to homogeneous catalysts. Since the active site exists only on the catalyst surface, this will reduce the overall reaction efficiency [5]. Therefore, in the future, we still need to continuously strengthen the price, cost, production technology and security.

1.4. Research motivation

With the development of science and technology, the problem of environmental pollution is increasing, which is more important for the design of some green materials. From a number of perspectives, we need to design a catalyst that can reduce the emission of harmful substances in chemical reactions, such as Carbon dioxide, carbon monoxide, sulfur dioxide, etc., and an indispensable feature as a catalyst: faster reaction rates. Nanomaterials as catalysts can improve the efficiency of the catalyst in the process, so that the generated products have high purity and high yield, reduce the generation of by-products, so that the reaction is carried out under more moderate conditions, reducing the input of equipment. From the design point of view, the nanomaterial catalyst we designed will be more environmentally friendly in green chemistry, and can help deal with pollutants and protect the environment. It is more economical, low-cost, and can be applied in many fields, which promotes technological innovation and increases economic benefits.

2. Design of nanomaterial-based catalyst

2.1. Raw material

2.1.1. Metal nanoparticles /metal oxides nanocatalysts

In recent years, metal nanoparticles have been a new term in the field of nanoparticles. Health-beneficial precious metals such as gold, silver, and platinum are used by scientists to synthesize new nanoparticles and are named metal nanoparticles [6]. The synthesis of metal nanoparticles and their structures and nanomaterials is the focus of current research in the scientific community. Due to their special characteristics, they can be used in catalysis, production of composite materials such as polymers, disease diagnosis and medical research, sensor technology, photoelectric recording media labeling [7], etc. The preparation and stabilization of metal nanoparticles are usually performed by different chemical and physical methods, such as electrochemical changes, chemical reduction, and photochemical reduction [8]. At the same time, the selection of the preparation method of metal nanoparticles is also crucial, because in the synthesis process of nanoparticles, the interaction

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kinetics of metal ions and reducing agents, the adsorption process of stabilizers and metal nanoparticles, and various experimental technologies on their morphology (structure and size), stability and physical and chemical properties will have a crucial impact on the final result. Silver nanoparticles have recently become the subject of intense research in the scientific community. Silver nanoparticles are particles of silver, ranging in size from 1 to 100 nanometers. Although often described as "silver", some are composed of a large proportion of silver oxide due to the large ratio of silver atoms on the surface to silver atoms in the body. At present, researchers have conducted research on the medical aspects of silver nanoparticles, including bone cement, surgical instruments, surgical masks, etc. In addition, studies have shown that appropriate amounts of ionic silver are suitable for wound treatment [9]. Due to the excellent and unique physicochemical properties of silver nanomaterials, these nanomaterials have received extensive attention in the use of SERS for biomedical imaging. In fact, the surface plasmon resonance and large effective scattering cross sections of individual silver nanoparticles make them ideal candidates for molecular labeling [10]. Therefore, many targeting silver oxide nanoprobes are currently being developed.

2.1.2. Carbon-based nanocatalysts

A carbon-based nanocatalyst is a kind of composite material that can load metal oxide nanoparticles on carbon-based material. High specific surface area, excellent electron propagation ability and chemical stability are the characteristics of this material, so it has great potential in the fields of energy conversion, environmental treatment and chemical synthesis [11]. Advantages: Nano-carbon materials (such as carbon nanotubes, nitrogen-doped carbon, etc.) provide a large number of active sites for catalysis, which significantly improves the catalytic efficiency. Electronic properties: by doping (such as nitrogen, phosphorus, etc.) or composite with other materials, the structure of carbon-based catalysts is changed, which greatly increases the catalytic performance [12].

2.2. Molecular structure

2.2.1. Catalytic activity

The catalyst has the ability to increase the reaction rate. This ability of the catalyst is called the activity of the catalyst. It is affected by the adsorption of reactants on the catalyst surface. One of the factors controlling catalyst activity is chemisorption. The bond formed between the catalytic surface and the reactants during the adsorption process cannot be too strong or too weak. The bond formed between the catalyst and the reactant must be strong enough for the catalyst to be active. If it is too strong, the reactant will be adsorbed on the surface of the catalyst, leaving no further adsorption space for the new reactant and unable to continue the reaction [12].

2.2.2. Catalytic selectivity

The catalyst is a highly specific compound. They have the ability to direct reactions to produce specific products. If you want to get different products, you need to use the same reactants, different catalysts. This is called catalyst selectivity. The special property of the catalyst is that it is highly selective. They can speed up one particular reaction while preventing another from occurring. Therefore, a specific catalyst can only catalyze a specific reaction. They cannot catalyze another reaction of the same type. For example, when nickel is used as a catalyst, hydrogen reacts with carbon monoxide to form methane; Methanol is produced when the mixture of zinc oxide and

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chromium oxide is used as a catalyst. Methanol is formed when only copper is used as a catalyst [13].

2.2.3. Catalytic stability

Catalyst stability refers to the ability of a catalyst to maintain its activity and structural integrity over a period of time under specific reaction conditions. This characteristic is mostly applied in industry, where the catalyst can run for a long time in the case of function loss, which will eventually affect the overall benefit and final result of the chemical reaction [13]. The catalytic stability of nanomaterials is closely related to their molecular structure, including the influence of molecular structure on the active site. The molecular structure of the catalyst determines the geometric and electronic properties of the active site, thus affecting its stability. For example, single-atom catalysts (SACs) show excellent stability and activity in various catalytic reactions due to their highly dispersed active sites and unique electronic structures [14].

3. Application

3.1. CO_2 reduction

From the mid-1960s to 1980, global temperatures increased by 0.2°C [15]. Exacerbating the greenhouse effect and causing the polar ice sheets to melt; Animals cannot live a normal life, but carbon dioxide emissions will cause some degree of environmental damage, such as melting glaciers, floods, heat waves, droughts, cyclones, hurricanes and food security problems [16]. In the chemical process, we want to do as much as possible to reduce carbon dioxide emissions, for the problem in the process, we can take the method of carbon dioxide reduction. The so-called carbon dioxide emission refers to the selective and efficient conversion of carbon dioxide into more valuable chemicals [17]. The nanomaterial catalysts we are studying now can just promote the reduction of carbon dioxide, which can be divided into the following types: electrocatalytic reduction [18], photocatalytic reduction and a small amount of [19] thermal catalytic reduction [20]. So-called photocatalysis [21] is the most important method of converting carbon dioxide into hydrocarbon fuels to mitigate the greenhouse effect and to ensure the global carbon cycle using inexhaustible solar energy resources. The electrocatalytic reduction mechanism of carbon dioxide involves multiple electron transfer steps and adsorption processes [22]. Changing the electronic structure is an effective method to improve the catalytic performance. For example, controlling the D-band center of Pt by alloying changes the adsorption energy of O_2 at the active Pt site, resulting in different performance in oxygen reduction reaction [23]. There is great interest in converting carbon dioxide into value-added products, such as formaldehyde, formic acid and methanol [24]. We have also mentioned the advantages of using nanomaterials as catalysts, including large surface-volume ratio, abundant active sites, atomic thickness and high proportion of coordination unsaturated surface sites, making them ideal candidates for carbon dioxide conversion materials with high photocatalytic activity [25]. Figure 2 shows schematic energy diagrams of photothermal catalytic carbon dioxide reduction over nanomaterials.

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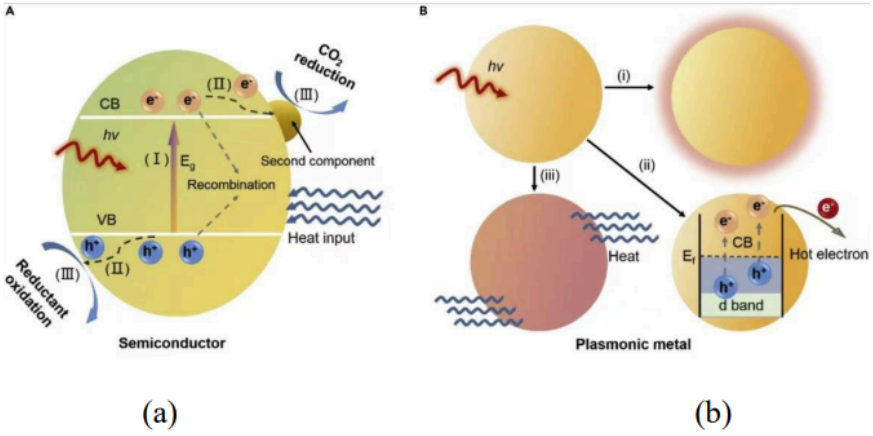


Figure 2. Schematic energy diagrams of photothermal catalytic carbon dioxide reduction over nanomaterials; (a) Schematic illustration of photothermal catalysis over a semiconductor with external heat input (CB, conduction band; VB, valence band; Eg, band gap): (I) light absorption, (II) charge separation, and (III) surface reaction.(b) Schematic illustration of the processes resulting from LSPR effect over plasmonic metal structures (Ef, Fermi level): (i) local enhancement of the electric field, (ii) hot-electron injection, and (iii) photothermal effect [20]

3.2. Water splitting

Hydrogen plays an important role in our lives, but from the current point of view, there is a shortage of hydrogen supply. To solve this limitation, we can make hydrogen by splitting water. The so-called water decomposition, in a simple sense, will be through some types of water into hydrogen and oxygen. These types mainly include: photocatalytic water decomposition [26], electrocatalytic water decomposition [27], thermocatalytic water decomposition [28] and photoelectro-catalytic water decomposition [29]. Where thermal decomposition catalyzes water decomposition, the main disadvantages are the low yield of hydrogen and the extremely high temperature requirements of the reaction [30]. However, photoelectrocatalytic water decomposition using nanomaterials is currently the most promising technology, which can make water decomposition easier and cheaper [30]. The basic principle of photochemical water decomposition is to convert solar energy into hydrogen gas by applying an external bias to a photovoltaic material immersed in an electrolyte that contains REDOX pairs, one of which is made of a semiconductor, exposed to light and capable of absorbing it. The electricity is then used for water electrolysis [30]. The structure of nanomaterials can directly control photon absorption and electrochemical catalysis, which has a greater impact on the electrocatalytic performance of photoelectrodes than the light collection ability, but this property is usually ignored. In fact, designing nanostructures is an adjustment process aimed at balancing a series of different processes that compete with each other in a complex system to optimize PEC performance. The most important task is to maximize the number of electrocatalytic sites to form a more efficient electrode/electrolyte interface, while reducing the number of charge recombination centers [31]. As mentioned above, due to the small size of nanomaterials, they have a large surface area, which speeds up the process of water catalysis and improves the reaction rate. All in all, nanomaterials have great potential and development prospects in catalytic water decomposition, reduce environmental pollution, and are environmentally friendly catalysts.

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3.3. Biomass conversion

Biomass conversion is the conversion of animal and plant waste (fallen leaves, apple cores, straw, bones, etc.) into useful resources in a specific way. Due to the scarcity of non-renewable energy and the increasing demand for energy in the world, biomass conversion is particularly important, which is an important direction in the field of renewable energy, providing the world with more diverse choices in energy, and biomass is low cost, easy to obtain, and environmentally friendly, which is in line with the characteristics of green chemistry that we often say. Biomass energy refers to the renewable energy that converts solar energy into chemical energy in plants through photosynthesis and then into heat energy and electric energy through different processing forms [32]. The ability of plants to use atmospheric carbon dioxide for photosynthesis makes it known as a "carbon neutral" fuel, which means that it does not introduce new carbon into the atmosphere [33], reducing carbon emissions, and catalysts still play an important role in the conversion process. Compared to traditional reactions, pyrolysis is used to continuously produce renewable energy and chemicals from biomass, but the production cost of biomass pyrolysis hinders its wider application [34]. Nano-catalyst is the most promising catalyst in the future. It has a high specific surface area and abundant active sites, which can catalyze the conversion reaction of biofuels more efficiently. Due to its high catalytic activity, it can achieve efficient catalytic conversion under low temperature and pressure conditions, thus reducing energy consumption and helping to improve the production efficiency and energy utilization efficiency of biofuels [35]. Therefore, they are widely used in the fields of green chemistry and renewable energy development.

4. Advantages of nanomaterial-based

4.1. Economic benefits (business/factory)

Nanocatalyst raw materials are principally categorized into metals, metal oxides, and carbon-based substances, each exhibiting distinct environmental trade-offs. Noble metal catalysts (e.g., Pt, Pd, Au) demonstrate superior catalytic activity, yet their environmental footprint is compounded by ecotoxicological risks from mining/refining processes, coupled with inherent scarcity and prohibitive costs. Metal oxide alternatives (e.g., Fe_3O_4, TiO_2) present improved cost-effectiveness and reduced ecological impact, though certain synthesis routes remain energy-intensive or reliant on hazardous reagents. Carbon-based materials (e.g., carbon nanotubes, graphene) emerge as sustainable candidates due to natural abundance and recyclability, yet industrial-scale production methods such as chemical vapor deposition necessitate rigorous emission mitigation protocols [36].

Advancements in environmental sustainability currently target three pathways: implementing green synthesis (e.g., bio-templated assembly, low-temperature hydrothermal methods); establishing closed-loop recovery systems for precious metals to alleviate resource depletion; and engineering biodegradable architectures like metal-organic frameworks. Future investigations must reconcile catalytic efficiency with ecological constraints through innovations in atom-economical synthesis and process intensification, thereby enabling practical deployment of green catalytic systems in energy conversion and environmental remediation [37].

4.2. Environmental benefits

Nano-catalysts are remarkably efficient because of their small particle size, which provides a significantly larger surface area compared to traditional materials. This distinctive feature enables

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them to accelerate chemical reactions, improve efficiency, and even operate effectively at lower temperatures and pressures, which yields substantial energy savings. These benefits make nano-catalysts as a game-changing innovation for industries and environmental protection [38]. One of the most remarkable aspects of nano-catalysts is their ability to be reused repeatedly. They are exceptionally stable, maintaining their activity through numerous reaction cycles. This means we do not need to continuously produce new catalysts, which conserves resources and supports sustainable practices, a win-win scenario for both industry and the environment [39].

Furthermore, nano-catalysts are instrumental in tackling major environmental challenges. They can purify air and water by breaking down harmful pollutants, thereby improving the health of our environment. Additionally, they enhance renewable energy technologies, such as enhancing solar energy capture and hydrogen production, marking a crucial stride towards a cleaner, greener future [40]. Nano-catalysts are also making waves in other domains. In medicine, they are being utilized to deliver drugs with greater precision, improving treatment efficacy while reducing side effects. In chemical manufacturing, they enable the creation of fewer byproducts and enhance the quality of the final product. In energy storage, they are extending the lifespan and performance of batteries [41].

In summary, nano-catalysts are unlocking new possibilities for cleaner, more efficient solutions across a wide range of fields. They are helping us utilize resources more intelligently, reduce waste, and mitigate pollution. As research continues, these tiny catalysts are poised to play an ever-increasing role in building a sustainable future.

5. Environmental impact of nanomaterial-based catalyst

5.1. The environmental friendliness of catalyst raw materials

But the synthesis of nano-catalysts is not without its environmental drawbacks. During production, chemical reactions can generate pollutants that pose risks to the environment. We introduce it from the following two aspects.

5.1.1. Pollution from raw material extraction and processing

The synthesis of metal-based nano-catalysts typically involves the reduction of metal precursors, such as metal salts or complexes, to form nanoparticles. This reduction process often employs reducing agents like hydrogen gas, ethanol, or other organic solvents. While effective, these agents can release harmful gases, such as hydrogen sulfide, carbon dioxide, or volatile organic compounds (VOCs)—into the atmosphere if not carefully managed. This not only contributes to air pollution but also exacerbates climate change. Moreover, the organic solvents used in these reactions pose another environmental risk: if not properly disposed of or treated, they can contaminate water sources. Solvent residues and by-products from the synthesis process can seep into waterways, harming aquatic ecosystems and underscoring the importance of effective waste management [42].

Carbon-based nano-catalysts, synthesized through methods like chemical vapor deposition (CVD) or sol-gel processes, come with their own set of environmental challenges. These techniques often operate under high temperatures and pressures and may involve toxic gases, such as carbon monoxide, ammonia, or other reactive species. Without stringent controls, these by-products can pollute both air and water, while also posing health risks to workers involved in the synthesis process. For instance, CVD methods frequently employ carbon-based precursors that generate fine particulate matter, a significant contributor to air pollution [40].

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5.1.2. Waste and byproducts from nanocatalyst synthesis

To address these environmental concerns, it is essential to adopt robust waste treatment and recycling practices throughout the synthesis process. The main waste generated during the production process is waste gas and wastewater. For waste gas, collection and purification can be carried out. Harmful gases produced during the synthesis process, such as hydrogen, carbon monoxide, and volatile organic compounds (VOCs), can be treated using waste gas collection systems such as activated carbon adsorption, catalytic oxidation, or condensation recovery. Activated carbon adsorbers are effective at capturing VOCs, while catalytic oxidation converts harmful gases into harmless substances (such as carbon dioxide and water) using catalysts. The captured waste gases can also be separated using gas separation membrane technology to recover valuable gases, such as hydrogen or other useful gases, for use in other reactions. Finally, a dynamic gas monitoring system should be installed to continuously monitor the concentration of harmful substances in the waste gas, allowing for timely adjustments to the reaction conditions and reducing pollutant emissions [43].

For wastewater, physical and chemical methods such as precipitation, filtration, and adsorption can first be used to remove heavy metal ions or dissolved pollutants. Activated carbon adsorption and ion exchange are common treatment methods. Additionally, for some organic pollutants, biological treatment methods can be applied, utilizing microorganisms to break down organic matter in the wastewater. Biological membrane reactors and biofilters can effectively remove organic pollutants from the wastewater, achieving purification. Finally, during the wastewater treatment process, membrane filtration (such as reverse osmosis technology) can be used to recover water resources and reduce water waste. The recovered water can be reused in cooling systems or other production processes, further improving resource utilization efficiency [44, 45].

In summary, for the waste generated during the production process, we need to carry out a process of collection, separation, and reuse to minimize the environmental impact.

5.2. Strategies to reduce pollution in the production process

Industrial nanocatalyst production requires integrated solutions to address metal waste, toxic emissions, and energy intensity. Green synthesis techniques demonstrate promise: biosynthesis using plant-derived reductants reduces toxic chemical use by 70%, while low-temperature hydrothermal methods (<200°C) achieve 30% energy savings with minimized by-products. Closed-loop resource recovery is critical—hydrometallurgical processes recover >95% of platinum group metals, and catalyst regeneration via thermal activation restores 80% initial activity. Process intensification strategies include microfluidic reactors, enhancing mass transfer efficiency (yield >90%) and plasma-assisted synthesis, reducing reaction time by 50%.

Renewable energy integration (e.g., solar-powered electrolysis) cuts Scope 2 emissions by 60%. For emission control, catalytic oxidizers degrade 99% of VOCs, while hybrid membrane-electrochemical systems remove 98% of heavy metals from wastewater. Biodegradable MOF catalysts with tunable hydrolysis rates (6-12 months half-life) require balanced Lewis acidity and hydrolytic stability. Regulatory frameworks should mandate life-cycle assessment (LCA) metrics, enforcing AE >85% and ISO 14001 compliance across supply chains.

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6. Conclusion

In this article, we have delved into the raw materials, preparation methods, application scenarios, advantages, disadvantages, and corresponding strategies to reduce the pollution of manufacturing nanocatalysts. Due to their high specific surface area and unique catalytic properties, nanocatalysts exhibit broad application prospects in fields such as energy, environment, and chemical industries industrial applications, especially in the green chemistry field. The raw materials for nanocatalysts typically include metals, metal oxides, and carbon-based materials. Preparation methods are diverse, and the application fields are also varied, leading to significant economic benefits. However, both the preparation and application processes can lead to environmental pollution. Therefore, it is crucial to emphasize methods that minimize the pollution associated with the production of nanocatalysts. In conclusion, nanocatalysts offer substantial potential for a variety of applications. By continually refining their preparation methods and treatment technologies, we can address existing challenges and unlock more extensive applications in the future.

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