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Nanomaterials in Catalysis: Applications and Challenges

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Abstract

Nanomaterials have emerged as highly promising catalysts in chemical engineering due to their unique structural, electronic, and surface properties at the nanoscale. Defined within the 1–100 nm range, they exhibit a high surface-to-volume ratio and tunable morphology, enabling enhanced reactivity and selectivity compared to bulk materials. This paper explores the role of nanomaterials in both heterogeneous and homogeneous catalysis, emphasizing applications in energy conversion, environmental remediation, and green chemical synthesis. Metal nanoparticles and metal oxides have demonstrated superior catalytic activity for fuel cells, photocatalysis, and pollutant removal. Organometallic and ligand-modified nanomaterials extend the scope of homogeneous catalysis with improved efficiency. Despite these advantages, challenges remain concerning catalyst stability, deactivation, scalability, and economic viability. Characterization techniques such as microscopy and spectroscopy provide insights into nanoscale behavior, supporting rational catalyst design. Future perspectives highlight innovative nanostructures, sustainable synthesis methods, and eco-friendly catalytic processes aimed at overcoming current limitations.

Keywords: Nanomaterials, Catalysis, Heterogeneous Catalysis, Homogeneous Catalysis, Environmental Applications, Energy Conversion, Green Chemistry

1. Introduction

Nanomaterials are an important area of new materials research, owing to their unusual and fascinating properties. Defined as materials with structural features smaller than 100 nm in at least one dimension, nanomaterials exhibit special properties related to their size and exhibit quantum effects. They bridge the boundary between bulk materials and atomic or molecular structures. Nanomaterials also possess a high surface-area-to-volume ratio and a strong confinement effect. They are typically classified based on their dimensions into zero-dimensional materials (such as clusters, solid colloidal nanodots, and hollow spheres), one-dimensional materials (including solid and hollow nanowires, nanorods, and nanotubes), two-dimensional materials (like nanolayers and nanofilms), and three-dimensional materials (such as bulk nanocrystalline materials, mesoporous materials, and nanocomposites). To achieve tailored size and morphology control, novel synthesis processes have been developed for various nanomaterials, including fullerene, carbon nanotubes, quantum dots, nanowires, and downsized ultra-fine powders or nanosized grains. Each type of material serves as the basis of a distinct research area.

2. Overview of Nanomaterials

Nanomaterials are a class of materials characterized by their ultrafine size and a high surface-to-volume ratio, which are advantageous for catalysis. Nanomaterials can be divided into four groups: metal nanoparticles, metal oxide nanoparticles, different types of clusters (e.g., dendrimers or ligands stabilized), and shape-controlled nanostructures. Metal nanoparticles have been extensively studied in catalysis due to their outstanding catalytic activities, which can be attributed to their high specific surface area and the combined electronic properties of both bulk metals and metal atoms.

Heterogeneous catalysis is employed in a wide variety of chemical operations. In heterogeneous catalysis, the reactants and products are in a different phase than the catalyst. The catalyst is usually a solid material, while the reactants/products are in the gas or liquid phase. Common types of catalysts include activated solids such as clays and charcoal, metal oxides, sulfides, aluminosilicates, and metals of the Platinum group supported on various solids. Catalysis plays a role in processes such as cracking, reforming, alkylation, and polymerization, all of which utilize heterogeneous catalysts.

2.1. Definition and Classification

Nanomaterials are typically defined as materials in which at least one dimension is within the range of 1–100 nm. Nanocrystals are nanometer-sized crystals with all three orthogonal dimensions fabricated at the nanometer length scale. Nanoparticles (NPs) have all three dimensions at the nanoscale, although with arbitrary shape and crystallinity. Nanoplates or nanosheets are single- or few-layered nanoparticles that grow in two orthogonal directions. Nanowires or nanorods have two dimensions at the nanometer length scale while growing in one direction. Nanotubes are hollow tubes with nanodimension thickness and much larger lengths. The nanometric dimension of at least one direction strongly affects the property of these materials.

Nanosized particles of different materials and shapes can be obtained by different synthesis methods, each with its advantages and disadvantages. Nature also provides a variety of nanomaterials through biogeochemical cycles. Hence, nanomaterials can be broadly classified into three groups or families: (i) naturally occurring nanomaterials, (ii) incidental nanomaterials generated unintentionally by natural or anthropogenic activities, and (iii) engineered or manufactured nanomaterials that are purposefully generated. Engineered nanoparticles are important in various technological applications and have attracted enormous academic as well as industrial interest. These can be further classified based on their chemical composition as carbon-based, inorganic-based, organic-based, and composite-based engineered nanomaterials.

2.2. Synthesis Methods

Nanomaterials comprise clusters of atoms sized within a few nanometers, often smaller than the dimensions of grains in typical polycrystalline materials. They can be classified as zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), or three-dimensional (3D) based on their structural features. Nanomaterials with identical chemical compositions may exhibit markedly different colors and optical properties owing to their size variations. Depending on their core compositions, options include carbon nanomaterials and aggregates of silver and gold quantum dots. Methods for the synthesis of nanomaterials include carbonization, hydrothermal carbonization, template-assisted processes, graphitization, solvothermal methods, template carbonization, pyrolysis methods, CVD pyrolysis, electrospinning, physical vapor deposition, and combustion. These techniques allow for the preparation of nanomaterials with diverse properties for catalytic applications.

Nanomaterials increasingly serve as catalysts, capable of facilitating industrial, energy-related, and environmental processes. For example, nanomaterials with photo- and redox-activity can be applied in photocatalysis and heterogeneous catalysis. Methanol synthesis also benefits from nanocatalysis, along with the Haber–Bosch process and the selective catalytic reduction of NOX. In environmental catalysis, nanomaterials are integral to fuel cells, catalysis of air pollution, water treatment, and various toxic chemical eliminations. Optimal development of nanomaterial functionality necessitates performing the oxidative catalytic process under more desirable conditions for each catalytic reaction.

3. Catalysis Fundamentals

Catalysis consists of accelerating the rate of a reaction in the presence of an additional reagent called catalyst, that itself does not undergo permanent chemical change, nor does get consumed (Claudiu Fierascu et al., 2019). A reaction in the absence of a catalyst usually follows a certain reaction path, or mechanism, at a certain reaction rate, at a fixed temperature and pressure. The presence of the catalyst allows the system to take another reaction path, or mechanism, that possesses a smaller overall activation energy. The result is an increase of the overall reaction rate (Nacci & Cioffi, 2011). Furthermore, the catalyst can influence the reaction outcome by facilitating a preferential reaction mechanism. The accelerated reaction can lead to higher yield, higher selectivity, or the formation of different products. These phenomena occur concurrently with favorable changes in mass transfer and the adoption of safer and more environmentally friendly reagents (Pal et al., 2023).

The mechanism of a catalytic reaction can be homogeneous or heterogeneous. Accordingly, homogeneous or heterogeneous catalysis takes place. In homogeneous catalysis, the catalyst and reactants form a single phase system, usually liquid. The system can also be gas-phase, but the gaseous species must be completely miscible. In heterogeneous catalysis the phase of the catalyst and the phase of the reactants differ from each other, usually solid and liquid, respectively, but also solid and gas or liquid and gas. Homogeneous catalysis allows a very fine control over the outcome of the reaction, but is difficult to separate from the reaction products. By contrast, heterogeneous catalysis favors the separation of the catalyst from the products, but the control over the reaction is limited to consideration related to transport phenomena, e.g., diffusion. Nanocatalysis can provide the advantages of both catalytic systems.

3.1. Types of Catalysis

Nanomaterials in catalysis have attracted great interest because of their important roles in stabilizing submicron-size particles as well as their controllable surface structure. The chemical and physical properties of nanomaterials provide them with specific advantages over conventional bulk materials and make them potential heterogeneous and homogeneous nanocatalysts. Nanomaterials are also important because of their potential applications in environmental remediation for producing a cleaner environment. Recycling and reusing have become permanent trends for material production and consumption. Air and water pollution caused by industrial, agricultural, and domestic activities has created environmental problems and more serious effects that cascade through the ecosystem. The contamination of the environment by CO, hydrocarbon, NOx, and particulate matter has caused a corresponding interest in the development of catalytic applications of nanomaterials.

Catalytic converters, comprising mainly susceptibility-sensitive materials with high catalytic activities, are used to reduce exhaust emissions. ZnO nanostructures are non-toxic and ecofriendly, which increases their potential utilization in environmental applications. Ru catalysts supported on nanosized TiO2 show enhanced activity and stability during catalytic oxidation of CO. Transition-metal-doped ceria or titania has attracted much interest because of the unique structures, textural properties, and redox properties of nanosized particles. Hydrogen production through nanotechnology has made possible the opening of new paths in the global energy market. The intermittent nature of solar energy sources, the exhaustion of fossil fuels, and the impact of greenhouse gas emissions make the development of clean and renewable sources of energy and fuel necessary.

3.2. Mechanisms of Catalytic Reactions

Catalytic reactions facilitate the transformation of reactant species into products via an alternative reaction pathway characterized by a lower activation energy; the catalyst remains unchanged after the reaction (Claudiu Fierascu et al., 2019). Depending on the number of phases involved, catalysis can be classified as homogenous (catalyst and reactants in the same phase) or heterogeneous (catalyst and reactants in different phases).

Five fundamental steps constitute the general mechanism of catalytic reactions: (a) reactant molecules diffuse and adsorb at active catalyst sites; (b) adsorbed reactants assemble into intermediates; (c) intermediates recombine into products; (d) products desorb from the catalyst surface; and (e) products diffuse away from the catalyst. Additional steps may be involved in complex reactions. The adsorption of reactants onto catalytic sites is a critical step that governs catalytic activity. In homogenous systems, catalysts possess inherently active chemical groups that readily adsorb reactants; therefore, catalytic activity is primarily dictated by the presence and availability of such groups. Conversely, in heterogeneous catalysts, activity depends on the nature and density of accessible active sites on the surface that interact with reactants.

Metal nanoparticles exhibit enhanced catalytic performance due to their high density of undercoordinated surface sites and modified electronic properties compared to bulk metals. The catalytic activity and selectivity of bimetallic nanoparticles can be precisely tuned through structural and compositional modifications, leveraging geometric and electronic effects of secondary metals. Intermetallic compounds, characterized by defined stoichiometry and ordered crystal structures, serve as ideal model catalysts for structure–property relationship studies. Encapsulation of nanoparticles within mesoporous silica shells imparts high sinter resistance, enabling their application under elevated temperatures and harsh conditions while facilitating investigations into catalytic mechanisms (Pei, 2018). Control over catalyst size from the bulk down to the atomic scale yields unique catalytic performances, as evidenced by the discovery that nanoscale gold particles exhibit substantially enhanced activity in oxidation reactions despite bulk gold's inertness relative to other precious metals (Pei, 2018).

4. Nanomaterials in Heterogeneous Catalysis

Metal Nanoparticles and Metal Oxides Nanomaterials have been applied in the catalytic synthesis of organic compounds and functional materials in heterogeneous catalysis. The kinetics and selectivity of heterogeneous catalytic reactions depend on the size and shape of metal nanomaterials. Metal nanoparticles (NPs) exhibit activity for various chemical reactions, including Suzuki–Miyaura cross-coupling reactions and Mielewicz-type cyclo-isomerization (Wang & Gu, 2015). Mono- and bimetallic catalysts such as FePt@Cu nanowires, Pt@Fe2O3 nanowires, bimetallic Pt@Ir nanocomplexes, Pt–Au heterostructures, Au–Pt bimetallic nanocomplexes, Pt/Pd nanodendrites, Au nanowires, CuO@Ag nanowires, and a wide range of Pd nanocatalysts have been synthesized. Although metal oxides, sulfides, and phosphides also serve as heterogeneous catalysts, ReOx species supported by mesoporous alumina (Al2O3) nano-rods demonstrate exceptional activity for selective aerobic aldehyde oxidation and ammonia activation in the hydroamination of alkyne to imine—one of the most challenging heterogeneous catalytic reactions. Catalytic metal oxide nanomaterials such as Pt/Ag3PO4, Pt/CeO2, CuO, ZnO, Mn2O3, Cr2O3, Ga2O3, and TiO2 exhibit catalytic activity, and various oxide nanomaterials with different molecular geometries have been synthesized (Claudiu Fierascu et al., 2019).

4.1. Metal Nanoparticles

Metal nanoparticles exhibit great catalytic potential and may serve as alternative replacements for bulk/unsupported nanomaterials due to their comprehensive range of applications and diverse metallic properties. Their catalytic activity arises directly from metal atoms, which provide an unlimited supply of active sites and active species (Narayan et al., 2019). Combined with high surface energy and a large surface-to-volume ratio, these properties justify the use of nanoscale metals in catalytic systems. Nanoparticles act as efficient bridges between the bulk phase and individual atoms, transiently influenced by thermal energy, and play a fundamental role in the catalytic conversion of targeted products (Wang & Gu, 2015). Their superior catalytic ability has been confirmed in various redox reactions. Active metal elements such as copper, ruthenium, platinum, silver, iridium, gold, and palladium demonstrate remarkable catalytic performance when employed in nanoparticulate form.

4.2. Metal Oxides

Metal oxide nanomaterials are widely applied heterocatalysts in both environmental and industrial catalytic processes. Their wide and tunable range of electronic and redox properties, their tunable morphology, crystal phase and size, and their resistance to oxidation and reaction conditions make these materials ideal as catalysts or catalyst supports. Environmental applications include the catalytic abatement of NO_x, VOC and CO from stationary and mobile sources, the catalytic degradation of harmful products in water, and the photocatalytic production of hydrogen as a fuel. Metal oxides also find applications in energy conversion, e.g., in catalytic fuel cell reactions as cathodes and anodes, in the oxidation of methane, and the electrocatalytic reduction of CO_2 to alcohols.

Nanostructured ceria, perovskites, and spinel groups, such as cobalt oxide, are the oxide materials most widely used in catalytic reactions. Ceria–zirconia solid solutions are highly catalytically active in methane oxidation due to the high oxygen ion conductivity provided by the shuttle mechanism. Additionally, perovskites have been tested as anode materials for solid oxide fuel cells. In another important application, spinel cobalt oxide, either pristine or doped with different metals, has been used to promote the oxygen evolution reaction at the anode in water-splitting electrochemical cells.

5. Nanomaterials in Homogeneous Catalysis

Homogeneous catalysis involves catalysts and reactants in the same phase, often liquid. Organometallic catalysts in homogeneous catalysis usually consist of a metal center and ligands; ligand modification adjusts both activity and selectivity. Molecularly defined nanomaterials are widely used as homogeneous catalysts, with catalyst sizes ranging from subnanomolecular scales to nanodimensions. Ligand-modified nanomaterials can catalyse various transformations, including multifunctional catalytic systems combining heterogeneous and homogeneous catalysts (Wang & Gu, 2015).

5.1. Organometallic Catalysts

Organometallic catalysis comprises reactions that utilize organometallic complexes as catalysts. Organometallic compounds contain at least one metal-to-carbon bond, with the carbon atom belonging to an organic group. Organometallic complexes formed by the combination of an active metal center with chelating ligands are widely applied in homogeneous catalysis. Such catalysts are tunable by electronic and steric means to achieve high activity and selectivity; however, this also implies multistep synthesis, limited catalyst lifetime, difficulties in recycling, and overall low catalyst usage efficiency. The immobilization of organometallic complexes onto solid supports offers a route to overcome these issues by combining the advantages of homogeneous and heterogeneous catalysis. Immobilization can occur through covalent bonding or noncovalent interactions, and the choice of support material (ceramic oxides, polymers, carbon-based materials) significantly influences catalytic behavior. Additionally, nanoparticles themselves can serve as catalytic supports that modify the electronic and steric properties of grafted organometallic complexes, enabling bifunctional catalysts with novel properties. Ligand-modified nanoparticles and metal–ligand cooperativity have been exploited for catalytic applications (Wang & Gu, 2015) (Pei, 2018).

5.2. Ligand-Modified Nanomaterials

The functionalisation of nanomaterials with ligands is an important approach to modulate their activity and selectivity as catalysts and catalytic precursors (Pei, 2018). Silica shells have been employed to enable sintering-resistant catalytic metal nanostructures of precisely controlled morphology and composition. The resulting catalysts can be used with good stability at high temperatures in various reactions, including CO oxidation, selective oxidation and hydrocarbon conversion. Additionally, the silica shells can be post-functionalised with catalytic active components to furnish bifunctional catalysts, which are active and selective in cascade reactions.

7. Applications in Energy Conversion

The distinct properties of nanomaterials, including an exceptionally high surface-to-volume ratio, enhanced surface properties, and tailored size and morphology, have led to their widespread exploration in a variety of catalytic reactions over the past few decades. While some nanomaterial-based catalysts offer superior catalytic activity, they experience rapid deactivation, and the synthetic procedures often entail complicated steps and low yields. The high surface area of nanomaterials provides abundant active sites for reactions, a favorable attribute for catalysts in fuel cells. In proton exchange membrane fuel cells (PEMFC), nanomaterials serve as catalyst supports and active catalysts to address sluggish oxygen reduction reaction (ORR) kinetics. Two types of functionalized carbon nanotube-based cathode materials have been synthesized and assessed for ORR activity. Likewise, Li-ion battery anode materials utilizing carbon nanotube-supported nanocrystals of Sn, SnO2, Ge, Si, and In2O3 demonstrate cathodic capabilities and specific capacities surpassing those of bulk materials.

7.1. Fuel Cells

Fuel cells are energy conversion devices that can operate efficiently even with practically zero emissions, utilizing oxidation reactions of hydrogen or other organic compounds at the anode and reduction of oxygen at the cathode to produce water, electricity, and heat. Employing hydrogen as an energy carrier offers advantages over the dominant use of carbon-based fuels, despite hydrogen storage challenges, because it reacts favorably with oxygen in fuel cells rather than being combusted. Continuous flow of hydrogen and oxygen through the electrodes of a fuel cell allows for the generation of electrical energy at a constant voltage. Efficient operation requires conducting materials with suitable catalytic activity for the half-cell reactions and facilitating ion transport. Impurities such as carbon monoxide poisoning during alcohol oxidation, oxidation and reduction of metals or nanomaterials used in catalyst layers, and poisoning by metabolites impede the reliable operation of alcohol/air fuel cells.

Nanomaterials have been employed as cathode catalysts in proton exchange membrane (PEM) fuel cells to confer better oxygen reduction reaction (ORR) activity, with the objective of enhancing current density. Carbon nanotubes (CNTs) are considered excellent reinforcing fillers in polymer membranes. The dispersion state of CNTs within the polymer can exert a significant influence on the electrical and mechanical properties of polymer membranes, a crucial consideration for practical applications. The resistance of Pd–Ni/CNT towards catalytic degradation in fuel cells has also been examined. Carbon nanotubes synthesized through chemical vapor deposition that exhibit good electrochemical activity for hydrogen evolution reaction (HER) and hydrogen oxidation reaction (HOR) have been doped with boron and phosphorus as well as metal nanoparticles of platinum, palladium, rhodium, and ruthenium. Metal hydroxide catalysts supported on calcium hydride (CaH_2) have been identified that effectively absorb O_2 and H_2O and catalyze the reactions of the absorbed species with CaH_2, resulting in in situ formation of oxide phases of the catalyst metals. These reactions proceed under reaction conditions of PEM fuel cells and eliminate poisoning species in the fuel streams.

7.2. Photocatalysis

Photocatalysis, often regarded as a branch of heterogeneous catalysis, involves catalysts activated by ultraviolet or visible light and has emerged as a powerful tool to reduce industrial energy consumption. Chemical transformations catalysed by light play a key role in applications framing the development of a more sustainable society, such as the production of solar fuels (e.g., hydrogen through Water Gas Shift and water splitting reaction), solar chemicals and the degradation of organic contaminants in water and air (Truppi et al., 2017). Notwithstanding recent progress, the development of new photocatalytic materials that can optimally couple sunlight harvesting, charge separation and surface reactivity remains fundamental (Likodimos, 2020).

8. Applications in Chemical Synthesis

Nanomaterials in chemical synthesis thus meet the increasing demands of green chemistry and represent a strong alternative to both traditional batch and flow Organic Synthetic methodologies (Narayan et al., 2019). Many chemical processes—such as the preparation of pharmaceuticals, fibers, fuels, detergents, polymers—undergo an acceleration due to the presence of a catalyst; besides lowering the activation energy and increasing the reaction rate, catalysts improve the efficiency of many processes, tackling the high exploitation of energy and the formation of un-desired by-products. Advanced catalytic processes contributed to the restoration of the cleanness of the environment, as multistep catalytic purification of exhaust gases and catalytic oxidation of pollutants to water and carbon dioxide, for waste waters treatment (Claudiu Fierascu et al., 2019). The impact, at different levels, of nanomaterials in organic synthesis is remarkable. Nanomaterials have been adopted as catalysts in several synthetic routes, ranging from degradable polyesters to heteroleptic Bis-arylimino-Pyridine iron dialkyl compounds (Wang & Gu, 2015).

8.1. Green Chemistry Approaches

Green chemistry has become an important part of current science and technology because of environmental concerns and increasing demand for novel, economic, and ecofriendly technologies—for example, catalytic reactions using nanomaterials in solvents that can reduce the formation of harmful byproducts, minimize the use of hazardous solvents or reagents or reduce the cost of production. When properly designed and fabricated, nanomaterial catalysts can overcome many of the disadvantages of conventional and homogeneous catalysts, such as the use of expensive materials and susceptibility to contamination of byproducts. Many groups have developed different protocols for versatile nanomaterial catalysts, involving transition metal and metal oxide nanoparticles; metal nanoparticles on supports like zeolite, carbon, and mesoporous materials; and gold nanoparticles on different supports for catalytic oxidation of alcohols to aldehydes, bases, and esters. Extraction of metals from solutions for reuse may be considered an application of a catalytic nature. Various metal additives explore easy industrial recycling for metals.

8.2. Selective Catalytic Processes

Catalysis is fundamental in the synthesis of the majority of industrial products. It induces a large increase in reaction speed while reducing the energy consumption and improving the yield. Furthermore, catalytic processes play a key role in protecting the environment, as they are essential in purifying exhaust gases and in water treatment (Claudiu Fierascu et al., 2019). Catalytic processes can be categorized into two types: homogeneous and heterogeneous, the latter being the most encountered in the industrial sector because of its advantages. The main disadvantage of heterogeneous catalysis is the difficulty in modeling and designing reactors, as these catalysts are solid porous materials and reagent diffusion and transport phenomena play a dominant role. Nanocatalysis has emerged as the solution to this dilemma, possessing the accessible catalytic activity of homogeneous catalysis and the improved selectivity, stability, reusability and recovery of heterogeneous catalysis. Nanotechnology has boosted catalytic performance, as the catalytic activity of materials such as cobalt oxide is significantly higher at the nanoscale than in bulk form.

The design of catalysts featuring high activity, selectivity, and stability has been a persistent challenge throughout the development of catalytic processes industrially and academically (Wang & Gu, 2015). Catalysts constructed on a nanoscale dimension have demonstrated enhanced catalytic activity and selectivity compared to previous generations of nanocrystal catalysts, exhibiting superior electro-catalytic activity for the oxidation of methanol. Nanocatalysts hold promise for addressing the growing energy and environmental crises engendered by traditional chemical engineering methods. Significant advances have been realized in the synthesis of various types of noble metal nanostructures, including FePt@Cu nanowires, Pt@Fe2O3 nanowires, bimetallic Pt@Ir nanocomplexes, Pt-Au heterostructures, and Au nanowires. As a critical component of the chemical industry, catalysis plays a key role in improving resource efficiency and reducing environmental pollution. Nanomaterials, straddling the boundary between atoms and bulk materials, present unique characteristics and have demonstrated great promise for a wide array of applications extending beyond catalysis to encompass biology and medicine.

9. Challenges in Nanomaterial Catalysis

Despite their attractive properties, several challenges can limit the use of nanomaterials as catalysts. These include stability and robustness, deactivation, reusability, large-scale production, and economic viability. Maintaining stability under catalytic conditions is difficult owing to sintering, particle growth (Ostwald ripening), dissolution, and leaching (Claudiu Fierascu et al., 2019). Deactivation may also occur through poisoning, blocking of active sites, or poisoning by reaction substrates, products, or intermediates. Reusability is crucial for industrial applications, yet nanoparticles may suffer from leaching, aggregation, and loss of active sites upon recycling. Large-scale production confronts challenges in achieving consistent size, shape, composition, and phase purity. Economic viability further hinders widespread use when fabrication relies on expensive precursors, complex synthesis, and costly ligands (Nacci & Cioffi, 2011).

9.1. Stability and Deactivation

Several factors influence nanomaterial stability and their catalytic applications: their dispersity and size distribution, the method of dispersion or anchoring on a support (or matrix), methods of reactant feeding (batch or continuous), temperature regimes, liquid or gas phase, and time on stream. Nanocatalysts often suffer from deactivation caused by particle sintering, leaching, or coking during catalytic reactions. Although nanomaterials demonstrate excellent catalytic activity, these disadvantages hinder their large-scale industrial applications in catalysis.

Deactivation of nanomaterial catalysts results in the loss of provided activity and selectivity. Several factors cause catalyst deactivation during catalytic reactions, including the accumulation of active site poisons on the catalyst surface, loss of activity due to active site loss, and changes in catalyst structure resulting in decreased activity. Nano-sized components in supported metal catalysts can migrate and move closer to other components at reaction temperatures, and physical interactions between the support and nanoparticle surface change with particle size or reaction conditions, making particles very unstable. To address these challenges, efforts in reducing nanocatalyst deactivation and enhancing stability are essential.

9.2. Scalability and Economic Viability

A significant obstacle lies in the efficient scale-up of laboratory-derived nanomaterials to commercial volumes, where synthesis remains complex and costly. Reactor design and production economics present additional complications. Although many novel nanomaterials display exceptional catalytic activity, their high production costs hinder practical implementation outside laboratory settings. For instance, platinum-based nanomaterials dominate catalysts in fuel cell technologies. Despite active research aimed at reducing platinum usage, the indirect cost transferred to the end user continues to surpass that of gasoline-powered vehicles. The challenge is not only in reducing platinum quantity but also in developing catalysts based on more abundant and cheaper transition metals that do not compromise cell performance.

In environmental catalysis, optimization of materials—accounting for performance, toxicity, and lifetime—is necessary both in single-step air pollutant removal and integrated multi-step fuel cell systems. TiO-based catalysts are widely utilized for air purification because of their photocatalytic activity combined with oxygen scavenging properties. Still, the economic viability of such systems must be carefully evaluated, particularly considering establishing costs and operational savings. Justification for significant initial investments requires either the achievement of so-called zero-emission standards within urban environments or a demand for improved fuel efficiency and reduced greenhouse gas emissions.

10. Future Perspectives in Nanocatalysis

Researchers actively explore new materials for catalysis, seeking accessible, robust, and selective catalyst architectures that remain cost-effective and environmentally friendly. Nanostructured materials represent a promising class of candidates that can satisfy multiple requirements. For example, by embedding metal nanoparticles in an oxide support, the interfaces between the two materials enhance charge transfer, catalytic activity, and selectivity (Claudiu Fierascu et al., 2019). Further advances in catalyst development include photochemically and electrochemically active structures that enable light-driven or electro-driven catalysis. Typical reactions include carbon dioxide conversion, hydrogen evolution, and fuel cells, requiring efficient, stable, and scalable photo-electrocatalysts. Copper oxide and copper silicide nanowires stand out as low-cost catalysts in these domains (Narayan et al., 2019). Alternative nanomaterials under study include germanium, boron nitride, and diamond nanostructures. Attempts to enhance catalyst durability have led to investigations of highly stable, dispersed catalysts such as the ultra-stable single atom-embedded nitrogen-doped graphene framework.

10.1. Emerging Nanomaterials

The ability to manipulate matter at the nanoscale provides robust platforms to engender unique and enhanced catalytic performance, including improved selectivity and recyclability (Claudiu Fierascu et al., 2019). Nanostructures occupy a perplexing middle ground between single atoms and bulk materials that are difficult to investigate, yet they comprise the active phase of many important industrial catalysts (Pal et al., 2023). Due to their large surface-to-volume area ratio, the reactivity of nanoparticles is often set by factors traditionally considered to have minimal impact on activity and selectivity, such as the size of surface features, local strain, and electronic effects (Nacci & Cioffi, 2011). By tuning these parameters, simple metallic materials can be developed into versatile catalytic platforms capable of manipulating reaction pathways, inducing chirality, and performing tandem or multi-step catalytic sequences. Considerable research is focused on enhancing atomic utilization efficiency by decreasing particle size. However, while smaller nanoparticles often exhibit more active sites, fewer atoms contribute meaningfully to the catalytic cycle, and essential surface interactions become increasingly energetically unfavorable.

10.2. Innovative Catalytic Processes

Several catalytic processes related to nanomaterials are of considerable interest. Among them, liquid-phase catalysis using metal or metal oxide nanoparticles and the mechanism behind their poisoning under reaction conditions are important. Environmental catalysis has received special consideration because the use of nanomaterials could help to eliminate pollution products, such as air and water purification. In addition, catalytic processes implicated in energy production, such as proton exchange membrane fuel cells, are not properly implemented because of the high cost and stability of the catalysts; nanomaterials are promising candidates for this type of system. Green chemistry approaches that also employ nanomaterials have been investigated, aiming to obtain products selectively while avoiding the use of excess reagents or toxic solvents. Finally, photocatalysis denotes a catalytic process activated with photons to produce radical species that enable complex reactions. The photocatalyst is excited when the energy of a photon is greater than the energy gap between the valence and the conduction band, thus promoting an electron from the valence band to a position on the conduction band and generating a hole.

Currently, two challenges remain: understanding the catalytic processes related to these applications and controlling the efficiency and activity of catalytic centers in order to achieve industrial processes. In catalysis, the effect of a catalytic center on a reaction is clarified with mechanistic proposals, which in turn allow the design of highly active and stable catalysts. Heterogeneous catalysts are generally less active yet more stable than homogeneous ones; combining the best properties of these materials has led to the development of active and stable catalysts for each process. Homogeneous catalysis is mainly carried out by organometallics or organocatalysts, which after reaction generate selective products but present stability problems. To overcome these problems, metals, oxides, or metal oxides may be functionalized with organic species that modify the catalytic mechanisms and prevent deactivation phenomena under reaction conditions. Both catalysis mechanisms share approaches based on molecular activation, in which the reagent is activated before the rate-determining bond-breaking or bond-forming step. In this context, nanotechnology knowledge, especially related to nanomaterials, is exploited to break the restrictions of heterogeneous catalysis.

11. Conclusion

Nanomaterials possess unique physicochemical characteristics distinct from their bulk counterparts. Over the last two decades, they have been investigated extensively for catalytic applications due to unique optical, electronic, electrical, mechanical, thermal, magnetic, and chemical properties. Nanomaterials are classified as one-dimensional, two-dimensional, or three-dimensional based on their exposed structural architecture, and synthesis methods include gas-phase condensation, chemical vapour condensation, chemical reduction, and photoreduction. Catalytic reactions transform starting materials into products through different reaction pathways; catalysts facilitate this by accelerating the rate without being consumed. Primarily, catalysis is recognized in two types: homogeneous and heterogeneous catalysis. Mechanisms include Langmuir-Hinshelwood (both reactants adsorbed), Eely–Rideal (one reactant adsorbed), and Mars vd Waal (lattice oxygen as reactant) mechanisms.

At a molecular level, metallic nanoparticles in heterogeneous catalysis act by offering large accessible catalytic sites, with stability, selectivity, easy recovery, and reusability. Metal nanoparticles are exploited due to their small size and nature, and are widely distributed in various catalytic fields; nanometal oxides are among the most studied catalytic materials because of their fundamental and industrial applications; and organometallic complexes are widely used in homogeneous catalysis. Ligand-modified nanoparticles maintain the homogeneity of homogeneous catalysts, while morphologically selective nanoparticles retain the heterogeneous catalytic advantage. Nanomaterials have versatile applications, including air purification and water treatment, fuel cells and photovoltaic cells, photocatalytic degradation and sustainable chemical processes, and selective oxidation and green chemistry. These applications indicate nanomaterials' considerable potential, even in the face of multifaceted challenges. However, extensive practical use faces several challenges. Stability concerns include nanoparticle structure, shape, composition, and surface sensitivity, with agglomeration and sintering arising from high surface-to-volume ratios influencing active surface areas. Poisoning and coking introduce deactivation risks through irreversible adsorption, site blocking, lattice penetration, metal implantation, and strong chemisorption of carbonaceous species. Scalability issues encompass laboratory production limitations, batchwise methods, process complexity, and reproducibility. Economic consideration remains critical as several noble metals and transition metals employed in catalysis are costly (Narayan et al., 2019) (Claudiu Fierascu et al., 2019)

(Wang & Gu, 2015).

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