



RECENT ADVANCES IN NANOCATALYSTS FOR ENVIRONMENTALLY SUSTAINABLE CHEMICAL TRANSFORMATIONS

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ABSTRACT

The area of nanocatalysis has become a significant research challenge towards building environmentally sustainable chemical process due to the high surface area, electronic tunability, availability of many active sites, and control of surface chemistry on the nanometer scale. Over the period 2020-2024, research within nanocatalysis has advanced from traditional metallic and metal oxide nanoparticles to advanced supported nanocatalysts, heterostructures, two-dimensional materials, magnetic nanocatalysts, single atom catalysts, biomass-based catalysts, and photoactive nanocomposites. The advances made within the area of nanocatalysis have widened their applications from traditional organic synthesis to biomass transformation, carbon dioxide conversion, hydrogen generation, water splitting, pollutant degradation, and wastewater treatment. This paper critically assesses these advances in relation to green chemistry, resource efficiency, catalyst recycling, energy efficiency, and circularity. Special attention will be paid to the interplay between nanometer-scale structure and catalyst performance, sustainable catalyst synthesis, single-atom catalysis, photonic catalysis, biomass-derived catalytic systems, and environmental applications. From the latest literature, it is clear that SAs present high efficiency in terms of metal loading, whereas biomass-based supports can bring about catalyst development through recycling and reuse. (American Chemical Society Publications) On the other hand, issues related to stability, metal dissolution, aggregation of nanoparticles, toxicity, scale-up, and sustainability should not be overlooked. It seems that the combination of nanocatalysis with renewables, wastes, artificial intelligence, and the concept of the circular economy will decide on its future importance.

Keywords: *Nanocatalysis; sustainable chemistry; green catalysis; single-atom catalysts; photocatalysis; biomass valorization; environmental remediation; circular economy.*

INTRODUCTION

The chemical industry is crucial for modern society; however, traditional chemical synthesis entails substantial energy and material consumption, hazardous waste production, reliance on fossil sources, and greenhouse gas emissions. Catalysis is the most promising strategy to tackle these problems since catalysts are able to speed up chemical reactions by diminishing the activation energy barrier and possibly cutting down the energy/material expenses of reactions. However, the demands for catalytic

systems of modern time have changed significantly. In addition to obtaining high conversion and selectivity, the catalyst has to work under milder conditions, utilize renewable or abundant materials, avoid hazardous reagents/solvents, maintain high operational stability, and enable facile regeneration/reuse of the catalyst. The role of nanocatalysis in this shift has become especially significant. Nanocatalysts include particles whose size allows changing their surface atoms, defects, interfaces, and electronic structure compared to bulk counterparts. Thus, such parameters as particle size, morphology, crystallinity, surface defects, oxidation state, and metal support interaction can be controlled in order to tune the catalyst's activity and selectivity. According to a 2023 review, nanocatalysis is becoming an important part of green chemistry due to a great surface area and increased interfacial functionality of nanomaterials.

This significance is especially apparent when it comes to heterogeneous catalysis. Traditional bulk catalytic materials could be composed of a rather large number of atoms that cannot be reached by the reagents. The decrease in size will result in a larger number of surface atoms and hence higher active site density. The potential for this advantage is even higher in the case of single-atom catalysts (SACs). In SACs, isolated metal atoms are immobilized on specific supports. These catalysts can reach almost complete atomic efficiency and offer precisely defined coordination spheres that can affect the reaction course and the resulting product. During 2020 to 2024, significant changes in the research directions towards multifunctional and sustainable nanocatalyst development have been observed. In addition to the catalytic performance, researchers have started to focus on methods of catalyst synthesis, resource consumption, stability, recovery, toxicity, and impact on the lifecycle. The use of biomass-based carbonaceous materials is gaining popularity due to their potential ability to convert agricultural and biological waste into value-added products. Starch, cellulose, lignin, hemicellulose, proteins, and chitin have been reported in recent reviews as the raw materials used for SACs synthesis involving metals like Fe, Co, Ni, Cu, Zn, Mn, and Pt.

Another major development is the integration of nanocatalysis with photocatalysis and renewable energy. Semiconductor nanoparticles and nanohybrids can absorb light and generate electron-hole pairs that drive oxidation and reduction reactions. Such systems are particularly relevant to environmental remediation and energy conversion because solar energy can potentially substitute for externally supplied thermal energy. The development of heterostructures, defect-engineered materials, carbon-semiconductor composites, and atomically dispersed photocatalytic sites has improved control over charge separation and surface reactions. Nanocatalysis is also increasingly connected with biomass valorization. Biomass is the major renewable source of organic carbon capable of serving as an alternative to fossil-derived feedstocks. However, the chemical complexity and oxygen-rich nature of biomass make selective conversion difficult. SACs have emerged as promising catalysts because isolated active sites can be tailored to promote specific hydrogenation, oxidation, hydrodeoxygenation, dehydration, and bond-cleavage reactions. A recent review emphasized the growing role of SACs in converting cellulose, hemicellulose, lignin, and their derivatives into fuels and value-added chemicals.

Notwithstanding all these advancements, however, nanocatalysis cannot be automatically seen as equivalent to green chemistry. First, nanoparticles might be synthesized at high temperature, using toxic precursors and organic solvents, as well as with high energy consumption. Nanomaterials might also possess environmental toxicity and metal leaching during their application. Thus, the sustainability

of a nanocatalyst should be determined throughout the whole lifetime cycle of this material and not just by considering its catalytic activity. In this research, recent achievements in nanocatalysts used for sustainable chemical transformations in 2020-2024 are critically analyzed. It discusses the development in nanocatalysts design and synthesis, application for sustainable chemical transformations, environmental remediation and energy conversion, comparison of performance and sustainability problems, and prospects.

REVIEW OF RECENT LITERATURE AND RESEARCH GAP

According to recent literature, there has been a departure from the traditional paradigm of only reducing the size of the catalyst particles. The recent trends in this field are more concerned about controlling active sites, interfaces, defects, coordination environment, and interactions between the catalyst and the support. Nanocatalysis has been emphasized by Agarwal et al. (2023) in the context of its relevance in green chemistry, where the nanomaterials exhibit greater surface activity to carry out environmentally friendly reactions. One of the most significant advances made so far in this field is the advent of single-atom catalysis. In a review of the single-atom metal catalysts for biomass conversion, Chen et al. (2024) pointed out their significance in terms of high atom efficiency, catalytic activity, selectivity, and stability. The utilization of biomass as the source material for catalyst preparation is yet another notable breakthrough. Yu et al. (2024) highlighted the natural biomass-based SACs for energy and environmental applications, mentioning that natural materials such as starch, cellulose, lignin, hemicellulose, proteins, and chitin have been used as the source material. These biomass materials can act as a carbon and heteroatom source for isolated metal atoms stabilization. The significance of this method lies in the fact that catalyst preparation involves biomass usage.

Moreover, Zhu et al. (2024) showed the applicability of biomass-derived SACs in environmental remediation. In their review, they discussed the use of these SACs in pollutant removal, carbon dioxide reduction, and nitrate reduction, focusing on the interconnections between the biomass used, catalyst morphology, the structure of the active site, and the efficiency of the catalytic process. (Further developments in this field have been made concerning the development of sustainable SACs, not only from biomass, but also from solid waste. A review paper in 2024 noted that biomass- and solid-waste-derived SACs were a promising solution for low-cost catalyst synthesis, implementation of circular economy principles, and carbon-neutral chemical processes. Moreover, ultrafast synthesis and artificial intelligence-guided precursor choice were mentioned as emerging methods for scalability improvement. One of the emerging research areas is that of single-atom photocatalysis. Recently published in 2024, this research focuses on the ability of single-atom photocatalytic centers to perform biomass transformation under relatively mild light conditions.

Therefore, it could be argued that the body of literature shows considerable advancements, however several research issues still exist. Firstly, lab scale catalytic efficiency is usually reported in a manner that does not include adequate lifecycle assessment. Secondly, the majority of papers focus on conversion and selectivity of reactions, offering limited details on stability of the catalysts, metal leaching, reusability and environmental effects. Thirdly, some very advanced nanocatalysts need complicated preparation procedures which can potentially make them less sustainable. Fourthly, the reproducibility of nanoscale active sites still poses problems. Fifthly, the number of papers addressing

all four parameters – catalytic efficiency, economic viability, toxicity and lifecycle environmental effects – systematically, is rather low. Thus, the major research issue could be described as a lack of an integrated approach to the assessment of nanocatalysts based on catalytic efficiency + resource efficiency + environmental safety + reusability + scalability + lifecycle sustainability.

Nanocatalyst Design, Synthesis, and Characterization

The performance of nanocatalysts is fundamentally governed by the interplay between structure and function. Size, shape, porosity, oxidation state, surface defects, electronic structure, and support effects may affect reactant adsorption, activation, intermediate stabilization, and product desorption. Hence, the modern nanocatalyst design is trending towards a structure-oriented engineering process. Nanoparticles of Pt, Pd, Au, Ag, Cu, Ni, Co, and Fe continue to be significant due to their electronic structure which enables hydrogenation, oxidation, reduction, coupling, and other chemical reactions. However, an increased focus is being made on earth abundant elements due to the expense and resource limitations of noble metals. Nanostructures will enhance the performance of relatively abundant metals while lowering the amount of catalyst used. The importance of supported nanocatalysts cannot be overstated in relation to sustainability. Nanostructures of carbon, silica, alumina, zeolites, metal oxides, graphene derivatives, carbon nanotubes, and biomass-derived porous carbon can inhibit nanoparticle agglomeration and increase stability. Support effects may also tune the electronic structure of active elements and alter reaction pathways.

Another promising area of research is green synthesis. The traditional method for synthesizing nanoparticles might require chemical reducing agents, stabilizers, organic solvents, and highly energy-consuming processes. Living organisms can serve as substitutes for reducing and stabilizing properties. Biomolecules from plants, such as polyphenols, proteins, and carbohydrates, might take part in metal ion reduction and the stabilization of nanoparticles. However, the sustainability of biological synthesis depends on the whole chain of the process, from biomass harvesting to extraction, purification, reactions energy, and postprocessing. A step forward in nanocatalysis engineering is the single-atom catalyst (SAC). It implies a design where only one metal atom is stabilized on the support rather than nanoparticles with multiple atoms inside. The authors Chen et al. (2024) noted that the catalytic activity of SACs strongly relies on the character of the metal center as well as its coordination environment. Defect engineering has acquired special significance in the preparation of SACs. Vacancy defects, heteroatom defects, edges, and other defects act as the anchoring sites for isolated atoms. Thus, defect engineering will not only help to enhance dispersion but also alter the electronic structure of active centers. Synergistic interactions of defects with isolated metal atoms have been found in researches concerning biomass conversion.

Biomass-derived carbon supports have shown tremendous potential as well. Natural availability, carbon content, heteroatoms functionality and porosity structures allow these materials to enable stabilization of isolated metals. These systems also give rise to a method by which low value biomass/waste materials can be transformed into valuable catalysts. In fact, recent scientific advancements have revealed that biomass-based SACs can be synthesized using diverse natural materials for energy and environmental applications. Multimodal characterization becomes vital since the catalytic activity of nanomaterials can never be predicted based solely on the bulk composition of

these materials. Morphology and dispersion of particles can be analyzed via electron microscopy, whereas crystallinity and phases can be evaluated using X-ray diffraction. Surface chemistry can be determined using X-ray photoelectron spectroscopy, whereas coordination and oxidation environments can be elucidated using X-ray absorption spectroscopy. Isolated atoms can be detected using aberration-corrected electron microscopy in suitable systems. This increasing complexity of nanocatalysts has thus led to the need for multimodal characterization of these materials.

Applications of Nanocatalysts in Sustainable Chemical Transformations

The use of nanocatalysts in sustainable chemical synthesis is wide due to their potential to carry out reactions with good catalytic activity and selectivity in low concentrations of catalysts and mild reaction conditions. Hydrogenation has become a major area of application. Nanostructured catalysts such as Ni, Co, Fe, Pd, Pt and others have been used in hydrogenation reactions of alkenes, alkynes, nitro compounds, carbonyls and intermediates formed from biomass. The nanoscale dispersion of catalysts allows easy access to the surfaces and low use of catalysts. The use of nickel and cobalt based on earth abundant metals is very appealing since it can avoid the use of expensive precious metals. Oxidation reactions have also emerged as an important area of application. Sustainable oxidation reactions try to use molecular oxygen, hydrogen peroxide, air, oxygen activated through electrochemistry or photocatalytic reactions instead of stoichiometric oxidants.

Nanocatalysts are also useful in the formation of carbon-carbon and carbon-heteroatom bonds. Nanoparticles of palladium, nickel, copper, iron, and cobalt have been studied as coupling agents. Their immobilization on suitable supports could help separate and recycle the catalyst, thus overcoming the primary disadvantage of homogenous catalysis. Photocatalysis of organic compounds is a very significant recent advancement. Nanostructured semiconductors can absorb light and generate electrons and holes that would start oxidation and reduction reactions. The employment of visible-light-responsive materials could help perform chemical transformations with the use of solar rather than thermal energy. The transformation of carbon dioxide is another important sustainable application of nanocatalysts. CO₂ is quite stable thermodynamically and thus not easy to activate. Nanocatalysts can change the energy of adsorption and stabilize reaction intermediates, making electrocatalysis, photocatalysis, and thermocatalysis of CO₂ possible. The products include CO, methanol, formic acid, methane, and other carbon-based compounds.

Single atom catalysts are especially suitable for CO₂ utilization due to the fact that in these catalysts active sites are single atoms, which makes it possible to control their electronic properties. Coordination environment can be created in such a way that it will affect the adsorption and processing of important intermediates. Nevertheless, sustainable use of CO₂ is strongly dependent on the source of energy employed in this process. If the catalyst is very effective but its operation requires energy production from carbon sources, there may be no significant positive environmental effects from this process. The role of SACs has gained particular importance owing to their isolated metal sites that allow the selectivity of bond activation. Current studies focus on the fact that SACs can help with the transformation of cellulose, hemicellulose, and lignin via thermocatalytic, electrocatalytic, and photocatalytic routes. The development of single atom photocatalysts that would convert biomass using mild conditions is one of the promising areas of study for 2024. The sustainable importance of such

technologies is high as biomass can serve as a sustainable carbon source. Rather than burning biomass, catalytic conversion can help to obtain more valuable products. In combination with biomass-based catalyst supports, the whole cycle will be created, when biomass is used both as raw materials and catalyst precursors.

Environmental Remediation, Energy Conversion, and Biomass Valorization

Nanocatalysis application in environmental remediation is one of the most widely researched areas of nanocatalysis applications. Industrial wastewater comprises dyes, pharmaceuticals, antibiotics, pesticides, phenols, endocrine disruptors, and many other pollutants. The traditional ways of dealing with them can be inefficient or even shift pollution to other phases. Catalytic degradation, reduction, oxidation, adsorption, or transformation of these pollutants are possible by using nanocatalytic reactions. Photo-catalysis is especially interesting due to the fact that illumination of the sample creates reactive agents that can attack organic compounds. TiO_2 , ZnO , graphitic carbon nitrides, iron oxides, bismuth semiconductors, and composites were widely explored. Heterostructure formation is aimed at minimizing recombination processes of electrons and holes and improving charge transport. Formation of composites with semiconducting and carbon materials improves adsorption capacity and electron mobility. Through structural modifications, scientists can achieve optimization of light harvesting, pollutants' adsorption, and catalytic reactions' rates. Magnetic nanocatalysts offer an extra benefit in terms of sustainability since they can be recovered after the process. Using magnetic materials such as Fe_3O_4 or its modifications in catalytic structures enables magnetic isolation. This is especially beneficial for wastewater purification since uncontrolled discharge of nanoparticles after treatment might cause new environmental issues.

Environmental applications are increasingly common with respect to biomass-derived SACs. There have been some recent studies on the use of biomass-derived SACs for pollutant elimination, carbon dioxide reduction, and nitrate reduction, showing that biomass-derived SACs could be environmentally useful as well as sustainable materials.) Energy conversion is another application area. The use of nanocatalysts for hydrogen evolution reaction, oxygen evolution reaction, oxygen reduction reaction, and overall water splitting is observed. The reason why single-atom catalysts are more popular is that their high metal utilization ratio may reduce the usage of costly catalytic material. Biomass-derived SACs with different metals such as Fe, Co, Ni, Cu, Mn, Zn, etc., have been studied for energy-related applications. Water splitting is a significant process of hydrogen generation through renewable electricity. Hydrogen evolution reaction and oxygen evolution reaction need proper catalysts due to their kinetic difficulties. Nanostructuring can enhance active-site accessibility, whereas atomically dispersed metals can provide optimized adsorption of essential intermediates. The combination of renewable electricity and nanocatalysis may result in an avenue for the production of chemicals from carbon-neutral sources. This is because renewable electricity can be used in electrochemical reduction of CO_2 , hydrogen generation, nitrate reduction, and organic synthesis, among others. Sunlight, too, can be used to trigger photocatalytic reactions. Biomass utilization is another complementary method. Instead of utilizing biomass solely for energy, catalytic reactions can be used to generate platform molecules and high-value chemicals. Recent studies of SACs have shown how renewable feedstock can be used together with catalytically active atoms. In summary, the convergence of environmental

purification, renewable energy sources, and biomass utilization shows how nanocatalysis can be sustainable in several ways.

RESULTS, COMPARATIVE ANALYSIS, AND CRITICAL DISCUSSION

The literature discussed in this study shows that there has been a marked advancement in nanocatalysis from 2020 to 2024. There has been an increased development from conventional catalysis using nanoparticles to more advanced technology where catalytic activity can be achieved via manipulation of site structure, defects, support, light, and dispersion..

Nanocatalyst platform	Principal sustainable contribution	Major applications	Key limitation
Metal nanoparticles	High surface activity and lower catalyst loading	Hydrogenation, oxidation, reduction	Aggregation and leaching
Metal-oxide nanoparticles	Stability and photocatalytic functionality	Pollutant degradation, oxidation	Charge recombination
Carbon-supported nanocatalysts	Improved dispersion and recovery	Organic synthesis, biomass conversion	Support preparation
Photocatalytic nanohybrids	Utilization of light energy	Wastewater treatment, organic synthesis	Photostability and separation
Magnetic nanocatalysts	Easy catalyst recovery	Environmental remediation	Potential metal release
Single-atom catalysts	Very high atomic utilization	Biomass conversion, energy conversion	Complex synthesis and stability
Biomass-derived SACs	Renewable/circular catalyst production	Environmental and energy applications	Scale-up and reproducibility
Single-atom photocatalysts	Mild light-driven transformations	Biomass upgrading, environmental chemistry	Mechanistic complexity

From the above comparison, single atom catalysts and biomass-based catalytic systems are two of the most significant recent trends. The SACs solve the issue of inefficient use of metals, whereas biomass-based systems deal with the issue of sustainability of the support and precursors used. Thus, their combination can help improve efficiency while minimizing the environmental impact of the material. However, high catalytic activity by itself is not sufficient to guarantee sustainability. The catalyst which needs expensive precursors, complicated synthetic method, high temperature or rare metals can have excellent catalytic activity but has huge environmental impacts. Likewise, photocatalytic

decomposition might exhibit excellent pollutant decomposition efficiency under laboratory water, while becoming less efficient for real wastewater because of competitive ions and organic substances.

Thus, a good performance evaluation framework must incorporate conversion efficiency, selectivity, productivity, catalyst life cycle, energy cost, catalyst recycling, metal efficiency, environmental impact, toxicity and life cycle analysis. An interesting perspective on current literature review is that nanocatalysis has shifted from material-based to system-based approach in the process of development of sustainable nanocatalysis. Earlier studies usually posed the question like "How active is the nanocatalyst?", while recent studies pose the question "Is the whole catalytic system sustainable?"

This is especially noticeable in the case of research in biomass-derived SACs, where the catalyst itself forms part of a circular material cycle, where the biomass or the waste material could be used as the starting material, which forms the carbon material that helps in stabilizing the isolated metal atoms, and then acts as the catalyst to convert the biomass. Some of the recent 2024 trends include solid waste-derived SACs, rapid synthesis, and AI-assisted material selection.

Challenges, Sustainability Assessment, and Future Perspectives

Despite great success, several difficulties still need to be overcome in order for nanocatalysis to become widely implemented in industry.

First, it is necessary to deal with stability issues. The nanoparticles have high surface energy and tend to aggregate. SACs could migrate and aggregate into nanoparticles under harsh reaction conditions. Deactivation is, therefore, one of the significant problems.

Second, it is important to solve metal leaching issues. The metal species that are released during catalysis might contaminate the reaction products and treated water. It is especially relevant for environmental remediation, where it is required that the treatment material itself does not turn into a pollutant.

Third, there is an issue of nanotoxicity. The environmental fate of the nanomaterials is defined by the size, shape, surface chemistry, oxidation states, and solubility of the particles. Ecotoxicological assessment is thus required along with the creation of novel nanocatalysts.

Fourth, there is a scale-up problem. Many of the catalyst synthesis methods have been tailored for small-scale production and it is often hard to implement them on a kilogram or tonne scale.

The fifth and final challenge is the lifecycle sustainability of the catalyst. The process of assessment of the catalyst needs to start from extraction of the raw material, to manufacturing of the catalyst, its use in reactions, regeneration and transport, and finally the process of disposal at the end of the cycle. This is especially true for those cases when the catalyst uses noble metals, complex organic ligands or energy intensive methods of synthesis.

For future research, earth abundant metals, low temperature synthesis, solvent-free or aqueous processes, renewable sources, waste-derived supports and recyclable designs need to be used. Biomass and solid waste-derived SACs are very promising, as they combine the production of the catalyst with

recycling of resources. Another promising area of research is artificial intelligence. AI algorithms could be used for fast screening of the precursors, metal and support combinations, synthetic methods and reaction parameters. According to the literature of 2024, AI-based screening of precursors, design of catalysts, synthesis and analysis are among new sustainable SAC research areas.

Single-atom photocatalysis can be another important future trend. The capability of integrating atomically precise active sites with light-absorbing semiconductors could lead to efficient and selective biomass conversion and environmental transformations in a relatively mild manner. This recent 2024 research emphasizes this technology for the conversion of biomass to valuable chemicals and fuels. In the long run, a closed loop system of catalysts can be an ultimate goal. In this case, renewables or waste materials are converted into catalysts, renewable energy is used as reaction energy, wastes act as reactants, catalysts are recycled and regenerated, and valuable products are produced.

CONCLUSION

During 2020–2024, nanocatalysis has undergone fast development and became a valuable technology platform of sustainable chemical transformations. The main advances in nanocatalysis are as follows: supported metal nanoparticles, photocatalytic nanohybrids, carbon-based nanocatalysts, magnetic catalysts, single-atom catalysts, biomass-derived catalysts, and single-atom photocatalysts. The key feature of nanocatalysts is the possibility to design their catalytic properties on a nanoscale. Increased surface area, flexible electronic structure, defect-ridden surface, and engineered metal-support interaction are able to enhance the catalytic efficiency and selectivity of the catalysts. Single-atom catalysts can be called especially valuable as isolated active sites allow increasing the metal efficiency and controlling catalytic processes precisely. (American Chemical Society Publications) Biomass-derived catalysts increase the sustainability of nanocatalysts by allowing to transform renewable resources and wastes into valuable catalytic materials. Recent studies demonstrate their applicability in energy conversion, environmental protection, biomass upgrading, CO₂ conversion, and other similar reactions. In contrast, nanocatalysis should not be regarded as necessarily sustainable. Toxicity, leaching, stability, regeneration, scaling up, and other aspects of catalysts have to be analyzed thoroughly. Thus, instead of creating more active catalysts, the key trend in the future can be the creation of catalytic systems that are efficient and sustainable in terms of their performance, resource utilization, safety, recyclability, economic viability, and lifecycle. The combination of nanotechnology with biomass upgrading, renewable energy sources, single-atom catalysis, photocatalysis, principles of the circular economy, and artificial intelligence may significantly contribute to the transition towards sustainable chemical production. In this regard, sustainable nanocatalysis has the capacity to become one of the core technologies for the synthesis of chemicals, fuels, and environmental goods.

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