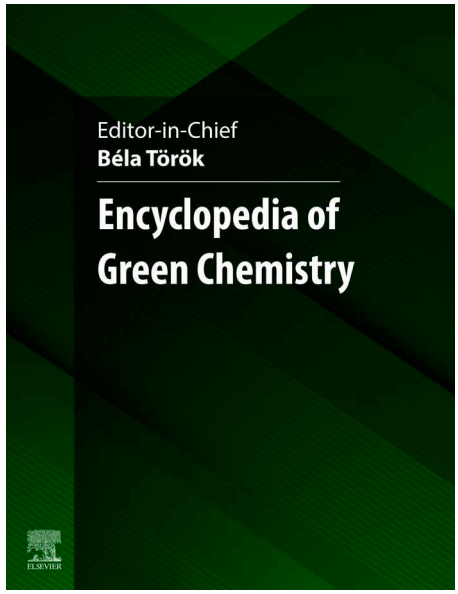




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# Single-Atom Catalysis

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## Abstract

Single-atom catalysts (SACs) are gaining significant attention in organic synthesis, providing a bridge between homogeneous and heterogeneous catalysis. These systems consist of individual metal atoms dispersed on solid supports, mimicking the precision and selectivity of ligand-based organometallic complexes. Compared to conventional catalytic systems based on supported metal nanoparticles, SACs offer several advantages, including efficient utilization of metal atoms, high stereo-, regio-, and chemoselectivity, and enhanced stability. Moreover, in contrast to conventional homogeneous organometallic catalysts, SACs eliminate the need for complex ligands, while overcoming challenges related to catalyst recovery, air/moisture sensitivity, and long-term structural integrity. The design of the support plays a critical role in maintaining atomic dispersion and preventing metal atom aggregation in SACs, with materials such as carbon nitrides, covalent organic frameworks, and metal-organic frameworks commonly employed to achieve this atomic-level dispersion. Advanced characterization techniques like aberration-corrected electron microscopy and X-ray absorption spectroscopy have been essential in studying SACs at the atomic level, allowing researchers to fine-tune their properties for targeted synthetic applications. This chapter provides an introduction to the principles, advantages, and applications of SACs, highlighting their potential in sustainable catalytic processes.

## Introduction

Fine chemical synthesis has long been critically important for the development of pharmaceuticals, natural products, agrochemicals, and polymers. The design of new catalysts is an integral part of this field, as these materials efficiently facilitate the formation or cleavage of chemical bonds (*1*). Catalysts often include molecularly precise organometallic complexes dissolved in organic solvents, such as the Wilkinson catalyst widely used for selective alkene hydrogenation (*2*). While these systems are highly active and selective, they present significant challenges, including expensive and time-consuming ligand design, high sensitivity to air and moisture, difficulty in separating catalysts for metal recovery, and limited stability (*3*). To address these issues, researchers have attempted to immobilize organometallic complexes onto solid supports, designing surface organometallic catalysts that have shown remarkable results for a variety of reactions (*4*). These systems are increasingly viewed as a potential bridge between heterogeneous and homogeneous catalysis. An alternative to surface organometallic catalysts is the use of single-atom catalysts (SACs) (*5*,*6*,*7*). In these catalysts, individual metal atoms are anchored onto the surface of a support via strong covalent interactions, without the need for additional ligands, which prevents the leaching and degradation commonly observed in homogeneous systems. The support, often composed of materials like carbon nitrides, covalent organic frameworks, or graphene, plays a crucial role by acting as a "ligand equivalent" that modulates the electronic properties of the metal atom, facilitating charge transfer to the metal (*8*).

This design maximizes atomic efficiency, ensuring that each metal atom is accessible during the catalytic process, which is especially beneficial when using expensive or rare transition metals. SACs also exhibit high selectivity, as the well-defined active sites of the isolated atoms lead to more targeted reactions with fewer by-products. Additionally, their distinct electronic structures can enhance catalytic activity. These factors, combined with their potential for improved stability, make SACs highly effective in a wide range of catalytic applications. Another important advantages of SACs is its efficient use of metal atoms (*5*,*6*,*7*). SACs, on the other hand, utilize every metal atom as an active site, reducing the amount of expensive and rare metals required for the catalytic cycle. This makes SACs a highly sustainable alternative to traditional organometallics-based processes, particularly for reactions that rely on precious metals like palladium, platinum, and rhodium. Moreover, in homogeneous organometallic catalysis, ligands are essential for stabilizing the metal center and controlling its reactivity. However, these ligands are often prone to degradation under reaction conditions, leading to catalyst deactivation and metal leaching into the reaction medium (*3*,*4*,*5*).

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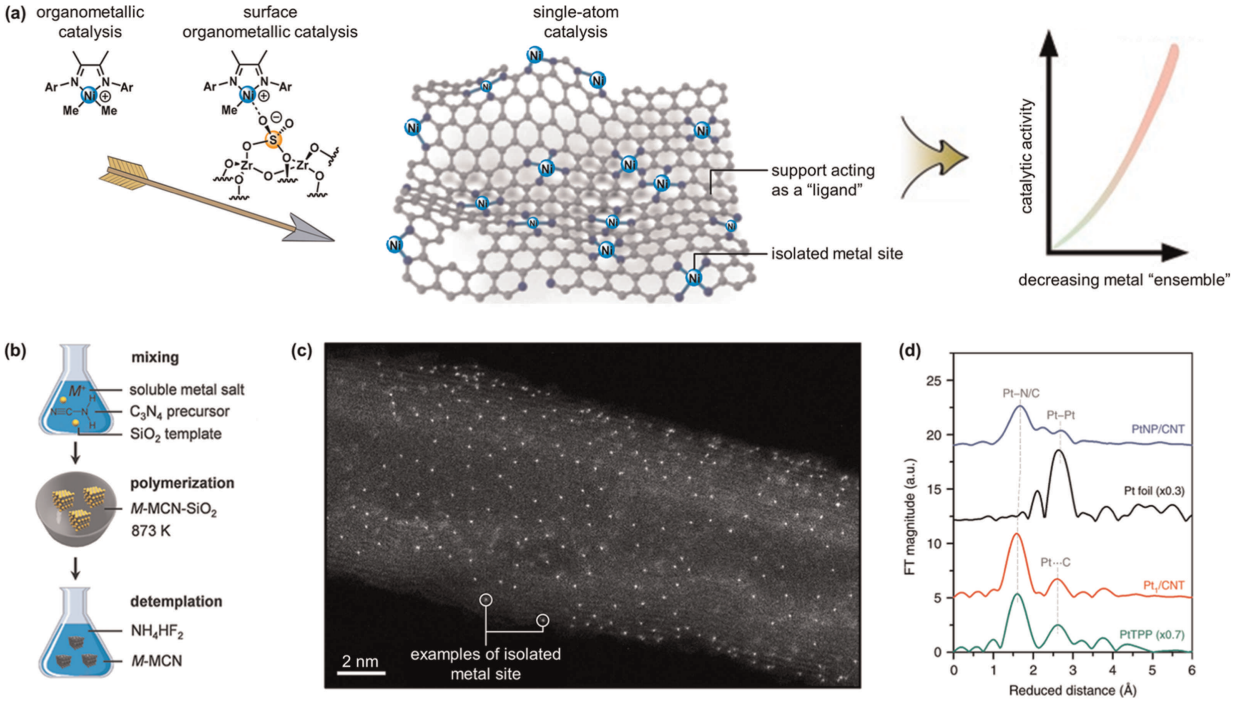



**Fig. 1** (a) Evolution of catalysis concepts in organic synthesis, from homogeneous organometallic chemistry to the emerging field of single-atom catalysis. On the side, it is shown the importance of decreasing the metal ensemble compared to conventional nanoparticle-based heterogeneous catalysts to enhance the catalytic performance. (b) Examplary sketch for the preparation of a class of SACs. For a deeper study of all other possibilities to make SACs, the reader is directed to more specialized reviews on the synthesis and characterization of SACs. (c) Aberration-corrected high-angle annular dark-field scanning transmission electron microscopy imaging of a single-atom $Pt_1$/CNT catalyst. The individual dots in the micrographs represent the isolated metal sites. (d) $k^3$-weighted Pt L3-edge extended X-ray absorption fine structure spectra of $Pt_1$/CNT and comparative Pt-based reference catalysts based on metal nanoparticles (PtNP/CNT), organometallic complexes (PtTPP), and foil (Pt foil). The absence of Pt-Pt bonds on the $Pt_1$/CNT spectra is demonstrated. Reproduced with permission from Saptal *et al.*, *Angew. Chem. Int. Ed.* **2023**, *62*, e202219306. Copyright 2023, Wiley-VCH.

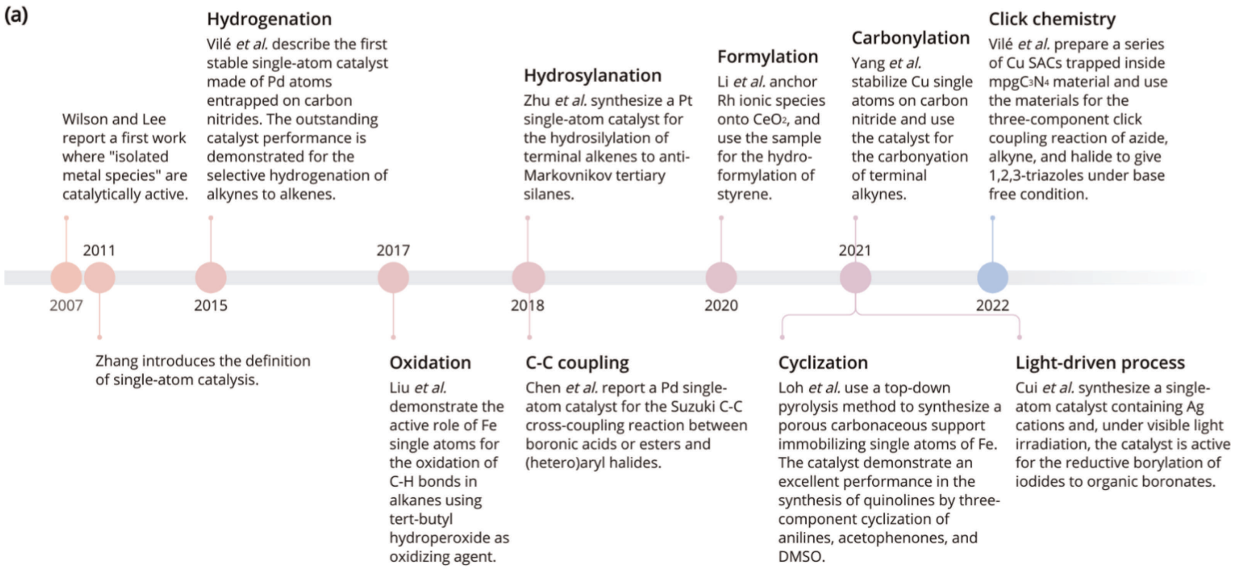
This not only reduces the efficiency of the catalytic process but also creates challenges for catalyst recovery and reuse, often resulting in significant amounts of metal waste. SACs overcome these issues by eliminating the need for complex homogeneous ligand systems. The solid support provides electronic stabilization to the metal atom, preventing it from aggregating or leaching under reaction conditions. This leads to a more stable catalyst that can be used over multiple reaction cycles without significant loss of activity (*8*). The ability to reuse SACs without extensive regeneration or replacement reduces also the consumption of materials and minimizes waste generation, further contributing to their environmental benefits. Moreover, the absence of ligands in SACs means that fewer chemical additives are required in the catalytic process, making the overall process cleaner and safer (**Fig. 1**).

## Historical Developments and Applications of Single-Atom Catalysts

The idea of isolated atoms as catalytic centers wasn't initially considered a viable strategy. Classical heterogeneous catalysis, particularly since the 20th century, revolved around nanoparticle-based catalysts. Researchers believed that the most efficient catalysts were those composed of nanoparticles or clusters of metal atoms dispersed on supports. This design allowed a significant number of atoms to be exposed on the surface while utilizing the catalytic properties of metals, particularly those in groups 8–10, such as platinum, palladium, and rhodium (*9*,*10*,*11*). However, this approach also meant that many atoms within nanoparticles were not involved in catalysis, as they were buried beneath the surface and thus inaccessible to reactants.

Theoretical work, beginning in the 1970s (*12*), hinted at the possibility of enhanced catalytic efficiency if all the metal atoms could be made available for reactions. Despite these ideas, the experimental tools and synthesis techniques available at the time made it difficult to stabilize and maintain single atoms on surfaces without their agglomeration into clusters. The rapid aggregation of metal atoms due to their high surface energy was a fundamental barrier that had to be overcome for single-atom catalysis to become a practical reality.

The concept of SACs began to take shape in the early 2000s (**Scheme 1**), with a growing interest in reducing the size of active catalytic materials to their theoretical limit—an individual atom. This period was characterized by advancements in materials




**Scheme 1** Timeline of the historic development of organic synthesis processes based on SACs. In particular, the figure shows the first synthetic application in each reaction class. Reproduced with permission from Saptal *et al.*, *Angew. Chem. Int. Ed.* **2023**, *62*, e202219306. Copyright 2023, Wiley-VCH.

science, especially in the development of more sophisticated supports, mainly metal oxides which could stabilize single atoms (*13*,*14*). One of the landmark moments in the development of SACs was the work by Professor Tao Zhang and his colleagues at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences. In 2011, they published a paper on the use of single-atom platinum catalysts for CO oxidation (*15*). In this study, platinum atoms were successfully stabilized on iron oxide supports, and the system exhibited high catalytic activity. This research highlighted the potential of SACs to combine the best features of both homogeneous and heterogeneous catalysis: the high activity and selectivity of single active sites, typical of homogeneous catalysts, with the robustness of heterogeneous catalysts. One key disadvantage was that the isolated metal atoms tend to aggregate under reaction conditions, leading to the formation of metal nanoparticles, which significantly reduces their catalytic activity. This instability arises because of the oxidic support used, where metal atoms were highly reactive and prone to migration. To address this challenge, in 2015 Vilé *et al*. used a N-coordinated carbon-based supports to stabilize SACs (*16*). The nitrogen coordination provided strong electronic interactions with the metal centers, increasing their stability while maintaining high catalytic performance. This approach represented a significant advancement in SAC design, allowing for improved reusability and efficiency in various catalytic reactions.

Support design is essential for producing stable SACs. Common supports include soft materials with high surface areas and active functional groups, such as carbon nitrides, covalent organic frameworks, metal-organic frameworks, and graphene. By manipulating the structure of the support, it becomes possible to control the surface free energy, which prevents the isolated atoms from clustering or aggregating (*17*). This spatial precision is absent in traditional nanoclusters or particles, where the active centers are often irregular in shape, size, and distribution (*18*). Consequently, SACs provide accessible and functional catalytic sites, which is crucial for minimizing the use of expensive and rare transition metals in catalytic reactions (*19*).

The synthesis of SACs is a rapidly evolving field in catalysis, driven by the need for highly efficient and atomically precise materials. However, synthesizing SACs requires overcoming significant challenges, particularly preventing the agglomeration of metal atoms into clusters or nanoparticles. To address these challenges, researchers have developed various synthesis methods, each with its advantages, limitations, and specific applications.

Wet impregnation is one of the simplest and most widely used methods for synthesizing SACs. It involves dispersing a metal precursor (typically a metal salt) into a liquid solution, followed by mixing the solution with a support material. After adsorption, the system is dried and subjected to calcination or reduction to anchor the metal atoms onto the support. By controlling factors such as metal precursor concentration, pH, temperature, and the calcination environment, it is possible to achieve the desired dispersion of single atoms (*20*). Wet impregnation is commonly used for the synthesis of SACs with metal atoms dispersed on metal oxide or carbon-based supports. One of the main advantages of wet impregnation is its simplicity and scalability. It does not require complex equipment, making it suitable for large-scale production. However, achieving uniform dispersion of single metal atoms is challenging. Without careful control of the conditions, metal atoms may agglomerate during the drying or calcination steps, forming clusters or nanoparticles instead of isolated atoms. To improve the effectiveness of wet impregnation for SAC synthesis, researchers often use low metal loadings or modify the support surface to enhance atom stabilization.

In co-precipitation, a metal precursor and a support precursor are mixed in solution, followed by the addition of a precipitating agent, such as sodium hydroxide or ammonium carbonate (21). The precipitating agent causes both the metal and support precursors to co-precipitate, forming a solid material. The resulting material is then filtered, dried, and calcined to obtain a catalyst with single metal atoms dispersed on the support. Co-precipitation offers better control over metal dispersion than wet impregnation, as the metal and support precursors are intimately mixed at the molecular level. This leads to improved stabilization of metal atoms and reduces the likelihood of atom agglomeration. However, like wet impregnation, co-precipitation requires precise control of the synthesis conditions to achieve the desired outcome. Factors such as pH, temperature, and the concentration of the precipitating agent must be carefully tuned to prevent the formation of metal clusters.

Atomic Layer Deposition (ALD) is a highly precise technique for synthesizing SACs, allowing for the controlled deposition of metal atoms onto a support material one atomic layer at a time (22). ALD involves exposing a support material to alternating pulses of a metal precursor and a reducing or oxidizing agent, separated by inert gas purging steps. Each precursor pulse reacts only with the surface of the support, ensuring that metal atoms are deposited in a uniform and controlled manner. ALD can achieve atomic-scale precision in terms of metal dispersion and loading, making it an ideal technique for synthesizing SACs. One of the key advantages of ALD is its ability to deposit single metal atoms on a wide range of support materials, including oxides, carbides, and nitrides. The high level of control over atom dispersion and surface coverage also allows for the precise tuning of catalytic activity and selectivity. Additionally, ALD can be used to deposit a variety of metal species, including noble metals (e.g., platinum, palladium) and non-noble metals (e.g., nickel, cobalt). However, the main limitation of ALD is its relatively low throughput and the need for specialized equipment, which may limit its scalability for large-scale SAC production.

Strong Electrostatic Adsorption (SEA) is a synthesis technique that exploits the electrostatic interactions between metal cations and the charged surface of a support material (23). In SEA, a support material with a charged surface (such as an oxide or carbon material) is placed in a solution containing metal cations. The electrostatic attraction between the positively charged metal ions and the negatively charged surface leads to the adsorption of the metal ions onto the support. Subsequent reduction or calcination steps are used to convert the adsorbed metal ions into single metal atoms. SEA provides a high degree of control over metal dispersion, as the strong electrostatic interactions help prevent the aggregation of metal atoms. It also allows for selective deposition of metal atoms at specific sites on the support, leading to uniform distribution and enhanced catalytic activity. SEA is particularly effective for synthesizing SACs with low metal loadings, as it minimizes the risk of atom aggregation. However, the method is sensitive to the pH and ionic strength of the solution, which must be carefully controlled to achieve optimal results.

Defect engineering is an approach to SAC synthesis that involves creating specific defects or vacancies in the support material to stabilize isolated metal atoms (24). Defects such as oxygen vacancies, nitrogen-doped sites, or sulfur vacancies can serve as anchoring points for metal atoms, preventing them from agglomerating into clusters. This approach is particularly effective for carbon-based supports, where defects such as nitrogen or sulfur doping can create strong binding sites for metal atoms. Defect engineering offers a high degree of stability for single metal atoms, as the defects act as traps that prevent atom migration and aggregation. This method is often used in combination with other techniques, such as wet impregnation or SEA, to enhance the stability and dispersion of metal atoms. However, creating and controlling defects in the support material can be challenging, as the defect density and distribution must be carefully optimized to achieve the desired catalytic performance.

Galvanic replacement is a synthesis method based on a redox reaction between a metal precursor and a sacrificial support material (25). In this process, a more noble metal precursor (such as platinum or palladium) is reduced by a less noble metal (such as copper or silver) on the surface of the support. The less noble metal is oxidized and dissolved, while the more noble metal is deposited as isolated atoms on the support. Galvanic replacement offers a straightforward and effective way to synthesize SACs with noble metals, as it allows for the deposition of single metal atoms without the need for complex synthesis steps. The method also enables precise control over the metal loading and dispersion by adjusting the concentration of the metal precursor and the sacrificial support. However, galvanic replacement is limited to metals with significant differences in redox potential, and it may not be suitable for all metal-support combinations.

High-temperature pyrolysis involves the thermal decomposition of a metal-organic framework (MOF) or other organometallic precursors at high temperatures in an inert or reducing atmosphere (26). During pyrolysis, the organic components decompose, leaving behind a carbonaceous support with single metal atoms dispersed on the surface. Pyrolysis is a versatile technique that can be used to synthesize SACs with a wide range of metal species, including transition metals and noble metals. One of the advantages of high-temperature pyrolysis is its ability to produce SACs with high metal loadings, as the metal atoms are stabilized by the carbon matrix formed during the decomposition process. The resulting SACs often exhibit excellent stability and catalytic activity, making them suitable for various applications, such as energy conversion and environmental catalysis. However, the high temperatures required for pyrolysis can lead to the aggregation of metal atoms if not carefully controlled, which may reduce the effectiveness of the catalyst.

Characterizing single-atom catalysts (SACs) requires a combination of conventional and advanced techniques to fully understand their atomic structure, electronic properties, and interactions with the support material (27). These methods provide insights into the catalyst's activity, stability, and selectivity, which are essential for optimizing performance. For example, aberration-corrected scanning transmission electron microscopy (STEM) is a crucial tool that allows direct visualization of individual metal atoms on the support surface. This high-resolution imaging technique enables researchers to confirm atomic dispersion, ensuring that metal atoms remain isolated rather than forming clusters or nanoparticles. By distinguishing single atoms from larger aggregates, STEM helps verify the fundamental structural integrity of SACs, a key factor

in their catalytic efficiency. Combined with electron energy loss spectroscopy (EELS), the technique can also be used to distinguish catalytic single atoms from isolated metal impurities coming from the synthesis (28). In Fourier-transform infrared (FTIR) spectroscopy, often with carbon monoxide (CO) as a probe molecule, researchers can investigate the electronic environment and coordination state of the metal atoms. CO adsorption shifts the vibrational frequencies of its stretching modes, and these shifts provide valuable information about the electron density on the metal atoms and their interaction with the support. This technique is highly effective in understanding the charge transfer between the support and the metal atoms, which directly affects catalytic behavior. X-ray absorption spectroscopy (XAS), particularly extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structure (XANES), offers detailed insights into the local coordination environment and electronic configuration of SACs. EXAFS provides information about bond distances and the coordination number surrounding the metal atoms, which helps determine whether they remain isolated or form clusters. XANES, in turn, reveals the oxidation state and electronic structure of the metal atoms, offering a window into the charge transfer dynamics crucial for stabilizing SACs. In addition to these conventional methods, several emerging and computational approaches have proven instrumental in SAC characterization. Density functional theory (DFT) plays a key role in modeling the electronic structure and reaction mechanisms at atomic resolution (29). DFT calculations can simulate catalytic behavior and help predict how metal atoms interact with their support, providing theoretical insights that guide experimental efforts in catalyst design. Another innovative approach involves machine learning (ML), which has increasingly been applied to analyze large datasets from experimental techniques like XAS (30). By training models on large databases of XAS spectra, ML can help automate the interpretation of spectral features and predict catalyst performance. This data-driven approach accelerates the discovery process by providing more accurate predictions of the local environment and electronic properties of the metal atoms (31). X-ray photoelectron spectroscopy (XPS) is another essential technique used to analyze the surface composition and oxidation state of SACs. XPS provides information about the chemical environment of the metal atoms and the extent of charge transfer between the metal and the support. By measuring the binding energies of core electrons, XPS helps to elucidate the electronic structure of SACs, especially regarding their catalytic sites. Less conventional but increasingly relevant techniques such as atomic force microscopy (AFM) and scanning tunneling microscopy (STM) have also been used to explore surface interactions and the electronic environment of SACs at the atomic scale. By combining these experimental techniques with computational methods like DFT and machine learning, researchers can develop a comprehensive understanding of SACs. This multi-faceted approach allows for the precise tuning of their catalytic properties, advancing the field of single-atom catalysis by providing deeper insights into the structure-performance relationships that govern their catalytic behavior.

One of the key catalytic advantages of SACs is their chemical orthogonality, meaning they exhibit high stereo-, regio-, and chemoselectivity toward specific reactions and functional groups (32). This orthogonality stems from the unique nature of SACs, where the single metal atom has a limited number of adsorption configurations due to its isolated positioning on the support. In fact, unlike conventional metal surfaces, which have multiple and often non-specific binding sites, SACs provide a well-defined active center that facilitates selective interactions with reactants. This precision ensures that only specific bonds and functional groups participate in the catalytic process, enabling SACs to exhibit high levels of selectivity in complex organic transformations. Because of these properties, SACs have shown remarkable efficiency in various cross-coupling reactions, such as Suzuki (33), Ullmann (34), Sonogashira (35), and Heck couplings (36), which are fundamental in the formation of C–C, C–O, and C–N bonds. These reactions typically involve a dynamic change in the oxidation state of the metal center during the oxidative addition and reductive elimination steps. Specifically, hydrogenation reactions play a critical role in the production of chemicals, pharmaceuticals, and fuels. The efficiency and selectivity of SACs have proven especially beneficial in these reactions, where isolated metal atoms provide precise control over hydrogen activation and transfer. Palladium and platinum SACs have demonstrated high activity in the selective hydrogenation of unsaturated compounds. For example, palladium SACs supported on carbon-based materials are commonly used in the hydrogenation of nitroarenes (37), producing anilines, which are valuable intermediates in the chemical and pharmaceutical industries. The atomically dispersed palladium atoms selectively activate the nitro group while avoiding the over-hydrogenation of other functional groups, such as carbonyls or alkenes. This selectivity is vital in fine chemicals synthesis, where the ability to control reaction pathways is crucial. Similarly, platinum single-atom catalysts have been employed in the selective hydrogenation of alkenes. These catalysts offer excellent selectivity towards terminal alkenes, which are important intermediates in the production of polymers, surfactants, and other fine chemicals. The isolated platinum atoms promote selective hydrogenation by minimizing side reactions, such as isomerization or over-hydrogenation, thereby increasing product yield and purity.

The hydrogenation of carbon dioxide ($CO_2$) is a key reaction in efforts to mitigate climate change by converting this greenhouse gas into useful chemicals and fuels. SACs have shown considerable potential in $CO_2$ hydrogenation due to their ability to activate $CO_2$ under mild conditions. Rhodium (38), copper (39), and nickel (40). SACs have been extensively studied for their role in the conversion of $CO_2$ to valuable products such as methane, methanol, and other hydrocarbons. In the reference provided, rhodium single-atom catalysts supported on metal oxides have been shown to efficiently catalyze the hydrogenation of $CO_2$ to methane, a reaction that holds promise for synthetic natural gas production. These catalysts are highly selective for methane, thanks to the well-defined electronic structure of the single rhodium atoms, which promotes $CO_2$ activation and hydrogenation without leading to over-reduction or the formation of unwanted byproducts. Copper SACs have also proven effective in the hydrogenation of $CO_2$ to methanol, a key feedstock for producing chemicals, fuels, and plastics. Single copper atoms supported on ceria ($CeO_2$) exhibit high selectivity towards methanol, driven by the ability of the ceria support to stabilize the copper atoms and facilitate $CO_2$ adsorption. This selective behavior is especially important in industrial applications, where methanol serves as a precursor for various chemicals and fuels.

Oxidation reactions are fundamental to many industrial processes, including the production of fine chemicals, environmental remediation, and energy conversion. SACs offer unique advantages in oxidation catalysis due to their high activity and selectivity, which stem from the atomic-level dispersion of active metal atoms. Palladium and platinum SACs have been successfully applied in the oxidation of hydrocarbons, alcohols, and carbon monoxide (CO) (*5*). For example, palladium SACs supported on ceria have been used to catalyze the low-temperature oxidation of methane, converting it to methanol. This reaction is particularly important for natural gas utilization, as methane is abundant and can serve as a valuable feedstock for producing methanol, which is used in a variety of chemical processes. In the oxidation of alcohols to aldehydes, platinum SACs have shown remarkable selectivity. Platinum atoms dispersed on metal oxide supports, such as titania ($TiO_2$), can catalyze the oxidation of alcohols to aldehydes with minimal formation of over-oxidation products, such as carboxylic acids. This selectivity is crucial in the fine chemicals industry, where high-purity products are required for pharmaceutical and agrochemical applications.

Dehydrogenation reactions are essential in the petrochemical industry, where they are used to produce alkenes from alkanes. Alkenes, such as ethylene and propylene, are important building blocks in the production of polymers, plastics, and other chemicals. SACs have shown significant potential in dehydrogenation reactions due to their high activity and ability to avoid side reactions, such as coking or over-dehydrogenation. Palladium and platinum single-atom catalysts have been successfully applied in the dehydrogenation of light alkanes, such as propane and ethylbenzene (*41*). Specifically, palladium SACs supported on alumina have been used to catalyze the dehydrogenation of propane to propylene, a key intermediate in the production of polypropylene. The isolated palladium atoms provide well-defined active sites for C–H bond activation, resulting in high selectivity for propylene and reduced formation of coke, a common issue in dehydrogenation reactions. Similarly, platinum SACs have been employed in the dehydrogenation of ethylbenzene to styrene, a precursor for polystyrene production. Platinum atoms dispersed on ceria supports exhibit excellent catalytic activity and stability, as the ceria helps to prevent the aggregation of platinum atoms and promotes the activation of C–H bonds. The high selectivity and stability of these SACs make them promising candidates for industrial dehydrogenation processes, where the efficient production of alkenes is critical.

The field of energy conversion, particularly in the context of renewable energy technologies, has benefited greatly from the application of SACs in electrocatalysis. SACs have been shown to enhance the efficiency of key reactions in fuel cells, water splitting, and $CO_2$ reduction by providing highly active and selective sites for electrochemical processes (*42*). Platinum and nickel SACs have been widely studied for their role in the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR) in fuel cells. For example, platinum single-atom catalysts supported on carbon-based materials exhibit high activity for the ORR, a crucial reaction in proton-exchange membrane fuel cells (PEMFCs). The isolated platinum atoms provide well-defined active sites for oxygen activation and reduction, leading to improved fuel cell efficiency and reduced use of expensive platinum. In the hydrogen evolution reaction (HER), nickel single-atom catalysts have shown great potential as a cost-effective alternative to platinum. Nickel SACs supported on nitrogen-doped carbon materials have demonstrated excellent activity and stability in HER, making them promising candidates for use in water-splitting devices. The atomic-level dispersion of nickel atoms allows for efficient hydrogen production, while the nitrogen-doped carbon support enhances the stability of the catalyst under electrochemical conditions.

SACs have also found applications in environmental catalysis, where they are used to degrade pollutants, convert harmful gases, and promote clean energy technologies. Their high activity and selectivity make them ideal for processes aimed at reducing environmental pollution and promoting sustainability. For example, SACs offer a promising strategy for removing pharmaceutical contaminants from wastewater due to their high catalytic efficiency, tunable selectivity, and minimized metal usage. Their application in advanced oxidation processes or photocatalytic degradation can significantly enhance the breakdown of persistent pollutants, reducing environmental impact (*43*).

The diverse applications of SACs in hydrogenation, oxidation, dehydrogenation, electrocatalysis, and environmental catalysis demonstrate their transformative potential in both industrial and sustainable chemistry. By providing atomically dispersed active sites, SACs offer significant advantages in terms of catalytic activity, selectivity, and metal utilization, making them ideal for a wide range of chemical processes. From the selective hydrogenation of fine chemicals to the oxidation of pollutants and the production of clean energy, SACs are paving the way for more efficient, cost-effective, and environmentally friendly catalytic technologies. As the field of SAC research continues to grow, it is expected that these catalysts will play an increasingly important role in addressing global challenges related to energy, the environment, and industrial processes. The ability to design and synthesize SACs with tailored properties opens up exciting possibilities for developing next-generation catalysts with unprecedented performance across a broad spectrum of applications.

## Conclusions

As it can be viewed from these examples, SACs have opened up new possibilities for greener reaction conditions. Traditional organometallic catalysis often requires harsh conditions, such as high temperatures, pressures, or the use of toxic solvents. SACs, on the other hand, have shown to operate effectively under milder conditions, thanks to their high reactivity and selectivity. Future directions in single-atom catalysis could focus on improving the stability of these catalysts under industrially relevant conditions, expanding their applicability to multi-step cascade reactions, and developing SACs for electrocatalytic and photocatalytic processes. Moreover, integrating SACs with automated high-throughput screening and artificial intelligence for catalyst design could significantly accelerate the discovery of new SACs with tailored properties. These advancements would not only broaden the scope of single-atom catalysis but also align catalysis research with global sustainability goals.

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