
Single-Atom Catalysts in Electrocatalytic Urea Synthesis: A Survey

www.surveyx.cn

Abstract

Single-Atom Catalysts (SACs) have emerged as transformative materials in electrocatalytic urea synthesis, offering enhanced efficiency and selectivity under ambient conditions. This survey paper explores the pivotal role of SACs in converting nitrogen (N) and carbon dioxide (CO) into urea, aligning with sustainable chemistry principles. The precision in engineering active sites facilitates overcoming challenges in nitrogen reduction reactions, improving charge transfer and reaction pathways. SACs also present an economical alternative to noble-metal-based catalysts, reducing reliance on costly platinum-group metals. The structural design and classification of SACs are crucial, with substrate materials and active site configurations significantly impacting performance. Advanced computational methods, including Density Functional Theory and machine learning, are employed to predict and optimize SAC behavior. Despite their potential, challenges in stability and reaction kinetics remain, necessitating innovative SAC designs. Recent advances demonstrate SACs' potential in achieving high catalytic activity and stability, paving the way for sustainable chemical processes. Future research should focus on optimizing catalyst performance through alternative nitrogen sources, refining support materials, and integrating computational techniques to enhance prediction capabilities. By expanding the library of SACs and exploring their catalytic properties, researchers can develop efficient, stable, and environmentally friendly catalytic systems for broader applications in renewable energy and green chemistry.

1 Introduction

1.1 Significance of SACs in Electrocatalytic Urea Synthesis

Single-Atom Catalysts (SACs) represent a transformative advancement in electrocatalytic urea synthesis, markedly improving catalytic efficiency and selectivity. Operating under ambient conditions, SACs facilitate the conversion of nitrogen (N₂) and carbon dioxide (CO₂) into urea through electrochemical reactions, embodying a sustainable synthesis method aligned with green chemistry principles [1, 2].

The atomic-level precision in engineering active sites is essential for optimizing catalytic performance, particularly in overcoming the inert N-N bond activation challenges associated with the nitrogen reduction reaction (NRR) [3]. SACs enhance charge transfer and reaction pathways, improving overall catalytic efficiency [4].

Additionally, SACs mitigate the inefficiencies and costs of traditional noble-metal-based electrocatalysts in urea oxidation and hydrogen evolution reactions, reducing reliance on expensive platinum-group metals (PGMs) [5, 4]. This economic advantage is complemented by their enhanced stability and durability, crucial for long-term applications in renewable energy contexts [6].

The integration of SACs into electrocatalytic systems is vital for advancing sustainable urea production. While electrochemical synthesis holds promise, the mechanisms involved are not fully

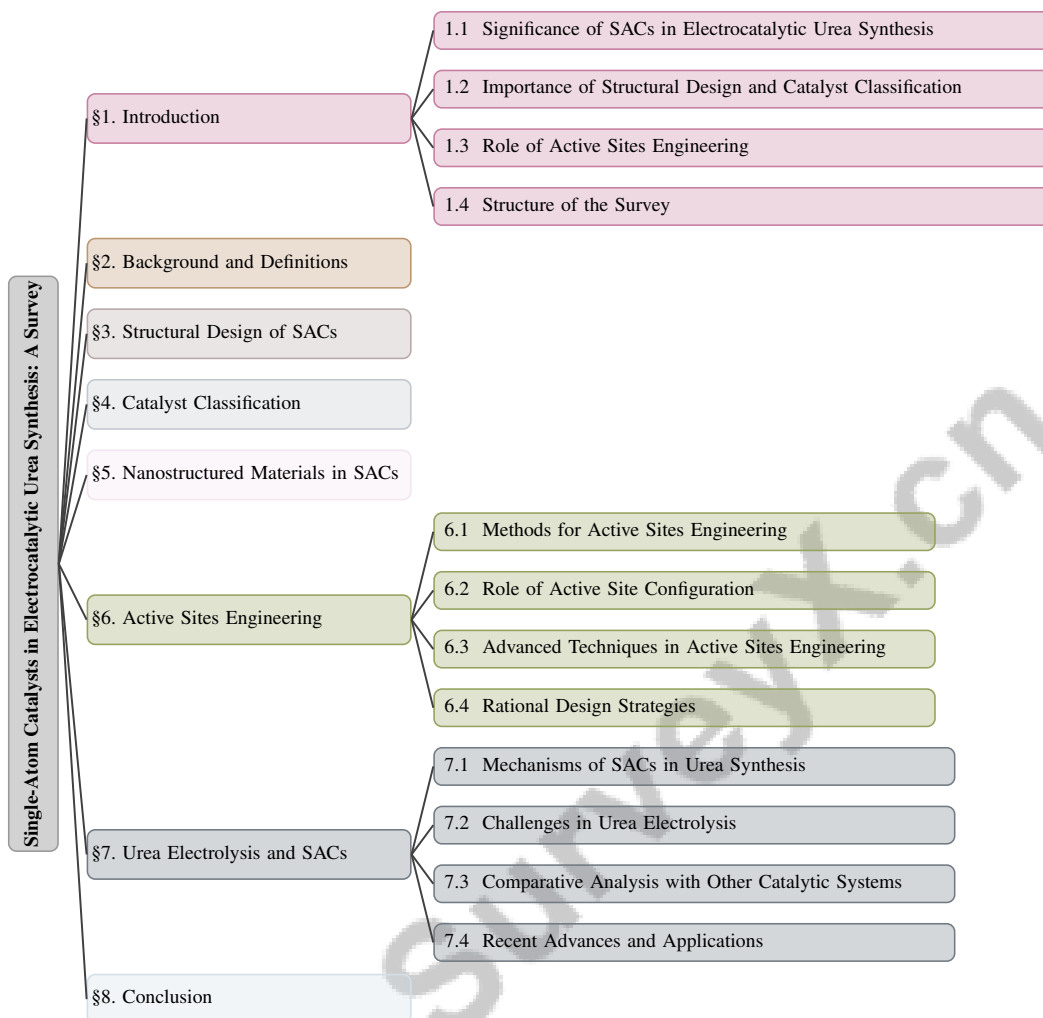


Figure 1: chapter structure

understood, and SACs serve as a critical tool in elucidating these processes [7]. Their capacity to enhance catalytic sensitivity and efficiency is further exemplified in applications involving atomically-thin metals like platinum, illustrating their transformative potential in catalysis and chemical detection [8].

1.2 Importance of Structural Design and Catalyst Classification

The structural design and classification of SACs are pivotal in determining their catalytic performance, especially in electrocatalytic urea synthesis. The structure-performance relationship is fundamental for developing efficient bifunctional electrocatalysts, as indicated by the categorization of these materials [9]. This classification not only elucidates the intrinsic properties of catalysts but also informs the strategic design of SACs for improved catalytic activity.

Optimizing SACs presents challenges in accurately predicting catalytic activity due to the diverse combinations of active elements and support materials [10]. Understanding the structural characteristics influencing catalyst behavior is essential; for example, specific MBenes like Mo_2B_2 , Ti_2B_2 , and Cr_2B_2 have been identified as effective for electrochemical urea synthesis from N_2 and CO_2 [2].

Furthermore, integrating SACs on modified graphene surfaces exemplifies a strategic method to enhance catalytic performance while decreasing dependence on PGMs [4]. This approach underscores the importance of substrate selection and modification in SAC design, leading to improved stability and efficiency.

1.3 Role of Active Sites Engineering

Active sites engineering is crucial for enhancing urea electrolysis efficiency by optimizing catalyst-reactant interactions. This strategy significantly influences catalytic performance, as demonstrated by indium hydroxide's role in promoting direct C–N coupling while suppressing competing reactions [1]. The arrangement and composition of active sites, such as atomically dispersed titanium on graphene, facilitate critical reactions like hydrogen dissociation, highlighting the potential of active site engineering to improve catalytic efficiency [11].

SACs maximize catalyst utilization by enabling each atom to participate in reactions, thereby enhancing overall efficiency [4]. In NRR, SAC activity is influenced by the number of unpaired d electrons in transition metals and the charge state of adsorbed transition metals [3].

The development of bifunctional electrocatalysts capable of catalyzing both the hydrogen evolution reaction (HER) and urea oxidation reaction (UOR) underscores the significance of active sites engineering in achieving superior catalytic performance [5]. However, challenges remain in creating electrocatalysts that effectively catalyze both oxygen evolution reaction (OER) and HER while maintaining stability over extended use [6].

Advanced computational techniques, including multi-branch Convolutional Neural Network (CNN) models, show promise for predicting SAC catalytic activity by utilizing electronic density of states (eDOS) to identify optimal active site configurations [10]. Additionally, *ab initio* Molecular Dynamics simulations have been employed to elucidate the C–N coupling mechanism in urea synthesis, emphasizing the critical role of active site configuration [12].

Innovative methodologies, such as the Single Atom Platform (SAP), enhance catalytic efficiency by improving electron transfer and reactant interaction through asymmetrically coordinated metal atoms [13]. This approach not only optimizes the active site environment but also facilitates dynamic interfacial behavior, crucial for forming C–C and C–N bonds necessary for synthesizing complex molecules [14].

1.4 Structure of the Survey

This survey is systematically organized to provide a comprehensive analysis of SACs in electrocatalytic urea synthesis, highlighting their potential to enhance efficiency and sustainability in urea production through innovative electrochemical methods while addressing catalyst design and performance optimization challenges [2, 13, 1, 9]. The introduction emphasizes the significance of SACs and the importance of structural design and catalyst classification.

The second section, "Background and Definitions," establishes a foundational understanding of SACs, defining key terms and elucidating their relevance to catalysis and sustainable chemistry, ensuring readers are equipped with essential concepts for subsequent discussions.

The third section, "Structural Design of SACs," explores various structural designs and the role of substrate materials and single atom arrangements, highlighting recent advancements in structural engineering that enhance SAC performance.

The fourth section, "Catalyst Classification," examines SAC classification, focusing on composition and support materials, which aids in understanding and improving catalyst performance through insights into hybrid, co-doped, and transition-metal-based structures.

The fifth section, "Nanostructured Materials in SACs," discusses the integration of nanostructures and their impact on catalytic activity, exploring the synthesis and characterization of these materials and their advantages in enhancing SAC properties.

The sixth section, "Active Sites Engineering," details methods for engineering active sites in SACs, emphasizing configuration importance and providing examples of successful practices from recent studies.

The seventh section, "Urea Electrolysis and SACs," analyzes SACs' roles in urea electrolysis, discussing mechanisms, challenges, and recent research findings related to their application in urea synthesis.

Finally, the conclusion summarizes key points, reflects on the current research state, and suggests future directions and potential applications of SACs in sustainable chemistry. Each section builds

upon the previous, ensuring a logical flow and comprehensive coverage of the topic. The following sections are organized as shown in Figure 1.

2 Background and Definitions

2.1 Overview of Single-Atom Catalysts (SACs)

Single-Atom Catalysts (SACs) represent a transformative advancement in catalysis, utilizing isolated metal atoms, such as titanium on graphene, to enhance catalytic efficiency [11, 4]. This atomic-level exposure maximizes catalyst utilization, significantly improving bifunctional catalysis, notably in urea electrolysis [5]. Maintaining the dispersion of single metal atoms without aggregation is critical, requiring precise substrate selection [15]. Advanced computational methods have been crucial in understanding SACs' unique properties, linking atomic-scale data to macro-scale functionalities [16, 10].

SACs face challenges in complex reactions, such as C-C and C-N bond formations, particularly with nickel-based catalysts [14]. Furthermore, there is a notable gap in understanding how varying electrode potentials affect reaction mechanisms and activity [7]. Addressing these challenges requires a deep understanding of atomic interactions and innovative enhancement strategies.

SACs are poised to revolutionize sustainable chemistry through their unique properties that enable the development of efficient catalytic processes. Their atomic-level operation and integration with advanced computational techniques position SACs as promising candidates for overcoming traditional catalyst limitations, especially in the electrosynthesis of urea, a vital chemical industry raw material [2].

2.2 Key Terms and Definitions

Understanding key terms is crucial for grasping SACs' role in electrocatalytic urea synthesis. 'Single-Atom Catalysts' involve isolated metal atoms, often from platinum-group metals, to enhance catalytic efficiency and selectivity [4]. These catalysts are pivotal in energy conversion applications, where atomic precision is essential for performance improvement.

'3D atomic structures' refer to the spatial arrangement of atoms in catalysts, influencing reactivity and chemical properties [17]. 'Chemical order/disorder' within these structures significantly impacts catalytic activity, as seen in FePt nanoparticles used in electrocatalysis [17]. 'Atomically-thin metals', such as platinum, are essential for developing advanced catalytic systems, enhancing sensitivity and efficiency in various applications, including SACs [8].

Traditional methodologies' reliance on 'linear assumptions' poses challenges in accurately representing catalytic systems' complex structures [18]. Advanced analytical techniques are necessary to decode intricate interactions, enhancing SAC design and functionality.

Understanding these terms is vital for appreciating advancements in SACs and their applications in sustainable chemistry and electrocatalytic urea synthesis. Recent developments in computational chemistry and nanomaterial engineering provide foundational knowledge for exploring innovative strategies in designing and optimizing efficient catalytic systems. These advancements include multiscale modeling approaches for catalyst discovery that categorize materials based on experimental viability, alongside precise engineering of atomic sites in single-atom catalysts and metallic 1T-MoS₂, which enhance catalytic activity and performance [16, 19, 13].

2.3 Relevance to Catalysis and Sustainable Chemistry

SACs play a crucial role in sustainable chemistry by providing efficient, environmentally friendly catalytic pathways for urea synthesis. These catalysts address the need for advanced systems that operate under ambient conditions, reducing energy consumption and environmental impact compared to traditional methods [1]. SACs' unique attributes, particularly their use of isolated metal atoms, allow precise control over catalytic processes, essential for enhancing selectivity and efficiency [20].

Transition metal-based SACs offer a cost-effective and sustainable alternative to noble metal catalysts in urea electrolysis, demonstrating superior economic and environmental benefits [9]. This shift

towards sustainable materials is vital for developing scalable and economically viable catalytic systems, aligning with green chemistry principles.

A significant challenge remains in identifying suitable electrocatalysts for the efficient electrochemical coupling of N_2 and CO_2 for urea production. Applying machine learning techniques to identify key descriptors predicting nitrogen reduction reaction (NRR) performance offers a promising strategy. By focusing on charge transfer and electronic structure modifications, such as boron doping, researchers can enhance SACs' catalytic efficiency [3].

3 Structural Design of SACs

3.1 Substrate Materials and Single Atom Anchoring

The choice of substrate materials is pivotal in the anchoring process of single atoms in Single-Atom Catalysts (SACs), directly impacting their catalytic performance. Graphene and its derivatives, such as N-doped, B-doped, and graphene with single vacancies, have proven effective for single atom anchoring, ensuring optimal exposure and engagement of metal atoms in catalytic reactions [4]. In bifunctional electrocatalysts, the electrochemical deposition of NiFeCo layered double hydroxides on nickel foam substrates exemplifies how substrate selection can enhance catalytic efficiency [6]. Additionally, the growth of Ni_2P/Fe_2P nanohybrids on Ni foam underscores the importance of tailored substrates in improving atom-support interactions [5]. Advanced strategies, including heteroatom doping and controlled nanostructures, further facilitate single atom anchoring, enhancing catalytic performance [9]. The spatial arrangement of atoms, as seen in carbon zero-layers on silicon carbide for atomically-thin platinum layers, is crucial for maintaining single-atom dispersion and optimizing performance [8]. Thus, the careful selection and engineering of substrate materials are essential for effective single atom anchoring in SACs, affecting their catalytic efficiency and potential applications in sustainable chemistry.

3.2 Innovative Structural Designs

Innovative structural designs in SACs have significantly enhanced their performance through advanced techniques that ensure the stability and activity of single atoms. Integrating single platinum (Pt) atoms into hybrid organic-inorganic perovskite structures exemplifies a method that anchors these atoms while preserving their catalytic activity [15]. This approach diverges from traditional methods by creating a stable environment that maximizes atomic utilization and efficiency. Uniform atomic doping of nickel and oxygen into 1T-MoS₂ represents another breakthrough, improving catalytic performance through enhanced electronic properties and active site accessibility [19]. Such atomic-level modifications optimize SACs, facilitating tailored electronic modulations that enhance activity across various applications [15, 16, 19, 13, 3]. By focusing on atomic arrangements and interactions, researchers can significantly enhance SAC efficiency and selectivity, paving the way for their application in sustainable chemical processes.

3.3 Precision and Stability in SAC Fabrication

Precision and stability in SAC fabrication are crucial for optimizing catalytic performance. The Single Atom Platform (SAP) method exemplifies this approach by utilizing organic polymers with functional motifs to anchor metal atoms post-synthesis, maintaining atomic dispersion vital for maximizing catalytic efficiency and longevity [13]. Substrate materials also play a key role in enhancing SAC stability. For example, indium hydroxide catalysts with well-defined 100 facets significantly improve urea synthesis efficiency by providing stable active sites [1]. SACs supported on graphene with single vacancies exhibit remarkable stability and reactivity due to strong interactions between single atoms and defect sites [4]. The development of atomically-thin platinum gas sensors further emphasizes the importance of surface effects in determining SAC stability and sensitivity [8]. Recent advancements in SAC fabrication techniques underscore the importance of precision and stability, facilitating the development of catalysts that exhibit high efficiency and durability for sustainable chemistry applications. Innovations such as engineered metal-organic platforms and hybrid organic-inorganic perovskites enhance structural precision, while atomically engineered activation sites on materials like 1T-MoS₂ improve electronic properties and atomic utilization efficiencies [15, 16, 19, 13, 14].

3.4 Advanced Computational Methods

Advanced computational methods are essential in the design and optimization of SACs, offering insights into their structural and electronic properties. Density Functional Theory (DFT) is widely used to analyze the thermodynamic stability of SAC structures under varying electrochemical conditions, providing a detailed understanding of catalyst-environment interactions [20]. This approach is crucial for predicting SAC stability and reactivity, enabling the design of more efficient catalytic systems. Machine learning techniques, such as Convolutional Neural Networks (CNNs), enhance predictive capabilities by analyzing electronic density of states (eDOS) and employing hybrid descriptor approaches to predict catalytic activity with greater accuracy [10]. Myopic Multiscale Sampling (MMS) uses multiscale modeling to optimize SAC structural design, facilitating a comprehensive exploration of catalyst properties [16]. Ab initio Molecular Dynamics (AIMD) simulations provide a robust framework for investigating reaction pathways, such as C-N bond formation during urea synthesis, under varying electrode potentials [12]. These simulations yield valuable insights into dynamic atomic-level processes essential for optimizing SAC performance. Additionally, the GENFIRE method employs advanced computational techniques to reconstruct atomic models, informing strategies for designing and optimizing SAC structures [17]. The integration of advanced computational methods, including DFT and AIMD simulations, offers a robust framework for the rational design and optimization of sustainable electrocatalysts for urea synthesis. By systematically evaluating the catalytic properties of two-dimensional metal borides (MBenes) and elucidating C-N bond formation mechanisms, these approaches enhance our understanding of electrocatalytic processes, addressing critical challenges in the electrochemical conversion of nitrogen and carbon dioxide into urea under ambient conditions. This progress significantly contributes to advancing the field of electrocatalytic urea synthesis, promoting environmentally friendly alternatives to traditional methods reliant on harsh conditions and ammonia feedstock [2, 12].

4 Catalyst Classification

4.1 Hybrid and Co-doped Structures

Hybrid and co-doped structures are pivotal in advancing Single-Atom Catalysts (SACs) by strategically combining elements and materials to enhance performance. The Myopic Multiscale Sampling (MMS) approach reframes catalyst discovery as a classification challenge, facilitating the identification of promising hybrid and co-doped SACs for experimental exploration [16]. The synergistic effects introduced by co-doped elements improve catalytic activity and stability. The Single Atom Platform (SAP) method exemplifies this by allowing post-synthesis chelation of diverse metal atoms, optimizing catalytic activity and selectivity [13].

Hybrid structures such as organic-inorganic perovskites and engineered metal-organic frameworks enhance electronic and structural diversity, facilitating precise SAC arrangement on inert substrates, thereby improving efficiency and stability. Incorporating single transition-metal atoms into perovskite surfaces enables uniform anchoring and electron donation, enhancing reactivity in reactions like CO oxidation and CO₂ reduction. Atomically engineered activation sites on catalysts like 1T-MoS₂ modulate electronic properties and improve atomic utilization, leading to superior performance in electrochemical reactions such as hydrogen evolution [15, 16, 11, 19, 13]. The tailored structural and electronic characteristics of hybrid catalysts open avenues for advanced catalytic applications.

Classifying hybrid and co-doped SACs is crucial for enhancing their efficacy in sustainable chemistry and electrocatalytic processes. This classification supports the identification of optimal catalytic properties and the development of advanced materials, significantly improving performance in reactions like CO oxidation and nitrogen reduction [16, 19, 3, 15]. Leveraging advanced computational and experimental techniques, researchers can systematically explore potential SAC configurations, leading to effective and sustainable catalysts.

4.2 Substrate-Based Classification

Substrate-based classification of Single-Atom Catalysts (SACs) is crucial for optimizing catalytic performance and stability. Different substrates interact uniquely with single metal atoms, influencing activity and selectivity. Graphene and its derivatives, such as N-doped and B-doped graphene, are prominent substrates due to their high surface area, excellent conductivity, and ability to stabilize

single atoms [4]. Heteroatom incorporation into graphene enhances metal atom anchoring strength and modulates electronic properties, improving catalytic efficiency.

Transition metal oxides and carbides serve as effective substrates for SACs, providing robust support that prevents aggregation and maintains high dispersion, crucial for catalytic activity [15]. MBenes, such as Mo_2B_2 and Ti_2B_2 , exemplify the potential of these substrates in facilitating electrochemical urea synthesis by enhancing N_2 and CO_2 interactions [2].

Organic-inorganic hybrid materials further enrich substrate-based classification, combining organic flexibility with inorganic stability. These hybrid substrates provide a versatile platform for single atom integration, allowing precise control over local environments and electronic interactions [13]. This classification aids in understanding substrate roles in SAC performance and guides the rational design of catalysts for sustainable chemistry and electrocatalysis applications.

By systematically classifying SACs according to their substrates, researchers enhance their understanding of complex interactions between support materials and catalytic behavior. This approach facilitates identifying promising catalysts for experimental investigation and designing effective, durable catalysts, crucial for optimizing diverse chemical transformations and advancing catalysis [15, 16, 10, 13, 14].

4.3 Bifunctional and Hybrid Catalysts

Bifunctional and hybrid Single-Atom Catalysts (SACs) represent significant advancements in catalysis, enabling simultaneous catalysis of multiple reactions and enhancing chemical process efficiency. These catalysts exhibit dual functionalities, such as promoting both the hydrogen evolution reaction (HER) and the urea oxidation reaction (UOR), critical for efficient urea electrolysis [5]. Developing bifunctional SACs is crucial for sustainable chemistry, as integrating multiple catalytic activities within a single system can substantially reduce energy consumption and improve process efficiency.

Hybrid structures in SACs involve strategically combining different materials or phases to achieve enhanced catalytic performance. For example, integrating single metal atoms into hybrid organic-inorganic perovskite frameworks maintains high catalytic activity while providing stability for the metal atoms [15]. This approach leverages the unique properties of both organic and inorganic components, resulting in catalysts that are efficient, durable, and adaptable to various reaction conditions.

The design of hybrid SACs often employs advanced structural engineering techniques to optimize interactions between different catalytic sites. The precise arrangement of active sites is crucial for maximizing efficiency and selectivity, allowing fine-tuning of electronic properties and reaction pathways [14]. Such control is essential for developing catalysts that effectively facilitate complex reactions, including the electrochemical synthesis of urea from N_2 and CO_2 [2].

4.4 Transition-Metal-Based Catalysts

Transition-metal-based Single-Atom Catalysts (SACs) are pivotal in catalytic research, enhancing reaction kinetics and selectivity across various chemical processes. These catalysts utilize isolated transition metal atoms, particularly from platinum-group metals, to maximize exposure and reactivity, achieving high catalytic efficiency [4]. The unique electronic properties of transition metals, characterized by their d-orbitals, facilitate versatile interactions with reactants, making them ideal for catalyzing complex reactions such as nitrogen reduction (NRR) and urea synthesis [3].

Integration of transition metals into SACs is often supported by advanced substrate materials, such as graphene and its doped derivatives, which provide stable and conductive environments for single atoms [4]. These substrates enhance dispersion and modulate electronic properties, improving catalytic performance. Transition metal oxides and carbides further exemplify the versatility of these supports in maintaining high catalytic activity and stability [15].

Recent advancements in computational methods have significantly enhanced the understanding and optimization of transition-metal-based SACs. Techniques such as Density Functional Theory (DFT) and Convolutional Neural Networks (CNNs) effectively predict catalytic activity and stability under various conditions. By integrating multi-branch CNN models with hybrid descriptor-based volcano plots, researchers can systematically screen diverse SAC systems, identifying optimal

catalyst candidates for specific reactions, such as CO₂ reduction. Multiscale modeling strategies allow for estimating bulk catalyst properties and accelerating classification of catalysts for experimental investigation, providing insights that inform both theoretical design and practical applications in catalysis [16, 10, 20, 13, 3]. These computational approaches enable the rational design of SACs with tailored properties, facilitating their application in sustainable chemistry and electrocatalysis.

The development of transition-metal-based SACs is essential for enhancing sustainable chemical processes, as these catalysts consist of minute amounts of transition metals precisely anchored to inert substrates, providing a cost-effective and highly efficient alternative to traditional catalysts. Recent advances in nanomaterials and engineered metal-organic platforms have stabilized single atoms, overcoming clustering challenges. This innovation enhances catalytic reactivity and enables fine-tuning of active sites, unlocking new functionalities and applications in catalysis [16, 13]. By leveraging the unique properties of transition metals, these catalysts can significantly enhance the efficiency and selectivity of chemical transformations, paving the way for more sustainable and environmentally friendly catalytic systems.

In the exploration of Single-Atom Catalysts (SACs), understanding the hierarchical structure of nanostructured materials is crucial. As depicted in Figure 2, this figure illustrates the intricate relationships within SACs, emphasizing various integration methods and their impact on catalytic activity. Furthermore, it outlines the synthesis and characterization techniques employed in the development of these materials, while also highlighting the advantages that nanostructures offer in enhancing catalytic performance. This comprehensive overview not only aids in grasping the complexity of SACs but also serves to underscore the significance of nanostructured materials in advancing catalytic science.

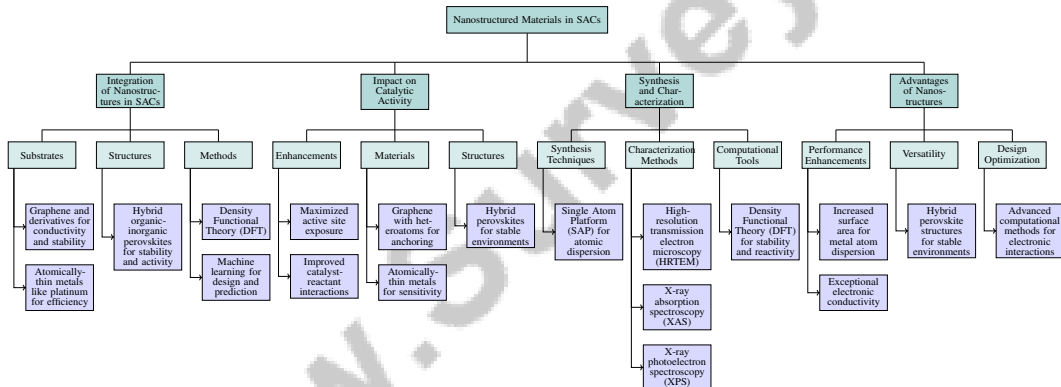


Figure 2: This figure illustrates the hierarchical structure of nanostructured materials in Single-Atom Catalysts (SACs), highlighting integration methods, impact on catalytic activity, synthesis and characterization techniques, and the advantages offered by nanostructures.

5 Nanostructured Materials in SACs

5.1 Integration of Nanostructures in SACs

The integration of nanostructures into Single-Atom Catalysts (SACs) is pivotal for enhancing catalytic efficiency through increased surface area and optimal dispersion of metal atoms. Graphene and its derivatives, known for their superior conductivity and stability, serve as effective substrates, facilitating the anchoring of single metal atoms and maximizing their catalytic exposure [4]. Atomically-thin metals, such as platinum, exemplify the enhancement of catalytic efficiency and sensitivity in applications like gas sensing [8]. Precise control over nanostructure thickness and arrangement optimizes interactions between single atoms and supports, thereby improving performance.

Hybrid organic-inorganic perovskite structures provide stable environments for single atoms, leveraging the unique properties of both components to enhance catalytic activity in sustainable chemistry and electrocatalysis [15]. Advanced computational methods, including Density Functional Theory (DFT) and machine learning, predict electronic properties and guide the rational design of nanostructured SACs, fostering the development of efficient catalytic systems [10].

5.2 Impact on Catalytic Activity

Incorporating nanostructures into SACs significantly enhances catalytic activity by maximizing active site exposure and improving catalyst-reactant interactions. Graphene, especially when doped with heteroatoms, strengthens metal atom anchoring and modulates electronic properties, boosting efficiency [4]. Atomically-thin metals improve catalytic sensitivity and efficiency, particularly in gas sensing applications [8]. Hybrid perovskite structures further enhance activity by providing stable environments for single atoms [15]. Computational methods like DFT and machine learning aid in predicting electronic properties, optimizing catalytic performance, and guiding rational catalyst design [10].

5.3 Synthesis and Characterization

Synthesis and characterization of nanostructured SACs are crucial for assessing catalytic performance and stability. Techniques such as the Single Atom Platform (SAP) method ensure precise atomic dispersion, essential for maximizing efficiency [13]. Integrating single atoms into nanostructured supports like graphene enhances dispersion and activity [4]. Characterization methods, including high-resolution transmission electron microscopy (HRTEM), X-ray absorption spectroscopy (XAS), and X-ray photoelectron spectroscopy (XPS), analyze structural and electronic properties [15]. Computational tools like DFT complement these techniques by predicting stability and reactivity under various conditions, guiding SAC design [20].

5.4 Advantages of Nanostructures

Nanostructures in SACs offer significant advantages, enhancing catalytic performance and applicability in sustainable chemistry. Increased surface area from nanostructures allows for higher dispersion of metal atoms, maximizing active site availability [4]. Exceptional electronic conductivity of materials like atomically-thin metals and graphene derivatives is vital for efficient electron transfer in electrocatalytic processes [8]. Hybrid perovskite structures exemplify the versatility of nanostructures, providing stable and active environments for single atoms [15]. Advanced computational methods, such as DFT and machine learning, optimize SAC design by providing insights into electronic interactions, thereby guiding the development of high-performance catalysts [10].

6 Active Sites Engineering

6.1 Methods for Active Sites Engineering

Method Name	Optimization Techniques	Structural Features	Material Composition
ML-AS[3]	Machine Learning	Boron Substitution	Boron-doped MoS ₂
GENFIRE[17]	Dft Calculations	3D Atomic Positions	Fept Nanoparticles
E-SU[1]	Electrochemical Coupling	Defined 100 Facets	Indium Hydroxide Catalyst
Pt-chemiresistor[8]	Sensor Design Optimization	Atomic Positions	Atomically-thin Platinum
RSGS[4]	Dft Calculations	Atomic Positions	Single Atom Catalysts
Ni ₂ P/Fe ₂ P/NF[5]	Manual Shaking Reaction	Conductive 3D Network	Ni ₂ p/fe ₂ p Nanohybrids

Table 1: Overview of various methods for active site engineering in Single-Atom Catalysts (SACs), highlighting the optimization techniques, structural features, and material compositions employed. The table includes methods such as machine learning, electrochemical coupling, and DFT calculations, demonstrating their applications in enhancing catalytic performance and efficiency.

Active site engineering in Single-Atom Catalysts (SACs) employs advanced techniques to optimize catalyst-reactant interactions, enhancing catalytic performance. Table 1 presents a comprehensive summary of the methods employed for active site engineering in Single-Atom Catalysts, detailing the optimization techniques, structural features, and material compositions that contribute to improved catalytic interactions and performance. Machine learning algorithms are pivotal in predicting the catalytic efficacy of transition metals on boron-doped MoS₂, identifying optimal configurations for improved efficiency [3]. The GENFIRE method refines active site engineering by accurately determining atomic positions and chemical species, allowing tailored configurations that ensure optimal catalytic activity and selectivity [17]. Optimizing indium hydroxide catalysts has shown high

Faradaic efficiency and selectivity in urea production, highlighting the importance of precise catalyst composition and structure [1].

Atomically-thin platinum layers as chemiresistors enhance sensitivity in detecting chemical species at low concentrations, emphasizing the role of ultrathin metal layers in improving active site accessibility and reactivity [8]. Density Functional Theory (DFT) analysis investigates interactions between metal single atoms and modified graphene supports, revealing electronic and structural factors influencing performance [4]. The rapid formation of conductive 3D networks in $\text{Ni}_2\text{P}/\text{Fe}_2\text{P}/\text{NF}$ systems enhances electron transfer and active site availability, demonstrating the efficacy of constructing conductive pathways to improve catalytic activity [5]. Synergistic interactions among transition metal hydroxides enhance charge transfer and catalytic activity, highlighting cooperative interactions' importance in active sites engineering [6].

Sophisticated methods focus on optimizing the catalyst-reactant interface. Advanced computational techniques, such as myopic multiscale sampling, improve catalyst classification efficiency, while experimental strategies using engineered metal-organic platforms stabilize single atoms on surfaces. These innovations significantly enhance catalytic performance, evidenced by improved reaction efficiencies in hydrogen evolution and CO/CO_2 gas trapping applications. This multidimensional focus aims to optimize existing catalysts and explore new avenues for catalytic functionality through precise atomic engineering [16, 19, 13], crucial for developing efficient and sustainable catalytic systems in electrocatalytic urea synthesis.

6.2 Role of Active Site Configuration

Method Name	Structural Features	Catalytic Enhancement	Computational Methods
Ti-SAC[11]	Ti Atoms	Hydrogen Spillover	Cnns
RSGS[4]	Single Vacancy	Graphene Surfaces	Density Functional Theory
HOIP-SAC[15]	Perovskite Structure	Charge Transfer	First-principles Calculations
CPM-ISM[7]	CU Surfaces	Electric Double-layer	Density Functional Theory
HDCNN[10]	Coordination Environments	Substrates IN Facilitating	Multi-branch Cnn

Table 2: Overview of various single-atom catalyst (SAC) methods, highlighting their structural features, catalytic enhancements, and computational methods used for optimization. The table provides a comparative analysis of the methods, emphasizing the role of active site configuration in enhancing catalytic performance.

Active site configuration is crucial in determining SACs' catalytic efficiency, directly affecting catalyst-reactant interactions. The precise arrangement of atoms within the catalyst structure is vital for optimizing performance, as seen in the interaction between titanium and graphene, which enhances hydrogen storage efficiency [11]. This configuration ensures full exposure and engagement of metal atoms in catalytic reactions, maximizing reactivity [4]. Table 2 presents a comprehensive comparison of different single-atom catalyst (SAC) methods, illustrating the interplay between structural features, catalytic enhancements, and computational techniques in optimizing active site configurations.

SAC effectiveness is amplified by substrates like hybrid organic-inorganic perovskites, which facilitate charge transfer to platinum atoms, enhancing reactivity and performance [15]. These substrates' ability to modulate electronic interactions is critical for achieving high catalytic activity, particularly in complex processes such as electrochemical urea synthesis [7]. Advanced computational methods, including Convolutional Neural Networks (CNNs), offer significant advantages in predicting SAC activity by managing complex electronic interactions efficiently [10], providing insights into optimal active site configurations and guiding SAC design with enhanced performance.

6.3 Advanced Techniques in Active Sites Engineering

Advanced techniques in active site engineering for SACs are essential for improving performance and stability. Atomic electron tomography combined with GENFIRE enables precise reconstruction of atomic structures, providing insights into active site arrangement and chemical composition [17]. This visualization aids in optimizing configurations for enhanced efficiency.

Integrating advanced computational methods, including DFT and machine learning algorithms, enhances active site engineering by predicting electronic properties and reactivity under diverse conditions. This approach addresses catalyst discovery challenges, translating atomic-scale calcu-

lations to macro-scale properties while optimizing performance within an exploratory framework. Employing a multiscale modeling strategy that integrates DFT predictions with machine learning allows classification of potential catalysts based on experimental viability, leading to efficient identification of promising candidates. Analyzing unpaired d electrons and charge transfer mechanisms in SACs provides critical insights into catalytic activity, particularly in nitrogen reduction reactions, informing rational design of more effective catalysts [16, 3]. These computational approaches offer a comprehensive understanding of interactions between single atoms and supports, guiding rational catalyst design with tailored properties.

The advancement of hybrid organic-inorganic frameworks, particularly hybrid organic-inorganic perovskites, presents a highly adaptable platform for optimizing active sites, significantly enhancing stability and reactivity. These frameworks serve as effective substrates for SACs like platinum (Pt), providing uniform anchoring sites and facilitating electron donation, improving performance in reactions like CO oxidation and CO reduction [16, 15]. Leveraging unique properties of organic and inorganic components allows fine-tuning of electronic interactions and active site configurations to achieve superior performance.

Employing these advanced techniques enables systematic exploration of SAC potential, leading to more efficient and sustainable catalytic systems. These strategies are crucial for advancing electrocatalytic urea synthesis, facilitating nitrogen and carbon dioxide conversion into urea under ambient conditions, overcoming traditional methods' limitations requiring harsh environments and substantial ammonia consumption. Developing new electrocatalysts, such as two-dimensional metal borides, and understanding electrochemical mechanisms are essential for optimizing efficiency and selectivity in this sustainable production process [12, 2, 7, 1].

6.4 Rational Design Strategies

Method Name	Material Engineering	Spatial Configuration	Computational Integration
RSGS[4]	Modified Graphene Surfaces	Arrangement OF Atoms	Density Functional Theory
GENFIRE[17]	Substrate Materials Modification	Precise Control Arrangement	Dft Calculations Inputs
HDCNN[10]	Support Materials	Coordination Environments	Convolutional Neural Network
HOIP-SAC[15]	Suitable Perovskite Substrate	Uniform Distribution Atoms	Density Functional Theory

Table 3: Summary of rational design strategies for single-atom catalysts (SACs) detailing the integration of material engineering, spatial configuration, and computational methods. The table highlights various methods such as RSGS, GENFIRE, HDCNN, and HOIP-SAC, illustrating their specific approaches to substrate modification, atomic arrangement, and computational techniques.

Rational design strategies for optimizing active sites in SACs are crucial for enhancing catalytic efficiency and selectivity. Table 3 provides an overview of the rational design strategies employed in the optimization of active sites in single-atom catalysts, focusing on the interplay between material engineering, spatial configuration, and computational integration. A key approach involves strategic selection and engineering of substrate materials anchoring single atoms. Modified graphene substrates, doped with nitrogen or boron, provide robust platforms for anchoring single metal atoms, enhancing electronic interactions and performance [4]. This method stabilizes single atoms and optimizes their electronic properties, facilitating efficient charge transfer during reactions.

Precise control over spatial arrangement and coordination environment of active sites is another critical aspect. Techniques like atomic electron tomography and GENFIRE enable detailed reconstruction of atomic structures, offering insights into optimal configurations for enhanced reactivity [17]. Understanding atomic-level interactions within SACs allows tailoring active site environments to maximize efficiency and selectivity.

Advanced computational methods, including DFT and machine learning algorithms, guide rational SAC design. These techniques predict electronic properties and activity, allowing identification of optimal configurations [10]. Integrating computational predictions with experimental validation enables development of SACs with tailored properties meeting specific demands in electrocatalytic processes.

Incorporating hybrid organic-inorganic frameworks in SAC design offers a versatile approach for optimizing active sites. These frameworks leverage unique properties of organic and inorganic components, facilitating fine-tuning of electronic interactions and configurations to achieve superior performance [15].

7 Urea Electrolysis and SACs

7.1 Mechanisms of SACs in Urea Synthesis

Single-Atom Catalysts (SACs) significantly enhance urea synthesis by enabling precise atomic-level interactions that boost catalytic efficiency and selectivity. Indium hydroxide catalysts, for instance, facilitate the direct coupling of nitrate and carbon dioxide, underscoring SACs' pivotal role in catalytic processes [1]. When supported on graphene, SACs offer isolated active sites, crucial for guiding reaction pathways in the conversion of nitrogen (N_2) and carbon dioxide (CO_2) into urea [4]. Additionally, hybrid organic-inorganic perovskites serve as effective substrates for anchoring platinum atoms, enhancing catalytic reactions like CO_2 reduction, which is essential for electrochemical urea synthesis [15].

The $Ni_2P/Fe_2P/NF$ electrode exemplifies outstanding electrocatalytic performance in urea electrolysis, achieving low overpotentials for both urea oxidation and hydrogen evolution [5]. This highlights SACs' potential to overcome the slow kinetics of these reactions, thereby enhancing urea synthesis efficiency. The $NiFeCo$ LDH/NF electrode also demonstrates excellent performance for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), with low overpotentials and high stability, vital for energy conversion technologies [6]. The electrochemical environment, including factors like electrode potential and pH, significantly influences the electronic structure and reactivity of SACs. Specific ions and the charge state of transition metals at active sites can alter catalytic efficiency [19, 4, 20, 3]. Understanding these conditions is crucial for optimizing SAC design and functionality, particularly in urea electrolysis, where computational and experimental approaches are vital for advancing SAC mechanisms and performance.

7.2 Challenges in Urea Electrolysis

Urea electrolysis using SACs encounters several challenges that limit efficiency and broader application. A key issue is the stability of SACs under electrochemical conditions, which can lead to aggregation of single atoms and a consequent loss of catalytic activity, especially in harsh environments with variable potentials and pH levels [15]. The slow kinetics of the nitrogen reduction reaction (NRR) and carbon dioxide reduction reaction (CO_2RR) present significant obstacles in urea synthesis. The strong triple bond of N_2 complicates activation, necessitating highly active and selective catalysts [3]. Moreover, the competitive HER often dominates the electrochemical environment, further complicating efficient conversion of N_2 and CO_2 into urea [5].

Developing SACs that efficiently catalyze both OER and HER while maintaining stability over time is a critical challenge. The bifunctional nature of these reactions demands catalysts capable of operating efficiently under dual functionalities, complicated by the distinct requirements of each reaction [6]. Precise control over reaction pathways and intermediates is essential for achieving high selectivity and yield in urea synthesis, necessitating advanced strategies for active site engineering and catalyst design [1].

Addressing these challenges requires a comprehensive understanding of electrochemical mechanisms and innovative SAC designs that enhance stability and reactivity. Advanced computational methods, such as Density Functional Theory (DFT) and machine learning models, offer promising avenues for predicting and optimizing SAC performance, guiding the rational design of catalysts to overcome these obstacles [10]. By integrating experimental and computational approaches, researchers can develop SACs that are efficient, selective, and robust, paving the way for sustainable and effective urea electrolysis.

7.3 Comparative Analysis with Other Catalytic Systems

Benchmark	Size	Domain	Task Format	Metric
-----------	------	--------	-------------	--------

Table 4: This table provides an overview of representative benchmarks used in the evaluation of single-atom catalysts (SACs) within various domains. It includes details on the size, domain, task format, and metrics employed to assess the performance of these catalytic systems, highlighting their applicability across different catalytic applications.

SACs provide substantial advantages over conventional catalytic systems, especially in enhancing the efficiency of electrocatalytic processes like urea synthesis. Engineered metal-organic platforms enable SACs to achieve atomic-level structural precision and stability, allowing for finely tunable local environments that enhance reactivity and selectivity. Recent advancements in bifunctional electrocatalysts highlight SACs' potential in urea electrolysis, contributing to sustainable hydrogen production while addressing environmental concerns related to urea-rich wastewater [15, 13, 14, 9]. The atomic dispersion of metal atoms in SACs maximizes active site exposure, enhancing catalytic activity and selectivity compared to bulk metal catalysts, achieving higher turnover frequencies and improved selectivity for critical reactions like NRR and CO₂RR.

Unlike conventional catalysts, which often suffer from agglomeration and limited active site accessibility, SACs maintain high catalytic activity even at low metal loadings, reducing reliance on expensive noble metals and improving economic viability. The precise control over the electronic structure of single metal atoms in SACs facilitates fine-tuning of catalytic properties, optimizing reaction pathways and kinetics. This capability arises from atomic-level structural precision achieved through innovative engineering methods, including organic templates and advanced computational simulations, enabling significant modifications in the local environment of metal sites for improved reactivity and selectivity across a broader range of catalytic applications [4, 13, 14].

Quantitative assessment of SAC performance can be achieved through techniques such as linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS). LSV measures current density at varying potentials, providing insights into catalytic efficiency, while EIS analyzes charge transfer resistance, deepening the understanding of electron transfer processes at the catalyst interface [6]. These techniques highlight the superior charge transfer capabilities and lower resistance of SACs compared to other catalytic systems, reinforcing their effectiveness in electrocatalytic applications. Table 4 offers a comprehensive summary of the benchmarks utilized in the comparative analysis of single-atom catalysts, showcasing their diverse applications and evaluation criteria.

The comparative analysis indicates that SACs offer significant advantages over traditional catalytic systems, particularly in enhanced efficiency, effectiveness, and economic viability. Their unique ability to facilitate a wide range of chemical reactions, along with precise control over active site configurations and integration of advanced computational methods like deep learning and multiscale modeling, aids in optimal design and screening of these catalysts. Furthermore, innovative substrates, such as hybrid organic-inorganic perovskites and engineered metal-organic platforms, enhance SAC catalytic performance, positioning them as promising alternatives to conventional catalysts [16, 10, 13, 15]. The unique properties and advanced characterization techniques of SACs make them a viable solution for sustainable and efficient catalytic processes, particularly in electrocatalytic urea synthesis.

7.4 Recent Advances and Applications

Recent advancements in Single-Atom Catalysts (SACs) for urea electrolysis underscore their potential to revolutionize sustainable chemical processes. SACs have shown remarkable efficiency in the electrocatalytic conversion of nitrogen (N₂) and carbon dioxide (CO₂) into urea, with research emphasizing the optimization of active site configurations and substrate interactions to enhance both catalytic efficiency and selectivity. This work is crucial for advancing sustainable nitrogen utilization and addressing environmental challenges associated with urea-rich wastewater, as highlighted in analyses of bifunctional catalysts for urea electrolysis [1, 9].

Notable advancements include SACs supported on modified graphene surfaces, which enhance stability and electronic properties, facilitating efficient charge transfer and reaction kinetics [4]. This approach improves catalytic performance while reducing reliance on expensive platinum-group metals (PGMs), enhancing economic viability [5].

The integration of hybrid organic-inorganic perovskite structures as SAC substrates effectively anchors single metal atoms, such as platinum, enhancing catalytic activity in the electrochemical reduction of CO₂, a critical step in urea synthesis [15]. This integration leverages the unique properties of organic and inorganic components, resulting in catalysts that are efficient, durable, and adaptable to various reaction conditions.

Advanced computational methods, including Density Functional Theory (DFT) and machine learning algorithms, have propelled SAC optimization by providing insights into electronic properties and

reaction mechanisms [10]. These techniques enable rational design of SACs with tailored properties, facilitating the identification of optimal configurations for enhanced catalytic performance.

Recent applications of SACs in urea electrolysis demonstrate their potential for achieving low overpotentials and high Faradaic efficiencies, indicating suitability for practical applications in energy conversion technologies [6]. The dual functionality of SACs in catalyzing both the hydrogen evolution reaction (HER) and urea oxidation reaction (UOR) further underscores their versatility and effectiveness in electrocatalytic processes [5].

8 Conclusion

8.1 Future Directions and Potential Applications

Future research on Single-Atom Catalysts (SACs) should prioritize the optimization of catalyst performance through the exploration of alternative nitrogen sources, which could significantly improve the electrocatalytic synthesis of urea [1]. Additionally, enhancing sensor design and investigating various metal candidates will be vital for increasing the selectivity and stability of SAC-based sensing platforms [8].

Optimizing support materials and examining different metal combinations are critical for further advancing SAC performance [4]. This includes refining synthesis processes and exploring alternative materials to bolster the long-term durability of SACs in practical applications [5].

The integration of advanced computational techniques with experimental validation will be essential for evaluating the impact of diverse environmental conditions on SAC performance. This approach encompasses the refinement of machine learning models to enhance predictive capabilities and the incorporation of experimental data into the classification processes of SACs, thereby expanding their utility in sustainable chemistry.

Moreover, broadening the library of atomically precise SACs developed through innovative methodologies and investigating their catalytic properties across various reactions will be crucial for the advancement of this field. By optimizing catalyst design and exploring additional coordination structures, researchers can improve catalytic performance across a wider array of reactions, paving the way for more efficient, stable, and environmentally friendly catalytic systems.

References

- [1] Chade Lv, Lixiang Zhong, Hengjie Liu, Zhiwei Fang, Chunshuang Yan, Mengxin Chen, Yi Kong, Carmen Lee, Daobin Liu, Shuzhou Li, et al. Selective electrocatalytic synthesis of urea with nitrate and carbon dioxide. *Nature Sustainability*, 4(10):868–876, 2021.
- [2] Xiaorong Zhu, Xiaocheng Zhou, Yu Jing, and Yafei Li. Electrochemical synthesis of urea on mbenes. *Nature Communications*, 12(1):4080, 2021.
- [3] Zheng Shu, Hejin Yan, Hongfei Chen, and Yongqing Cai. Mutual modulation via charge transfer and unpaired electrons of catalytic site for superior intrinsic activity of n₂ reduction: from high-throughput computations assisted with machine learning perspective, 2022.
- [4] Aleksandar Z. Jovanović, Slavko V. Mentus, Natalia V. Skorodumova, and Igor A. Pašti. Reactivity screening of single atoms on modified graphene surface – from formation and scaling relations to catalytic activity, 2021.
- [5] Lei Yan, Yulin Sun, Enlai Hu, Jiqiang Ning, Yijun Zhong, Ziyang Zhang, and Yong Hu. Facile in-situ growth of ni₂p/fe₂p nanohybrids on ni foam for highly efficient urea electrolysis. *Journal of Colloid and Interface Science*, 541:279–286, 2019.
- [6] Pravin Babar, Abhishek Lokhande, Vijay Karade, Bharati Pawar, Myeng Gil Gang, Sambhaji Pawar, and Jin Hyeok Kim. Bifunctional 2d electrocatalysts of transition metal hydroxide nanosheet arrays for water splitting and urea electrolysis. *ACS Sustainable Chemistry & Engineering*, 7(11):10035–10043, 2019.
- [7] Qian Wu, Chencheng Dai, Fanxu Meng, Yan Jiao, and Zhichuan J Xu. Potential and electric double-layer effect in electrocatalytic urea synthesis. *Nature Communications*, 15(1):1095, 2024.
- [8] Kyung Ho Kim, Hans He, Marius Rodner, Rositsa Yakimova, Karin Larsson, Marten Piantek, David Serrate, Alexei Zakharov, Sergey Kubatkin, Jens Eriksson, and Samuel Lara-Avila. Chemical sensing with atomically-thin metals templated by a two-dimensional insulator, 2020.
- [9] Zhijie Chen, Wei Wei, Ho Kyong Shon, and Bing-Jie Ni. Designing bifunctional catalysts for urea electrolysis: progress and perspectives. *Green Chemistry*, 26(2):631–654, 2024.
- [10] Haoyu Yang, Juanli Zhao, Qiankun Wang, Bin Liu, Wei Luo, Ziqi Sun, and Ting Liao. Convolutional neural networks and volcano plots: Screening and prediction of two-dimensional single-atom catalysts, 2024.
- [11] Hydrogen spillover and storage on graphene with single-site ti catalysts.
- [12] Xin Liu, Yan Jiao, Yao Zheng, Mietek Jaroniec, and Shi-Zhang Qiao. Mechanism of cn bonds formation in electrocatalytic urea production revealed by ab initio molecular dynamics simulation. *Nature Communications*, 13(1):5471, 2022.
- [13] Amogh Kinikar, Xiushang Xu, Takatsugu Onishi, Andres Ortega-Guerrero, Roland Widmer, Nicola Zema, Conor Hogan, Luca Camilli, Luca Persichetti, Carlo A. Pignedoli, Roman Fasel, Akimitsu Narita, and Marco Di Giovannantonio. Advancing single-atom catalysts: engineered metal-organic platforms on surfaces, 2024.
- [14] G. S. Priyanga and S. K. Behera. Interfacial dynamics and catalytic behavior of single ni atom site, 2024.
- [15] Qiang Fu and Claudia Draxl. Hybrid organic-inorganic perovskites as promising substrates for pt single-atom catalysts, 2018.
- [16] Kevin Tran, Willie Neiswanger, Kirby Broderick, Erix Xing, Jeff Schneider, and Zachary W. Ulissi. Computational catalyst discovery: Active classification through myopic multiscale sampling, 2021.

-
- [17] Yongsoo Yang, Chien-Chun Chen, M. C. Scott, Colin Ophus, Rui Xu, Alan Pryor Jr au2, Li Wu, Fan Sun, W. Theis, Jihan Zhou, Markus Eisenbach, Paul R. C. Kent, Renat F. Sabirianov, Hao Zeng, Peter Ercius, and Jianwei Miao. Deciphering chemical order/disorder and material properties at the single-atom level, 2016.
- [18] Juan Shen, Kaliappan Muthukumar, Harald O. Jeschke, and Roser Valenti. Physisorption of an organometallic platinum complex on silica. an ab initio study, 2012.
- [19] Yichao Huang, Yuanhui Sun, Xueli Zheng, Toshihiro Aoki, Brian Pattengale, Jier Huang, Xin He, Wei Bian, Sabrina Younan, Nicholas Williams, et al. Atomically engineering activation sites onto metallic 1t-mos2 catalysts for enhanced electrochemical hydrogen evolution. *Nature communications*, 10(1):982, 2019.
- [20] Ana S. Dobrota, Natalia V. Skorodumova, Slavko V. Mentus, and Igor A. Pašti. Surface pourbaix plots of m@n4-graphene single-atom electrocatalysts from density functional theory thermodynamic modelling, 2021.

Disclaimer:

SurveyX is an AI-powered system designed to automate the generation of surveys. While it aims to produce high-quality, coherent, and comprehensive surveys with accurate citations, the final output is derived from the AI's synthesis of pre-processed materials, which may contain limitations or inaccuracies. As such, the generated content should not be used for academic publication or formal submissions and must be independently reviewed and verified. The developers of SurveyX do not assume responsibility for any errors or consequences arising from the use of the generated surveys.

www.SurveyX.cn