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Review

Programmable Nanocatalysts in Circular Chemistry: Toward Self-Learning and Reconfigurable Reaction Networks

Aikhoje Ezekiel Fred[1], Garindo Boro[2], Ugochukwu Gladys Chioma[3], Abdullahi Bilyaminu[4,*]

[1]Department of Inustrial Chemistry, Federal University Wukari, Taraba State, Nigeria

[2]Department of Chemistry, Federal University Wukari, Taraba State, Nigeria

[3]Department of Chemistry, Delta State College of Education, Mosogar, Nigeria

[4]Department of Science Laboratory Technology, Federal Polytechnic Kaura Namoda, Zamfara State, Nigeria

[*]Corresponding author: Abdullahi Bilyaminu, bilyamuhammad@gmail.com

Abstract

Programmable nanocatalysis represents an emerging paradigm in sustainable chemistry, integrating nanoscale engineering, chemical feedback control, and artificial intelligence (AI) to achieve self-learning catalytic behavior. Unlike conventional static catalysts, programmable nanocatalysts programmableally modulate their structural and electronic properties in response to real-time reaction conditions, thereby enhancing activity, selectivity, and longevity. This research investigates the design principles, programmable mechanisms, and circular chemistry integration of programmable nanocatalysts, with emphasis on self-optimization, waste valorization, and energy-neutral reaction cycles. Through a systems-level framework combining molecular coding of reactivity, AI-driven performance optimization, and feedback-controlled reaction networks, the study demonstrates how self-regulating catalytic platforms can enable closed-loop, environmentally benign chemical processes. The findings reveal the transformative potential of self-learning materials in reshaping industrial catalysis, accelerating discovery-to-deployment timelines, and supporting circular economy objectives in chemical manufacturing.

Keywords

Programmable nanocatalysis, Chemical self-learning, Circular chemistry, AI-driven catalysis, Programmable reaction networks

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1. Introduction

The development of programmable nanocatalysts represents one of the most significant advances in sustainable chemistry. Unlike traditional catalysts with fixed, structure-defined active sites, programmable nanocatalysts are programmable, intelligent nanoscale materials that can autonomously optimize their catalytic performance in response to real-time reaction conditions. In other words, these materials are capable of self-learning catalytic behavior, where their structural and functional properties evolve programmatically under the influence of environmental stimuli and user-defined control parameters [1,2]. By contrast, conventional static catalysts are limited by non-programmable performance and fixed surface chemistries, which restrict their efficiency and responsiveness in complex chemical systems.

The integration of circular chemistry principles into catalytic design is a core aspect of sustainable catalysis. Circular chemistry emphasizes minimizing waste, maximizing resource efficiency, and designing catalysts and reactions that are self-refining and sustainable. Traditional catalytic systems, however, often hinder circular production because their optimization cycles are slow, energy-intensive, and incapable of responding to real-time changes in reactants or reaction environments. Programmable nanocatalysis addresses these limitations by incorporating self-learning capabilities, automated feedback loops, and programmable reactivity to optimize catalytic efficiency in real time [3,4].

Advances in artificial intelligence (AI), machine learning (ML), and robotics have further accelerated the development of programmable nanocatalysts. Modern AI techniques, including reinforcement learning (RL) and active learning, enable catalytic systems to continuously revise predictive models, incorporate new experimental data, and rapidly explore complex chemical spaces [5,6]. This predictive optimization reduces waste, improves energy efficiency, and accelerates the discovery of novel catalysts and reaction pathways, supporting the principles of green chemistry [4]. Closed-loop systems combining AI, automated experimentation, and high-throughput synthesis are increasingly transforming research and development into more efficient, reproducible, and scalable processes [7,8].

Large language models (LLMs) and multimodal AI systems are proving particularly powerful in programmable nanocatalysis. These models can process chemical literature, predict reaction outcomes, generate retrosynthetic pathways, and optimize catalyst structures, effectively bridging the gap between theory and experiment [9,10]. Advanced techniques, such as Bayesian optimization and RL, facilitate data-driven decisions that surpass the capabilities of inflexible, static catalytic systems. Collectively, these approaches represent a new digital paradigm in chemistry, sometimes described as the "fifth paradigm," characterized by the convergence of AI, automation, and robotics in chemical discovery [11,12].

In this paradigm, AI-driven models can autonomously design chemical spaces, predict multi-dimensional optimization outcomes, and programmatically modify reaction conditions to improve catalytic performance. Automated synthesis and computational chemistry enable unprecedented accuracy, speed, and scalability in catalyst screening, surpassing human-directed experimentation in both reproducibility and efficiency [13,14]. The combination of AI, robotics, and nanochemistry allows the creation of self-adjusting, programmable catalytic structures capable of learning from their environment, restructuring reaction pathways, and valorizing waste [5,15,16]. These innovations are crucial for achieving sustainable industrial chemical processes within the framework of circular chemistry [17,18].

Practical applications of AI in catalyst discovery include the identification of novel functional molecules through large-scale database analysis and predictive evaluation of thermoprogrammable and kinetic properties [3]. Collaborative AI/human interfaces, exemplified by tools such as CataLM, enable rational design of electrocatalytic materials and contribute to self-learning autonomous catalytic networks [19,20]. Together, these systems lay the foundation for a sustainable circular chemical economy driven by intelligent self-innovation.

This study aims to develop a scientific framework for programmable nanocatalysts that integrates programmable reactivity, AI-controlled self-learning, self-regulation, and energy efficiency within circular chemical processes. It seeks to define structural, mechanistic, and digital design principles required to transform nanocatalysts from passive materials into smart, programmable systems capable of autonomously improving catalytic performance, restructuring reaction pathways, and valorizing waste. Ultimately, this research identifies strategic approaches to translate programmable catalytic innovations from laboratory-scale studies to large-scale industrial applications within sustainable chemical networks.

2. Methodology

This study employed a mixed-method scientific approach integrating systematic literature mapping, conceptual modelling, and computational design analysis to investigate the principles and operational frameworks of programmable nanocatalysts within circular chemistry. A comprehensive evidence-synthesis protocol was executed across major scientific databases (Scopus, Web of Science, ScienceDirect, SpringerLink, and PubMed), using Boolean keyword combinations related to programmable catalysis, AI-guided optimization, reaction feedback systems, and circular chemical processes, with the search restricted to 2020-2025 publications. All records underwent PRISMA-based screening and quality assessment, and relevant studies were thematically categorized to extract mechanistic, structural, and digital design parameters. These insights were used to construct a multi-criteria computational framework evaluating programmable reactivity, AI-driven optimization, and circular system efficiency. Comparative modelling, supported by surrogate thermoprogrammable and kinetic metrics, enabled the formulation of an integrated mechanistic architecture for programmable nanocatalysts, providing a scientifically grounded basis for their functionality, scalability, and sustainability in advanced catalytic applications.

3. Theoretical Underpinning of Programmable Catalysis

Programmable catalysis refers to catalytic systems whose active state is not static but programmatically modifiable by external stimuli (temperature, pH, solvent, gas composition, light, etc.) or by controlled periodic forcing. In such systems, the catalyst's structural, electronic, or environmental parameters (e.g., aggregation state, binding affinity, solvation environment) can be toggled or tuned in time to influence reaction kinetics and selectivity. Emerging work for example, programmable hydrogenation catalysts whose selectivity is reversibly switched by H_2/CO_2 equilibrium, or stimuli-responsive polymer-embedded nanoparticle catalysts—demonstrates that this approach can realize "programmable" or "switchable" behavior. In parallel, theoretical frameworks such as the Catalytic Resonance Theory show how time-dependent modulation of binding energies or surface states could overcome classical energetic trade-offs (e.g., Sabatier limits), enabling reaction control beyond what static catalysts permit. While these developments do not (yet) reproduce the full complexity of enzymatic regulation, they nonetheless mark a paradigm shift: From fixed, "mechanically determined" catalysis toward programmable catalysis, opening avenues for temporal control over rate, selectivity, and reaction pathways [21].

3.1 Thermoprogrammable Feedback and Reaction Memory

The principle of thermoprogrammable feedback underpins the programmability of catalytic reaction networks, whereby reaction intermediates possess specific energy states that influence the direction and outcome of subsequent catalytic cycles [21,22]. In this framework, intermediates act as transient stores of chemical "memory," providing a feedback mechanism that alters catalyst behavior based on prior reaction events. This concept of reaction memory is central to achieving kinetic asymmetry, enabling a system to operate away from classical equilibrium and to coordinate complex, multi-step networks [23,24]. Catalysts within such networks can self-regulate, programmatically managing turnover frequency and selectivity, and orchestrating multidirectional, reversible transformations in a manner reminiscent of the programmable control observed in biological systems. Indeed, enzymes within biological networks exploit intermediates to fine-tune reaction outcomes, maintaining flexibility and precision across interconnected pathways [25,26].

Synthetic analogues can be driven out of equilibrium by transducing chemical energy into mechanical or configurational work performed by the catalyst, leading to the formation of dissipative structures sustained by a steady energy inflow [21,27]. These non-equilibrium assemblies create the conditions necessary for programmable behavior in artificial catalytic systems, enabling functionalities such as controlled reaction timing, selective bypass of competing reactant streams, and primitive chemical communication across interconnected reaction networks. Furthermore, the simultaneous occurrence of multiple reaction intermediates generates distributed feedback control, imparting resilience to environmental fluctuations, substrate concentration changes, and flow rate variability [28]. This capability shifts the focus of catalyst design from static efficiency to programmable, responsive behavior, which is particularly critical for complex, multi-step catalytic cascades.

Reaction memory provides a mechanistic explanation for programmable selectivity, wherein the system retains information about prior states to preferentially guide reaction pathways. Certain intermediates may influence the orientation of subsequent substrate binding, stabilize transient transition states, facilitate cooperative interactions at active sites, and steer product formation while minimizing undesired byproducts [21,29]. This behavior has been exploited in the design of autonomous chemical engines capable of converting specified chemical feeds into ordered outputs and maintaining far-from-equilibrium steady states analogous to those observed in living systems [27]. The ability to sustain such steady states is especially advantageous in intricate catalytic cascades, where precise control over numerous consecutive reactions is required to achieve high yields and selectivity.

3.2 The Surfaces of Energy Modulation

Due to their flexibility, nanostructured materials can be adjusted programmatically to the potential energy surfaces of reactions to programmable catalysis. This versatility is due to the framework, surfaces, and active sites of a catalyst having the capacity to alter, both reversibly and programmably, with regard to the environment or the chemical environment. The changes that can be made are structural changes to the active site of the catalysts, rearrangement of the charge distribution of the catalysts on the cell surfaces, restructuring of the surfaces, and evolution of the active sites to adopt new geometries [25,26]. Catalysts may modify the activation energies of the reactions by modifying the electronic environment surrounding the reactions, regulate the strength of adsorbates, and redirect the reaction directions to operate in the optimum range dependent on the catalysts.

The programmable sites find a larger configurational space within the nanoscale development of programmable sites than visible materials do. This facilitates a sort of programmable reactivity that reacts to the concentration, temperature, or solvent characteristics of a substrate [29,30]. The programmable reactivity methods are analogous to enzyme catalysis, where the conformational changes of a protein scaffold are used to bind and stabilize transition states and react in many steps [25]. In artificial systems, these principles are applied to the design of materials with tunable lattice and surface morphology that react to feedback that is stored within reaction intermediates. These materials create energy surfaces, which lead to programmable generation of the surface with the catalytic cycle in real-time [30,31].

These modulations work programmatically in the engagement of catalysts in non-equilibrium when transformation of energy and structural readjustments occur, which are then succeeded by the reaction process acceleration [21,27]. Self-regulation of the energy profile by thermoprogrammable feedback and structural plasticity will ensure that the reactivity of the system is maintained at a constant level in changing reaction conditions. This stability of reaction in different conditions is particularly important in building dissipative catalytic systems, where sustained dissipation of energy plays a key role in the maintenance of activated states and emergent complex organizational structures [29].

The energy requirement for adaptive restructuring in catalysts differs significantly from conventional catalytic processes due to the dynamic nature of adaptive systems. In traditional catalysis, the catalyst is typically static, with fixed active sites, and the energy input is primarily used to overcome the reaction's activation energy and maintain operating conditions such as temperature and pressure. In contrast, adaptive or self-learning catalysts can reorganize their active sites in response to changes in reaction conditions, substrate types, or accumulated intermediates. This restructuring requires additional energy for atomic rearrangements, bond reorganization, and, in some cases, the operation of integrated feedback or sensing mechanisms. Despite this extra energy demand, adaptive restructuring can improve overall reaction efficiency by optimizing active sites in real-time, minimizing side reactions, and enhancing turnover frequency. Consequently, while the short-term energy cost of adaptive catalysts is higher, the total energy consumed per unit of product can be lower in the long term, particularly for complex, multi-step, or deactivation-prone reactions. Adaptive catalysts thus trade an initial energy investment for greater selectivity, activity, and sustainability over the course of extended reactions, as shown in Figure 1 that compares the energy requirements in conventional and adaptive (self-learning) catalysis, highlighting the efficiency gains over time.

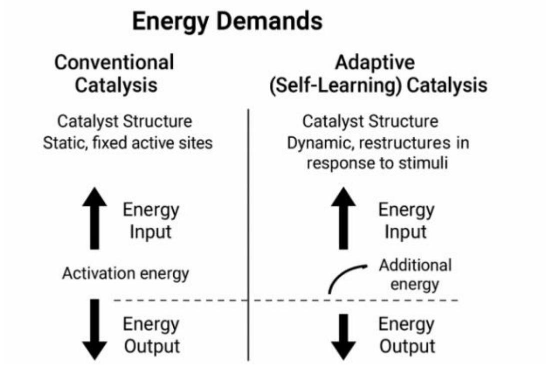

Figure 1. Comparison of energy requirements in conventional and adaptive (self-learning) catalysis.

Figure 1 illustrates the differences in energy demands between conventional and adaptive catalytic systems. In conventional catalysis, the catalyst possesses a static structure with fixed active sites, and energy input is primarily used to overcome the activation energy barrier, producing the corresponding energy output. In contrast, adaptive (self-learning) catalysts feature dynamic structures that can restructure in response to environmental stimuli. This adaptive behavior requires additional energy input to facilitate structural changes, but it allows for more efficient catalysis under varying conditions, potentially enhancing overall energy utilization and reaction performance.

Self-learning in catalysis can be quantified through measurable changes in efficiency, selectivity, adaptability, and responsiveness over repeated reaction cycles, often aided by real-time monitoring and AI-driven feedback. These metrics distinguish truly adaptive catalysts from static systems.

3.3 Kinetic Reconfiguration and Stimuli-Responsiveness

Besides the thermoprogrammable and structural features, the programmable catalysts also reform the kinetic features of their behavior in response to an external stimulus. The activity, selectivity, and mechanistic pathways of reaction steps can be modulated to respond to pH, light, and magnetism by stimuli-responsive systems, which adjust control over catalytic active site behavior [32,33]. These are seen in both biological oscillators and metabolic pathways in the control of reaction rates and the production of desired products [34].

The principles of supramolecular chemistry and systems chemistry support the concept of programmable catalysts with emergent behavior such as periodic switching, self-organization, and adaptable reactivity [35]. The intelligent control of chemical transformations and imitation of naturally regulated chemical transformations is possible through emergent self-organization, programmable reactivity, and self-organization, which are formed through interactions of molecular elements and a combination of external energy. Their inclusion of feedback loops and reconfiguration following a specific stimulus allowed the systems to maintain chemoselectivity and avoid the loss of reagents, both of which simplify the process significantly, and compares to the speed of enzymatic reactions [27,34].

The responsiveness of a catalyst is increased by reconfiguration of the programmable rearrangement of sites and spatial and temporal placement of substrates, energy input, or reaction conditions variability. An example of this is that the reaction pathways of photoresponsive catalysts are real-time modulated in the choice of selectable pathways on the basis of reversible electronic or structural changes on absorbing light [32]. Similarly, surface charge and other magnetic field responsive electrocatalysts and magnetically controlled electrocatalysts can be used to induce selective electrocatalytic reactions with significantly higher turnover rates [33]. In general, these flexible systems form part of the advancement of intelligent catalytic materials that possess self-regulation, memory, and reactivity to the environment.

The foundations of the catalytic systems that exhibit lifelike behaviors, such as sensing and actuation, communication, and energy transduction, as elaborated upon earlier in the paper [29,36], are outlined. With a continuous input of energy and in-and-out-of-equilibrium states, such systems can possess other properties not manifested in static classical thermoprogrammable systems, like homeostatic control, self-replication, and programmable network formation [27]. The combination of systems chemistry, materials science, and bio-inspired ideas results in the development of programmable catalytic systems, which can replicate the versatility and complexity of natural enzymes and are further adaptable and scalable to industrial demands.

3.4 Interaction among Feedback, Plasticity, and Stimulus Control

The rational design of programmable catalysts is offered by the incorporation of feedback provided by thermoprogrammables, modulation of energy surfaces, and kinetic reconfigurations. Catalysis may be subjected to constant self-optimizing behavior and versatile selectivity by feedback in reaction intermediates, active site modulation of nanostructural plasticity, and system response to stimuli [37,38]. Such a system-wide network of various components can be used to assemble chemically autonomous networks of decision-making, analogous to living cells, which integrate various signals in order to regulate metabolic fluxes [21,24].

The emergence of new system properties, such as the reaction memory, self-organization, and programmable reconfiguration, generates special opportunities for the efficient, selective, and sustainable change of the target chemicals [29,30]. Design principles of biological catalysis include preorganization of electrostatic fields and the effects of secondary coordination spheres, as well as flexible conformations that can be extrapolated to designing synthetic catalysts that can behave as enzymes can in non-equilibrium, energy-rich conditions, with an eye towards sustainable catalysis [25,31].

Theoretical investigations indicate the influential innovations programmable catalysis can bring, putting a shadow over the imposing design to a new level where catalysts act as intelligent chemical systems. These systems adapt to changes in the surrounding environment, include the reaction history, and exploit performance optimization by making nanostructural features programmatically change. The feedback of thermoprogrammables, structural plasticity, and reactivity to stimuli combine to offer the best advanced reconfigurable architectures in the design of catalysts that process information, store memory, self-regulate, and perform other intelligent processes other than mere autonomy [27,35].

The code of programmable catalysis lies in the combination of reaction memory, energy surface modulation, and stimulus-controlled kinetic reconfiguration. Self-optimising catalytic systems can be designed by imitating the principles of biological catalysis and by combining biological nanostructures, supramolecular chemistry, and systems chemistry. Programmable catalysis enables the design of life-like, intelligent materials that operate smoothly under far-from-equilibrium states of matter. This approach provides greater control over chemical transformations, enhances selectivity, and strengthens the foundations of sustainable and programmable catalysis, as illustrated in Table 1 which outlines the mechanistic drivers of programmability in nanocatalysts, which are essential for optimizing catalytic processes [29,34,36].

Table 1. Mechanistic drivers of programmability in nanocatalysts.

Mechanistic Driver	Functional Role	Representative Mechanisms	References
Thermoprogrammable Feedback	Enables reaction memory and programmable rate control	Far-from-equilibrium steady states, energy transduction via intermediates	[21,26,29]
Nanostructural Plasticity	programmable reconfiguration of active sites	Lattice breathing, electronic redistribution, programmable surface restructuring	[28,30]
Stimuli-Responsive Kinetics	On-demand modulation of selectivity and turnover	pH-responsive gating, photo-switching, magneto-electronic activation	[27,37]
Molecular Logic Operations	Encodes catalytic decision-making	Molecular gates, allosteric control, cooperative amplification	[32,33]

The interplay between feedback mechanisms, catalytic plasticity, and stimulus-responsive control forms the foundation of adaptive behavior in nanocatalytic systems. By dynamically modulating active sites in response to environmental cues, catalysts can "learn" from previous reactions, adjust their structural and electronic properties, and optimize reaction outcomes in real time. Understanding these interactions is crucial because they define the system's capacity for self-regulation, autonomous optimization, and resilience under fluctuating conditions. Building on these insights, the next step is to translate these principles into the rational design of programmable nanocatalysts, where structural, mechanistic, and digital design considerations are integrated to create fully adaptive and intelligent catalytic networks.

4. Principles of Design Programmable Nanocatalysts

Programmable nanocatalysts are developed by bringing together a number of disciplines: Materials science, computational chemistry, and systems intelligence. These catalysts no longer have the programmable constraints of the catalysts of yesterday, with the combination of structural precision, AI-based predictive modelling, and the developments of functional molecular logic. The programmable self-optimization behavior and self-optimizing functionality in these programmable nanocatalysts are observed in a very large multiplicity of chemical transformations and processes [39]. In this section, we consider three fundamental aspects of the design of programmable nanocatalysts: The structural design of intelligent catalytic systems, the implementation of AI and automated data-driven rationalization, and the molecular programming of the catalyst to allow selective control of activation and deactivation.

4.1 Intelligent Reactivity Architectures

The design of the nanocatalysts is the key to intelligent reactivity, namely how they are built. It dictates the orientation of the reacting species to the exposures to the catalytic active sites and the variations in the catalytic paths and changes as a result of modulated feedback. The programmable metal-organic frameworks (MOFs), single-atom catalysts (SACs), and the hybrid of enzymes and nanoparticles are some of the most exciting architectures. As a result of the structural modularity of the programmable MOFs, tunable frameworks with variable pore sizes, regulated chemical environments, and spatially organized catalytic active sites can be constructed. This provides the frameworks the ability to adsorption selectivity with activation and confinement of multi-stage transformations. MOFs also provide the introduction of stimuli-responsive units that can regulate the electronic and steric characteristics of the operational catalytic centers in response to external stimuli [40].

This capability of SACs to form active sites on single atoms provides challenges to control the coordination chemistry and electronic structure to a level never before achieved. This is because of the high atom economy of the catalysts and their responsiveness to chemical fields and directly attached ligands (programmable), enabling the attainment of control of catalysts to a similar degree as the enzymatic process [41]. Conversely, enzyme-nanoparticle hybrids have the desired characteristics of specificity, programmability, adaptability of biological catalysts, and inorganic nanostructure of the required robustness and tunability. These hybrid systems have demonstrated self-regulation in catalytic processes that are autonomous and coordinated with biomolecular recognition when external metallic or semiconducting surfaces are present and have catalytic self-stimulation and reversible control over activation and deactivation in response to externally applied stimulus [39,42].

The hybrid systems derived in this work are particularly significant to the area of photocatalysis, where several hurdles like low photon-to-chemical energy transformation efficiency, feeble chemical stability in redox conditions, and low reusability have existed for decades [41]. The operating envelope of such systems is greatly increased by the use of highly sophisticated photocatalytic architectures that combine hierarchical structuring, nanoscale confinement, and responsive surface chemistry. These features enable high photocatalytic activity to be sustained even when irradiance drastically varies and chemical conditions change to differing degrees [42]. The given qualities can be directly translated into the problem of sustainable energy for water splitting and CO_2 reduction, as illustrated in Figure 2. This figure showcases intelligent reactivity architectures in programmable nanocatalysis, including MOFs, SACs, and enzyme-nanoparticle hybrids integrated for adaptive catalytic performance.

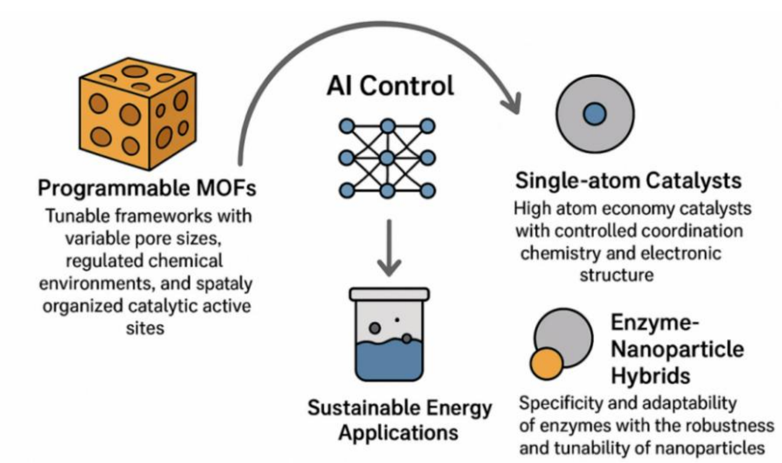

Figure 2. Intelligent reactivity architectures in programmable nanocatalysis: MOFs, SACs, and enzyme-nanoparticle hybrids integrated for adaptive catalytic performance.

Figure 2 illustrates the core intelligent reactivity architectures that enable programmable and adaptive catalysis. Programmable MOFs provide tunable pore structures, regulated chemical microenvironments, and spatially organized catalytic sites for selective adsorption and multi-stage transformations. Single-atom catalysts offer atom-level precision in coordination and electronic structure, enabling enzyme-like control of catalytic pathways. Enzyme-nanoparticle hybrids integrate the specificity and responsiveness of biological systems with the robustness and tunability of inorganic nanomaterials, allowing self-regulating and stimulus-responsive catalysis. Together, these architectures support high-performance photocatalytic and sustainable-energy applications by maintaining activity under variable light and reaction conditions.

4.2 Data-Driven Chemistry and Integrating AI

The integration of AI and data-based strategies will allow achieving programmable catalytic systems with self-optimizing and predictive reactivity. The space of reaction parameters and catalytic configuration can be easily sampled to self-optimize the reaction parameters and catalytic configuration by using a variety of ML methods such as the artificial neural network, programmable neuro-fuzzy inference system, and the Bayesian optimization frameworks [43,44].

In the case of photocatalytic systems, AI can predict the band gap, the surface reaction energetics, the programmability of charge carriers, and the synthesis of the material predictor, which is combined with experimental feedback to refine the catalyst iteratively [44]. This method can help to reduce severe inefficiency in reactors due to heterogeneous light distribution, charge recombination, and mass transport [45,46]. The simulations of thousands of possible material compositions are possible with the use of ML algorithms, and photocatalytic heterostructures, co-catalysts, and van der Waals assemblies with predefined properties can be synthesized on a high-throughput scale [47].

The highest stage of AI analysis involves optimization of new strong separators in real-time using the analytical algorithms of AI on layered catalysts. These are the algorithms that are most suitable to the layered architectures, and they are the ones that are used in the prediction of high-concept value range parameters. This enables the production of automated changes in the parameters of the reaction (including temperature, pH, and light intensity) whenever they do not reach optimal values [44,48]. This is necessary in the highly developed catalytic converting systems, particularly the removal of the poisonous by-products [49].

Autonomous reaction and catalyst system machine-learning algorithms are optimized to focus on predictive modelling such that seamless integration continuously optimizes reaction systems and catalytic layers to achieve the desired thermoprogrammable parameters. This integration ensures that maximum efficiency, selectivity, and stability are achieved, as demonstrated in Table 2. This table outlines the AI and machine-learning functions supporting programmable catalysis, which are key to enhancing catalytic performance and system optimization [43,44].

Table 2. AI and machine-learning functions supporting programmable catalysis.

AI Capability	Purpose in Catalysis	Impact on Performance	References
Predictive Modelling (ML/ANN/PINN)	Band-gap prediction, charge-transfer modelling	Reduces trial-and-error, enhances catalyst design speed	[46,48]
RL	Closed-loop reaction optimisation	Real-time programmable correction for selectivity & yield	[10,7]
Autonomous Robotic Experimentation	High-throughput catalyst discovery	Accelerates discovery cycles from weeks to hours	[50,51]
LLM-Enabled Chemical Reasoning (e.g., CataLM)	Retrosynthetic guidance, catalyst selection	Enhances decision-making and knowledge-driven exploration	[20,16]

4.3 ML and AI in Real-Time Control of Programmable Nanocatalysts

ML and AI are central to enabling real-time, self-learning control of programmable nanocatalysts. Predictive modeling using techniques such as ML, artificial neural networks (ANNs), and physics-informed neural networks (PINNs) allows the simulation of electronic properties, band-gap prediction, and charge-transfer processes in catalytic materials. These models reduce reliance on trial-and-error approaches and accelerate the rational design of high-performance catalysts by anticipating reaction outcomes before experimentation [46,48].

RL provides a framework for closed-loop optimization, where the catalytic system is treated as an interactive environment. RL algorithms adjust reaction parameters such as temperature, flow rate, and catalyst composition in real time based on measurable outputs, including product yield, selectivity, and intermediate concentrations. This programmable approach ensures that the system continuously self-corrects to achieve optimal catalytic performance under programmable reaction conditions [10,7].

Autonomous robotic experimentation further enhances the efficiency of ML-guided catalysis. By integrating high-throughput synthesis and automated characterization, robotic platforms can test numerous catalyst formulations in parallel, reducing discovery cycles from weeks to hours. The combination of robotics with AI enables rapid iteration, programmable feedback integration, and real-time adjustment of reaction parameters, creating a closed-loop self-learning system [52,53].

LLMs such as CataLM contribute an additional layer of intelligence by providing retrosynthetic guidance and catalyst selection. These systems leverage chemical knowledge databases to support decision-making, prioritize experiments, and explore reaction networks effectively, bridging the gap between computational prediction and experimental implementation [20,16].

Together, these AI and ML strategies transform programmable nanocatalysts into autonomous, programmable systems capable of continuous optimization, minimal human intervention, and programmable response to fluctuating feedstocks and environmental conditions. By integrating predictive modeling, RL, autonomous experimentation, and LLM-guided reasoning, these systems represent a major step toward self-driving laboratories and circular, sustainable chemical processes.

4.4 Molecular Coding of Reactivity

The notion of programming, since logic gates are built into the nanostructures to regulate catalytic activity, has taken programmable nanocatalysis to a new dimension. These gates operate as digital circuits and switch the on or off state of catalytic sites in response to certain chemical or physical inputs [39]. This allows the catalysts to be able to process the information in the environment and modify their programmed reaction paths, like using one of two parallel reaction paths or changing selectivity to different concentrations of substrates or other stimuli.

Molecular coding can be realized in a number of strategies. As an example, stimuli-reactive ligands or surface-level changes can be used as an "input sensor," which changes the electronic structure or accessibility of the active site when a chemical or physical signal is detected [40,41]. The positive assemblies and the allosteric designs facilitate the propagation of the signal by cooperative interactions to form concerted responses in many active sites as observed in enzymes. This process is also especially helpful in selectivity in multicomponent reactions when it is important to minimize the formation of byproducts because control over sequential or competitive processes becomes paramount [42].

With the programmable programmability of nanocatalysts (reactivity can be changed by prediction), guided with an optimized knowledge provided by AI, it can also be achievable. The adaptation of the electronic surface state of embodied photocatalysts based on molecular logic can maximize the photon absorption and inhibit charge recombination and accelerate the rate of hydrogen evolution in response to various illuminations [44]. Similarly, in environmental catalysis, molecular coding can be used to selectively activate with respect to individual pollutants, thereby increasing the removal efficiencies with lesser energy needs in the wastewater treatment process, as shown in Figure 3. This figure illustrates the molecular coding of reactivity through logic-gate-based regulation of programmable nanocatalysts, which enhances the effectiveness of pollutant removal.

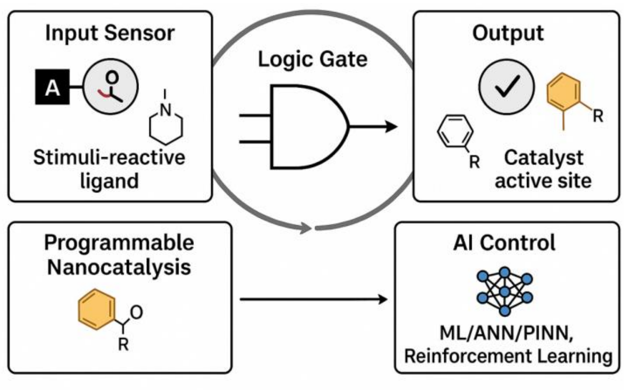

Figure 3. Molecular coding of reactivity: Logic-gate-based regulation of programmable nanocatalysts.

Figure 3 illustrates how molecular coding enables programmable control over catalytic reactivity using logic-gate principles embedded within nanostructures. Stimuli-responsive ligands act as input sensors, detecting chemical or physical signals and modifying the electronic or steric accessibility of active sites. These inputs are processed through molecular logic gates, which switch catalytic pathways on or off to determine the reaction outcome. The resulting output activates or deactivates specific catalytic sites, selecting between parallel pathways or modulating reaction selectivity. Integrated with AI-guided prediction and optimization, this molecular coding framework enhances photocatalytic efficiency, pollutant-specific activation, and adaptive environmental catalysis.

4.5 Synergistic Integration of Working Systems

The AI optimization-based intelligent architectures and the molecular coding in addition to them offer a collaborative system of programmable next-generation nanocatalysts. With the incorporation of correct nanoscale engineering into these systems with current computational prediction modelling and stimulus-responsive logic, they can operate independently and can also correct themselves to remain optimum in changing scenarios [39,40].

It is quite convenient in overcoming the common photocatalysis issues that demand massive implementation with high photon-conversion efficiency, chemical stability, and cost efficiency [41,42]. The programmable nanocatalysts could be optimized to achieve a bandgap, surface reactivity, and energy alignment reducing trial and error at reduced environmental cost using AI to select the material and design programmable nanocatalysts [44,50].

Moreover, when catalysts are designed with molecular logic and feedback-sensitive properties, they can tune their activity in a programmable manner, avert deactivation, and retain high selectivity during extended reaction times. Through imitating natural enzymes, these versatile catalysts can be stabilized and reactive on a bigger scale, which is necessary during industrial application. Such a strategy will make it possible to build useful catalytic systems and help establish autonomous chemical networks that are able to learn on their own, perceive their surroundings, and intelligently adjust their reactivity.

The rational design of programmable nanocatalysts establishes the structural, mechanistic, and digital frameworks necessary for adaptive and self-learning behavior. However, the full potential of these catalysts is realized only when their design principles are aligned with circular chemistry strategies, ensuring that catalytic processes are not only efficient but also sustainable and resource-conscious. Integrating circular chemistry principles requires that catalysts actively minimize waste, valorize by-products, and enable closed-loop reaction cycles, transforming catalytic systems from isolated reactive units into components of a broader sustainable chemical network. By embedding these considerations into the design of programmable nanocatalysts, it becomes possible to achieve a synergistic balance between autonomous catalytic performance and environmental responsibility, a critical step toward sustainable industrial applications.

5. Integration of Circular Chemistry

Circularity in programmable nanocatalysis will transform chemical production to a completely new stage, where we can build systems that are naturally self-governing, resource-efficient, and sustainable. Circular chemistry seeks to create closed-loop production circuits or reaction networks as opposed to a linear production pattern where the chemical processes follow the "take-make-dispose" pattern. In this case feedback controls reactions, and waste is minimized. Moreover, there is energy recovery, and it reuses materials in regeneration processes [51,52]. This part discusses the innovations in design, programmable catalytic, and energy control in circular chemical systems.

5.1 Linear Feedback-Controlled Reaction Networks

A majority of the batch and continuous chemical processes are bounded by fixed reaction conditioning. Their small range of programmableness in feed-to-product and linearity results in high amounts of byproducts. On the way, environmental burdens are also created. In contrast to this, reaction networks that are controlled by feedback provide programmable catalysts designed to monitor the changes in the environment, change activity, and change selectivity. The integration of programmable reactivity and programmable control into catalytic scaffolds can be used to provide reaction intermediates to supply thermoprogrammable and kinetic information, which, in its turn, can instruct the system to self-regulate [39,37].

In multistep cascade reactions, products derived during the initial steps may serve as regulatory information that either positively or negatively affects the other transformations to enhance the yield and reduce undesired side products [21, 24]. This architecture is self-learning; P allows reaction networks where the catalyst system retains memory of previous chemical reactions and evolves its energy landscape to maintain appropriate performance, like biological metabolic circuits [27].

Such networks work in reality by enabling live sensors, ML, and autonomous reactors. These systems monitor the reaction process. The system evaluates the resemblance between the result of the reaction and the target. In case a deviation has been found, the system changes one of the reaction conditions. This may be the pH, temperature, solvent composition, or other fields applied. And in this sense a closed loop is created [6,3]. The transitions between the fixed and the feedback-controlled networks will render the chemical processes far more efficient, which could also minimize the wastage and increase the resilience to changes in the feedstock quality of other environmental factors.

5.2 Recovery of Waste Using Catalytic Processes

One of the basic rules of circular chemistry is to reuse the waste to create something useful. Programmable catalysis can be achieved with programmable nanocatalysts, in which the selectivity of the catalyst and the reaction pathway can be programmatically adjusted based on the feedstock composition, suggest the use of the above with a waste stream containing CO_2, lignocellulosic biomass with agro-industrial residues of variable composition, and reactivity [54].

As an example, modified catalysts can selectively participate in the activation of different functional groups on the same type of biomass-derived molecule and convert a heterogeneous feedstock into a platform chemical, biofuel, or polymer precursor without the need to subject biomass to extensive pretreatment [55]. Similarly, it can be modified by changing properties of the active sites, electronic properties, and experimentation variables to make it desirable to the generation of carbonates, formates, or syngas according to the objective of a particular process [3].

Predictive models that run on AI could be used to predict changes in waste composition by catalysts. They are consequently able to modify their reactivity over such changes that enhance their efficiency and selectivity in conversion [23]. Application of a new catalyst enhances sustainability [23]. This plan decreases the reliance on prescribed conditions of reaction and discourages the development of undesired by-products. This will provide an economic benefit and is also aligned with principles of green chemistry like preventing waste, energy conservation, and also renewable feedstocks [52].

Also highly useful in valorization cascades (where multiple products can be extracted out of a waste stream) is programmable catalysis that can provide the ability to recycle and reuse a natural ecosystem. The programmable nanocatalysts can transform waste into wealth, leading to the creation of a sustainable and circular chemical economy, as illustrated in Table 3. This table outlines the circular-chemistry performance indicators for programmable nanocatalysts, which are essential for evaluating their efficiency and sustainability in such processes.

Table 3. Circular-chemistry performance indicators for programmable nanocatalysts.

Circular Metric	Operational Definition	Relevance to Programmable Systems	References
Waste-to-Value Conversion Efficiency (WVCE)	Fraction of waste transformed into useful products	programmable selectivity enables multi-stream valorization	[54,56]
Energy Neutrality Index (ENI)	Ratio of energy recovered to energy consumed	Stimulus-responsive systems optimize energy flows	[41,57]
Catalyst Regeneration Factor (CRF)	Ability to self-repair or self-regenerate active sites	AI-driven restoration prolongs catalyst lifetime	[8,36]
Cycle Stability and Reusability (CSR)	Number of cycles without performance loss	Feedback-controlled reactivity reduces deactivation	[52,55]

5.3 Regenerative Cycles and Energy Neutrality

Circular chemistry is interested in both material efficiency and energy neutrality, as well as regenerative catalytic cycles. It is possible to design nanocatalysts with programmable functionality to match the exothermicity of a reaction with an endothermic reaction to achieve intrinsic balancing of energy within the catalyst network [56]. The electrons are released in one of the reaction steps, and there is another step where the electrons generated in the first step are arrested. This way it reduces the amount of energy input into the environment and is sustainably friendly [51].

Combining the management of photocatalytic, electrocatalytic, and thermal energy into systems that can be programmed enhances the recovery of energy. Photocatalysts may utilize solar energy to promote endothermic reactions, but on electrochemical platforms, energy can be collected and recycled in a reaction network, leading to self-sustained reactions [45,46]. These strategies, together with regenerative cycles, not only enable the catalysts to undergo numerous cycles, but they also increase lifespan and eliminate repetitive replacement. This is what is necessary in scaling industrially.

The catalysts are able to adjust their structures depending on the varying energy conditions, assuring that no energy is wasted. All these catalysts are one-of-a-kind. To illustrate this, pH/light-responsive catalytic centers can selectively turn their active states to their inactive ones and vice versa to align with energy availability, thereby enabling the possibility of time-dependent energy optimization and avoiding wastage of energy [32,34].

The less energy-consuming designs are beneficial to the sustainable production in decreasing the reliance on the use of fossil fuels and decreasing the greenhouse gases when producing the chemicals. The net-zero energy chemical processes can be supported by integrating energy recovery and regeneration into programmable nanocatalysts. This implies that chemicals will be made in a sustainable and cyclical way.

5.4 Systems-Level Integration and Implications for Industry

To make a difference in scaled applications of circular chemistry, one should be able to bridge catalyst design, AI optimization, and process engineering at the systems level. The key component of this integration is programmable nanocatalysts, which integrate feedstock processing and energy management and product generation in coherent networks with feedback control.

Biorefineries represent the application of this idea and rely on interdependent catalytic modules to transform the heterogeneous agricultural residues into a plurality of products biofuels, platform chemicals, and functional materials. These plants are capable of adjusting programmatically the processing conditions under influences of feed variability, environmental conditions, and energy availability and maximizing efficiencies and product yields using programmable catalysts and real-time monitoring [53,54].

On an industrial level, there are numerous advantages of employing circular and feedback-based chemical manufacturing. As an illustration, it decreases the flows of waste, provides more flexibility of processes, reduces the usage of resources, and advances adherence to regulations. Besides, molecular logic and AI in catalytic structures work on a reactor scale and make decisions without the involvement of operator activation, minimizing the risk factor and making processes less dangerous [6,43].

By definition, circular and programmable chemical systems reduce greenhouse gas emissions, energy, and use of renewable feedstock. In this way, it is also useful in sustainability and recharging the climate. Circular chemistry is transforming itself into a strategy and molecular- and process-level embedded concept to ensure that the chemical industry actively innovates and actively solves urgent environmental issues [3,23].

The introduction of circular chemistry into programmable nanocatalysis is a radical and novel technological paradigm of chemical synthesis. It provides self-regulating, energy-efficient, and programmable systems. The combination of feedback-controlled reaction networks, waste valorization, and regenerative cycles provides the prospect of resource-efficient and environmentally friendly chemical reactions. Meanwhile, the integration of AI, stimulus-reactive design, and molecular logic provides the intelligence of the processes so that they can work on their own.

It is not possible to remove the thiophene in oil. Future studies will probably involve scaling programmable catalytic systems and optimizing AI-aided process control, feedstock, and product scope that involve circular processes. The implementation of cyclic chemistry incorporates a way to work towards the future of the self-educating, energy-neutral, and environmentally friendly chemical process by incorporating the principles of smart design and sustainability, as well as the use of advanced materials [51,52,56]. As shown in Figure 4, the multi-layer mechanistic architecture of programmable nanocatalysts can play a key role in advancing these innovations.

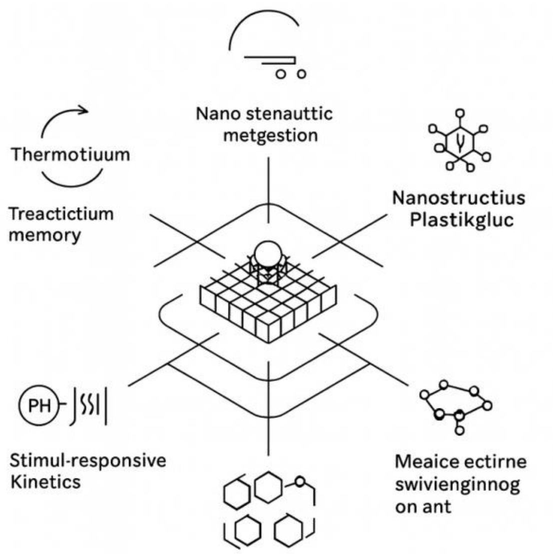

Figure 4. Multi-layer mechanistic architecture of programmable nanocatalysts.

Figure 4 illustrates the multi-layer mechanistic architecture that enables the design, modulation, and programmable control of programmable nanocatalysts. The central catalytic core is shown as a structured nanosurface, surrounded by five functional domains that collectively regulate catalytic behavior. These domains include:

(1) Thermal and reaction memory, which allows the catalyst to retain information about previous reaction states;

(2) Nano-scale motion and transport, governing the movement of reactive species across catalytic interfaces;

(3) Structural plasticity, enabling reconfiguration of nano-assemblies during catalysis;

(4) Stimuli-responsive kinetics, where catalytic rates adapt to external triggers such as pH, light, or electromagnetic fields;

(5) Molecular switching and electron transfer pathways, which fine-tune the reaction mechanism through controllable electronic modulation.

Together, these interacting layers create a programmable catalytic system capable of learning, adapting, and optimizing performance across complex reaction environments.

5.5 Programmable Nanocatalysts for Waste Recovery and Energy-Neutral Circular Processes

Programmable nanocatalysts enhance waste valorization and enable energy-neutral cycles by programmatically adapting their structure and electronic properties to heterogeneous feedstocks and fluctuating process conditions. These catalysts selectively convert complex waste streams including agro-industrial residues, lignocellulosic biomass, and CO_2 into high-value chemicals, fuels, and polymer precursors without extensive pre-treatment [54,55]. By actively tuning surface active sites in response to real-time reaction conditions, programmable nanocatalysts direct reaction pathways toward desired products while minimizing by-product formation, thus facilitating closed-loop chemical processes [3,4].

A key mechanism involves programmable active site modulation, where the catalyst reversibly adjusts coordination environments to favor specific intermediates. For example, SACs and MOFs can sense substrate composition and reorganize their electronic structure to enhance selective oxidation or hydrogenation in mixed waste streams. Another mechanism is feedback-controlled reaction regulation, in which integrated sensors monitor reactant and product concentrations and adjust turnover frequency, temperature, or applied potential to optimize energy efficiency and product yield. This programmable strategy effectively reduces external energy input while maintaining high selectivity, establishing a robust, self-regulated catalytic cycle [23,52].

Case studies demonstrate programmable nanocatalysts converting CO_2 and biomass into syngas, formate, or higher-value chemicals under mild conditions, achieving high selectivity and yield while minimizing energy consumption [54,55]. Similarly, programmable catalysts for lignocellulosic residue pyrolysis increase bio-oil yield, reduce char formation, and enable integrated heat recovery, exemplifying energy-neutral circular operation [55].

The integration of AI-guided predictive control further enhances efficiency. ML models anticipate variations in feedstock composition and programmatically adjust catalyst configuration, ensuring maximal waste conversion with minimal energy input [1,5,6]. These programmable catalytic systems thus exemplify sustainable, programmable, and energy-efficient approaches to circular chemistry, transforming waste streams into valuable resources while aligning with principles of green chemistry and circular economy [52].

Integrating circular chemistry principles into programmable nanocatalysts not only ensures sustainable and waste-minimizing processes but also amplifies the practical potential of self-learning catalytic systems. By combining adaptive design with circular resource management, catalysts can autonomously adjust their activity and selectivity to process diverse feedstocks efficiently, recover valuable by-products, and continuously improve reaction outcomes. This convergence of intelligent control and sustainability creates a platform where programmable nanocatalysts move from theoretical constructs to practical tools for industrial, pharmaceutical, and environmental applications.

6. Uses of Self-Learning Nanocatalysts

Self-learning nanocatalysts will help revolutionize the chemical sciences. One of the fundamentals of an autonomous, programmable, high-performance, and chemical catalytic system may be such self-learning catalytic systems. These systems are transforming the face of catalysis by introducing new possibilities of electrocatalysis, photonics, and environmental remediation by utilizing AI, robotic automation, and feedback-controlled architectures [57,58]. Here we will comment on the primary application places of programmable nanocatalysts. Besides, it will demonstrate their practical benefits and mechanistic innovations and influence sustainable chemistry.

Real-time reprogramming is most effective when catalysts are engineered at the atomic and nanoscale to dynamically adjust facet exposure, defect density, surface composition, and electronic properties, enabling continuous self-optimization under operational conditions. As shown in Figure 5, an AI-driven adaptive catalytic system integrates feedstock input, catalyst dynamics, reaction monitoring, and closed-loop control, enhancing the catalytic process in real-time.

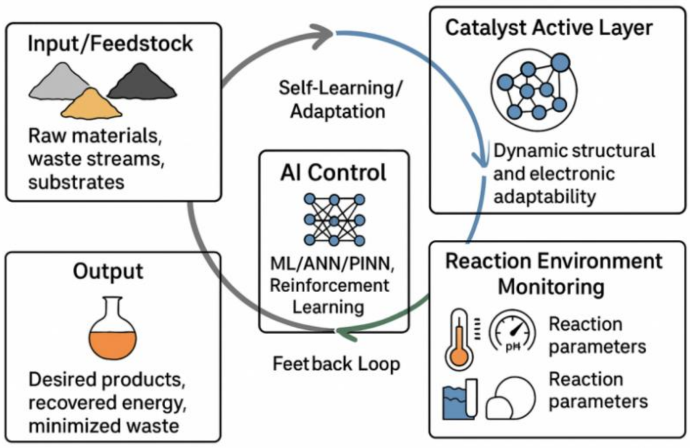

Figure 5. AI-driven adaptive catalytic system integrating feedstock input, catalyst dynamics, reaction monitoring, and closed-loop control.

Figure 5 illustrates an integrated AI-driven framework for adaptive catalytic processes. The system begins with the input/feedstock, which may include raw materials, substrates, or waste streams that enter the catalytic environment. The catalyst active layer exhibits dynamic structural and electronic adaptability, enabling real-time adjustments in response to changing reaction conditions. Continuous reaction environment monitoring including parameters such as temperature, pH, and reactant concentrations provides the system with essential operational feedback.

These data streams are processed by the AI control module, which employs ML, ANN, PINN, and RL to make informed decisions. The AI continuously optimizes reaction conditions through a feedback loop, enhancing catalytic performance, stability, and efficiency. Ultimately, the system yields desired outputs, such as target products, recovered energy, and minimized waste, while simultaneously improving process sustainability. The closed-loop design enables self-learning and adaptation, ensuring long-term optimization of catalytic behavior under variable operating environments.

6.1 Transformable Electrocatalysis

Electrocatalysis refers to various reactions that accelerate an electrode reaction that has been catalyzed by a molecule, solid, or polymer. They are widely involved in energy conversion reactions like those related to the hydrogen evolution reaction, which is HER, the oxygen evolution reaction (OER), and the CO_2 reduction reaction, which is CO_2RR. A number of renewable energy technologies are rooted in these reactions. Self-learning nanocatalysts have the ability to provide programmable electronic control through their active site qualities, electronic architectures, and reaction intermediates, which automatically adjust in reaction to feedback on the reaction conditions and AI algorithms [59,60].

As an example, programmable catalysts can quickly reorganize the local electronic density of the centers of metal to produce desirable effects on the proton adsorption rate or electron transfer rate, thereby switching HER and OER kinetics in different electrolytic conditions [57]. The alternative option is active site geometry, oxidation state, ligand environment, or programmable tuning of CO_2RR, which selectively reduces to produce formate, CO, or hydrocarbons [61]. It will self-improve without the human factor of researchers having to spin off experiments in order to find the most appropriate catalyst and operating conditions.

Robotic synthesis systems operate with spectroscopic and electrochemical sensors to analyze fidelity and efficiency by implementing closed-loop iterative optimization. The activity and selectivity of the catalysts can further be improved by systems that allow the catalysts to learn from the outcomes of reactions and optimize them [58]. This method allows the researcher to save on energy, reagents, and time in making faster discoveries. It is possible to change the composition of feedstock, like electrocatalytic platform composition, with temperature and high-performance energy conversion with programmable use of pH or applied potential depending on the performance of ML algorithms.

6.2 Photonic Reactivity of Hybrid Systems

Photocatalysis is another field that programmable nanocatalysts can be utilized in with great potential. In the traditional photocatalytic systems, the inefficiencies are usually a result of poor use of photons, recombination of charges, and incapacity to respond to changes in light. The interactions they mediate are controlled by self-learning catalysts via a programmable photonic reactivity that regulates photon absorption, charge separation, and surface reaction rates via an AI-assisted feedback mechanism [42,58].

The light-harvesting capacity of nanocomposites or hybrid nanomaterials incorporating semiconductor nanoparticles with plasmonic structure or enzyme mimetic will vary with the incident intensity of light, wavelength, and reaction intermediates [41,44]. ML Scaffolds predict the most optimal geometry of heterojunctions, surface defects, and co-catalysts to maximize quantum efficiency that controls autonomous reconfigurations to light-driven reaction networks [45].

Besides, systems may utilize logic gates at a molecular scale, whereby they would utilize particular photonic or chemical inputs to switch on or switch off catalytic sites selectively [39]. Complex photocatalytic process applications, which are required to produce solar fuels, selective reactions with organics, and degradation of pollutants under diverse solar conditions, also require the capability to program behavior. Very high efficiencies can be kept by a recently innovative photocatalytic system due to self-learned feedback. This represents a great enhancement compared to those with non-moving (stationary) components [40,43].

6.3 Environmental Remediation Networks

The most useful application of self-learning nanocatalysts would be in the physical removal of the environment. Independent catalytic cycles have the potential to reuse and restructure ecosystems and reduce pollutants with minimal human intervention. The use of these systems is based on the iterative feedback of AI that monitors the concentration of the pollution, the kinetics of the reaction, and the formation of byproducts. Depending on this data, catalytic activities are modified in order to have efficient degradation.

Programmable reaction pathways can be engineered into programmable nanocatalysts that can convert complex organic pollutants found in wastewater to either benign or valuable products, contingent on the chemical composition of the effluent [49]. The closed-loop control will enable the catalytic network to prevent over-oxidation and undesired side reactions and the accumulation of intermediate toxins automatically [61]. Effective systems are used when traditional remediations are not effective or when they are extremely costly in the case of persistent organic pollutants, pharmaceuticals, and complexes of heavy metals.

High-throughput analysis coupled with predictive modelling and robot experimentation capabilities provided by the platforms' corrective self-learning allow reaction conditions to be explored quickly in multidimensional chemical spaces. This capability will enable autonomous systems to find the most favorable catalyst composition, dosing, and reaction conditions depending on various environmental matrices, reducing the number of trials and errors and reducing the time of remediation [58,62].

Also, the environmental remediation networks may be integrated with resource recovery systems whereby the degraded pollution may be converted into reusable chemicals, fuels, or materials that are sustainable and circular [56]. The use of AI-based decision-making ensures catalyst reactions are performed with minimum material and energy and a low environmental footprint to achieve maximum possibilities in the remediation and valorization process [51].

Emergent behavior leads to the formation of a new form of intelligence, which is a result of a large population of catalytic units that interact with each other. These catalytic units are able to communicate with each other using chemical signals or might utilize digital feedback as well. They work as a group, collectively, and therefore optimize the performance of treatment works at a large scale. This method is quite analogous to the processes present in nature, such as a self-organizing process that performs the equilibrium and resilience processes. This also indicates that the programmable nanocatalysts can consider programming of life-like functional change in artificial chemical systems [27,29].

6.4 Collaboration with Self-Driving Laboratories

One of the enablers of such applications is the integration of AI, characterization, and robot experimentation with programmable nanocatalysts into self-driving laboratories. The databases rely on the design-make-test-analyze cycle to optimize their predictive models automatically using data in what they test, which is enabling the development of new catalysts at an astounding rate [59,60].

Multi-component nanomaterials can be studied using self-driving laboratories. Consequently, we are in a position to evaluate an enormous amount of compositions, morphologies, and surface functionalizations in days, as opposed to months. Neural networks build quantifiable correlations between material properties and engineering performance, which are used to direct further manufacturing towards efficiency and longevity of catalysts [58]. Using this repetition technique to optimize electrocatalytic, photonic, and remediation systems, among others, for a selected application yields the highest performance, selectivity, and ecocompatibility ever.

In addition to this, the scalable and modular self-driving laboratory also enables the straightforward introduction of new catalytic modules or optimization of various properties, including biological activity, solar absorption efficiency, or selective adsorption without impacting on current workflows. The scalability of catalyst design also allows the investigators to be able to keep up with shifting requirements and develop and engineer next-generation catalytic systems in a short period [58,61].

Self-learning nanocatalysts avoid over-adaptation by combining feedback-controlled response, structurally resilient designs, stimulus thresholds, self-limiting chemical networks, and AI-guided predictive constraints, ensuring that adaptive behavior improves performance without compromising stability or selectivity.

6.5 Problems and Future Research

Although self-learning nanocatalysts can transform the game, there appears to be many issues left out. Predictive models should be able to capture the range of chemical spaces as well as not only fitted on a single dataset. Several methods, including the transfer learning, active learning, and ensemble modelling, prove important towards standard performance under heterogeneous conditions of reactions [58]. In addition, in the practical industry and environmental uses of autonomous systems, hardened hardware, strong nanomaterials and reliable sensor networks must be capable of enduring changing environments.

Other aspects to be considered include energy efficiency and scalability, and lifecycle sustainability. As an example, catalysts must be active and selective at an extended period and not foul, aggregate or deactivate to be useful at large scale. The development of AI-controlled regeneration systems, self-repairing materials, and surfaces with stimuli responses are considered to be the possible solutions to these problems [32,33].

The complete potential of programmable nanocatalysts might be achieved in the future through the assistance of materials science, chemical engineering, robotics, and AI. Such progress as the creation of universal predictive models with the capability to sample complicated chemical spaces and self-teaching frameworks is going to yield fast performance enhancement to take advantage of new chemicals and environmental circumstances. The integration of AI and catalysis will result in the creation of automated and efficient catalytic processes to address various international problems. More specifically, these catalytic reactions are applicable in the generation of energy and alleviation of environmental problems. These opportunities demonstrate how bright AI in catalysis will be in the future. More studies in this field will definitely reveal a number of other opportunities.

While the practical applications of self-learning nanocatalysts demonstrate their transformative potential across chemical synthesis, industrial manufacturing, and environmental processes, several challenges remain before these systems can achieve widespread adoption. The integration of adaptive catalytic behavior with autonomous control, circular chemistry, and large-scale industrial processes introduces technical, computational, and material complexities that require careful consideration. Understanding these limitations is critical for guiding the next generation of programmable nanocatalyst development and for bridging the gap between laboratory-scale innovations and scalable, sustainable chemical networks.

The emergence of self-educating nanocatalysts and chemical intelligence systems are new opportunities of autonomous science but need strong scientific, computational, and ethical advances to become a reality. These frontiers are promoted by integration at various scales, programmable computation, and responsible innovation to guarantee safe self-regulation of chemical systems. Three fundamental frontiers outlined in the path taken by research and innovation in this emerging field include multi-scale synchronization, computational translation, and ethical and environmental implications.

7. Challenges and Frontiers

7.1 Multi-Scale Synchronization

One of the biggest challenges towards self-learning nanocatalysis is multi-scale synchronization through feedback chains at nano, molecular, and reactor scales [21]. Nanocatalysts have the ability to self-optimize on a molecular scale, but to introduce these phenomena to macroscopic reactor conditions, there has to be smooth interplay between extremely different spatial and time scales. Recently, an article in Nature explains that chemical self-regulation can be done on different scales. Successful self-regulation of complicated chemical systems thus relies on cross-scale communication assemblies that permit information exchange amid local and global reaction settings [63].

It is against this that scientists are developing hierarchical feedback loops to bridge the gaps between the nanoscale processes that regulate stability, such as charge transfer, adsorption/desorption, and process parameters at meso- and macro-scales, such as temperature, pressure, and flow. In order to bring about this parallelism in effort, it is necessary to be able to integrate real-time sensor data with a data-driven control model. These allow the catalyst to independently adjust its structure or reactivity according to reaction condition changes [21].

However, it is computer intensive to model. In order to coordinate well with real-time data, hybrid digital-physical control systems will be needed whereby ML algorithms with automatic updating of their model parameters will constantly renew the sensor data and future-state projections. The systems are required to consider the inherent stochasticity of the chemical reactions in addition to the delays, noise, and nonlinear behavior on different scales.

The deeper we know our response, the more we can eventually be in a reactive coherent state; the information that is taken in and shared between the nano- and macro-scale would enable it to respond in a predictive or programmable fashion. This will go a long way in developing catalytic networks that are self-regulating and can effectively perform in an industrial or environmental environment.

7.2 Computational Translation: Chemical Neural Networks

The reverse engineering of chemical reactions and their interpretation on computer architectures is the next frontier that will allow the creation of a chemical neural network that can inform not only on mechanisms of chemical reactions but also on biological and digital neural connections [64]. Things and individuals of the old have turned out to be unknown in the contemporary world. But as time has passed, our perception and observations have shifted from irrational vision to rational vision.

Because chemical networks are nonlinear, stochastic, and interactive by nature, compared to electronic circuits, modularity and scalability are more complex with more complex networks [18]. The unexpected properties of these can lead to phenomena such as waves, bistable behavior, or chaos that can be difficult to deal with using the old techniques. However, the tuning of these chemical systems may also be applied to exhibit emergent intelligence so that spontaneous behaviors, including the ability to discriminate between and remember objects and learn, become exhibited [35].

One of the recent papers is about the promise of realization of chemical reaction networks (CRNs) in the context of the development of autonomous architectures. In order to fulfill this promise, researchers are working on recurrent neural chemical reaction networks (RNCRNs). These RNCRN constructions will be capable of acquiring arbitrary programmable behaviors without a fixed initial condition and long recalibrations [18]. Some of the complicated behaviors that can be made by these robots include synchronization, decision-making, and chaotic pattern formation. They get to learn through the surrounding environment, and this makes them design molecular forms of biological cognition that are compatible with the chemical kinetics and AI.

This is a great departure from the conventional digital computers. Specifically, it is a bottom-up method that utilizes chemical complexity and does not eradicate it [11,32]. Molecules are not passive reactants but an active computational agent that is able to perform intelligent operations as a collective. These systems might have self-learning capabilities of feedback loops to hierarchically develop higher-order cognitive processes such as adaptation, abstraction, and goal-directed optimization [35].

These kinds of systems allow chemical artificial intelligence (ChemAI), in which chemical reactions themselves are used to reason. ChemAI will combine AI algorithms and physical reaction networks, which may enable materials to perceive and react to patterns in the surrounding environment, predict reaction outcomes, and self-correct in the event of their performance being below the intended level. This can provide the chemicals with functions similar to general intelligence analogues.

To enhance learning, ChemAI should be practicable. Due to their effectiveness, deep learning models are frequently poorly interpretable and empirically biased due to their heuristic training [21]. Such biases in chemical systems may be unstable and unpredictable. In order to ensure that learned behaviors do not contravene thermoprogrammable and kinetic principles, then, we are suggesting explainable AI architectures and PINNs (physically informed neural networks).

The end result is developing chemical robots–mechanical minds that carry out self-controlled responses, communicate with one another, and demonstrate an emergent intelligence as a team [35]. The networks would be able to perform predictive analysis and problem solving in functional equivalence to human cognition, and this resulted in the production of intelligent, distributed chemical systems capable of self-managing themselves in diverse environments.

7.3 Implications of the Procedure on Ethical and Environmental Concerns

With AI and chemical autonomy becoming increasingly similar, the ethical and environmental outcry is becoming more pronounced. The autonomy of self-learning chemical systems raises concerns of control, safety, and liability.

In case the autonomous nanocatalysts are not controlled properly, they may possess unexpected results such as uncontrolled reactions, bioaccumulation, and cross-reactivity. We must possess powerful principles and evaluations that gauge the influence of such things on the overall life, whether they are stable and recyclable [35]. Environmental monitoring and traceability technologies, such as the reaction logs of blockchain and sensing-based verification, may have a significant role in promoting self-learners' accountability.

Moreover, ethics do not only relate to the safety of the environment but also to algorithmic governance and data ethics. Chemical discovery is becoming influential with the AI-based systems. Nonetheless, the training data may induce bias that may change the behavior of materials or optimize unsafe strategies. Human-in-the-loop architectures are needed to facilitate the evolutionary impact and decisions alignment.

Finally, the self-learning chemical systems design will be based on green chemistry and circular economy concepts, like low toxicity and recyclability over the lifecycle. To self-adjust to one's environmental imprint and monitor it, eco-safety might also be fed back (with AI) [11].

The moral edge of chemical innovation will hence be dictated by the combination of autonomy, intelligence, and sustainability. It takes issue with responsible design models to make sure that the programmable chemical system guarantees global sustainability, as opposed to compromising it. Consequently, these frameworks should incorporate moral thinking, openness, and environmental responsibility [35].

7.4 The Path Forward

These frontiers will be achieved through deep interaction between fields such as chemistry, AI, systems engineering, and ethics. Future studies need to focus on:

Programmable digital twins model of the catalytic systems with built-in experimental feedback to multi-scale modelling construct.

Chemical neural networks based on the principles of physical chemistry that can be trusted and are safe.

Design the catalyst in an autonomous and ethical way, and at the same time be transparent.

Addressing the challenges and exploring the frontiers of programmable nanocatalysts requires robust experimental validation. While computational models, AI-driven predictions, and self-learning frameworks provide powerful guidance, experimental evidence is critical to verify adaptive behaviors, optimize reaction conditions, and ensure reproducibility in real-world applications. Integrating experimental insights into the design of programmable nanocatalysts not only strengthens their practical feasibility but also facilitates the alignment of these systems with circular chemistry principles, ensuring that sustainability targets are met without compromising catalytic performance.

8. Integration of Experimental Evidence in Programmable Nanocatalysts for Circular Chemistry

Programmable nanocatalysts in circular chemistry exhibit emergent self-learning behavior, where past catalytic events inform future reactivity, demonstrating a sophisticated level of autonomous control over reaction pathways [65]. Unlike conventional static catalysts, these systems integrate real-time feedback and programmable learning mechanisms, allowing them to programmatically adjust to fluctuating input streams and transient intermediates, thereby optimizing product formation while minimizing waste within complex circular economy processes [66]. This adaptability is particularly crucial for sustainable industrial applications, where feedstocks are often heterogeneous and require flexible catalytic systems for efficient valorization [66].

Experimental observation studies reveal that programmable nanocatalysts can modulate turnover frequency and selectively redistribute intermediates across parallel reaction pathways in response to environmental cues. This reaction memory effect enables continuous improvement in catalytic efficiency and selectivity over extended operational periods, aligning with principles of active learning and machine intelligence [67]. Such autonomous optimization reduces the reliance on human intervention, facilitating closed-loop operation in chemical networks and supporting the recovery of valuable components from spent materials [68].

Moreover, these catalysts are capable of self-reconfiguration, programmatically adapting reaction pathways in response to system feedback, which represents a significant step toward self-driving laboratories and AI-assisted chemical discovery [69,70]. Integrating mechanistic insights with machine-guided experimentation, these systems exemplify how catalytic networks can program their own behavior based on prior states, ultimately enhancing process robustness and sustainability [71].

Collectively, the findings highlight the transformative potential of programmable nanocatalysts in circular chemistry: They not only enhance efficiency and reduce waste but also provide a platform for autonomous, programmable chemical systems capable of learning and evolving within complex reaction environments [70].

Programmable nanocatalysts achieve self-regulated catalytic behavior through a sophisticated interplay of programmable structural restructuring and electronic tuning at the molecular level. Programmable restructuring involves the reversible reorganization of surface atoms, active sites, or lattice facets in response to changes in reactant concentrations, intermediate formation, or local reaction conditions. Such reconfigurations optimize adsorption energies, stabilize transition states, and facilitate efficient catalytic turnover, enabling continuous adaptation under fluctuating operational environments [72].

Complementing structural plasticity, electronic tuning allows active sites to programmatically adjust their charge distribution, oxidation states, and orbital occupancy. This modulation improves reactant binding, lowers activation barriers for preferred reaction pathways, and suppresses side reactions, effectively enhancing selectivity and catalytic efficiency [73]. Feedback from reaction intermediates or environmental cues acts as a chemical signal that informs subsequent cycles, enabling catalysts to "learn" from past reactions and adjust their behavior in real time [72,74].

Such programmable molecular behavior mirrors the induced-fit model observed in enzymatic catalysis, where conformational changes optimize active sites upon substrate binding [75]. Programmable nanocatalysts can perceive and respond to both weak and strong external signals, maintaining optimal performance across a range of reaction conditions, including temperature fluctuations and heterogeneous feedstocks [74,76]. This programmable adaptability ensures sustained catalytic efficiency and product yield, distinguishing programmable systems from static catalysts that often suffer from activity degradation or selectivity loss under non-ideal conditions [77].

The combination of structural and electronic responsiveness also enables intelligent sensing and reversible isomeric transformations, which are particularly useful for catalytic and sensing applications under varying thermal or chemical stimuli [78]. Collectively, these emergent properties facilitate the design of self-learning, reconfigurable catalytic networks that are capable of autonomous adaptation, real-time optimization, and continuous improvement, providing a foundation for sustainable, circular chemical processes.

The integration of experimental evidence into programmable nanocatalyst development provides a solid foundation for understanding adaptive behavior, optimizing reaction networks, and aligning catalytic systems with circular chemistry principles. Building on these advances, it is now possible to envision the next generation of intelligent catalytic systems, where experimental insights, AI-guided optimization, and autonomous self-learning converge to create fully adaptive and sustainable chemical processes. Considering the current achievements, challenges, and validated frameworks, a forward-looking perspective highlights the potential pathways and innovations that will shape the future of programmable nanocatalysis.

9. Future Perspectives

AI combined with nanocatalysis and circular chemistry is a game changer for chemical research. Nevertheless, one should not stop at a single avenue. A promising direction is quantum-informed catalytic learning, through which quantum computing systems can predict reaction paths and optimize catalysts more than they have ever been predicted or optimized in the past [79]. With quantum algorithms of complex multi-electron systems, quantum mechanical effects could be applied to construct predictive self-adapting catalyst designs with controls over the associated electronic landscapes [80]. It may revolutionize computational catalysis because reaction coordinate surfaces that are hard to solve with classical techniques can now be analyzed.

The creation of programmable reaction ecosystems where networks of nanocatalysts communicate with each other chemically in a manner optimizing them. These systems were motivated by living systems, which could change their reactivity programmatically and redistribute catalytic functions depending on stimuli and substrate availability. Through their collaboration, it is possible that such catalysts can assist products in achieving higher yields and being more productive in terms of consuming and utilizing energy and resources. It assists them to act as a self-organized chemical network. With the integration of feedback control, chemical memory, and logic reactivity, the intelligent design of functional materials and catalytic networks will allow the creation of learning communities of catalysts that are capable of continuous adaptability.

Self-learning catalytic platforms in the industrial circular loops are also an essential part of the practical application. To scale up laboratory-scale programmable nanocatalysts to self-regulating industrial reactors, it is necessary to have powerful architectures to support real-time monitoring, closed-loop feedback, and AI-controlled optimization [6]. It is not merely reducing the scaling of the physical systems but creating protocols of energy neutrality, regenerative cycles, and waste valorization at the levels of the throughput in industries [10]. Autonomous catalysis and the circular economy should be coupled, which may assist chemical manufacturing to pursue not a linear, resource-intensive model but a self-regulating, sustainable, and profitable one [81,82].

Collectively, these prospective directions imply that self-learning catalytic systems are transformative. Ecosystems of coordinated reactions based on quantum knowledge, detailed industrial integration, and whole-system discovery will compress the length of the discovery-to-delivery cycles and enhance sustainability. These discoveries will bring completely new chemical sophistication and efficiency both at the lab and in the industry. The difficult thing is to ensure that the sophisticated technology would be compatible with trusted data and understandable calculations to make it safely and reasonably and sustainably applicable in the autonomous catalysis.

10. Conclusion

Self-learning nanocatalysis Programmable Programmable self-learning nanocatalysis is a new paradigm in chemical science, fusing threads made of nanochemistry with threads made of AI and circular chemistry. These catalysts are not ordinary simple static designs due to the provision of thermoprogrammable feedback, programmable modulation of structure, and stimulus-responsive reactivity. Autonomous experimentation, closed-loop feedback systems, and AI modelling are used in assisting in the fast discovery, accurate optimization, and environmentally friendly process management. Multi-scale synchronization solutions, the implementation of chemical neural networks, and ethics are solutions that we will have to come up with as the field progresses. Future developments in quantum-informed computation, programmable reaction ecosystems, and industrial circular integration will allow the demonstration of catalytic systems being moved off the shelf and into scalable industrial platforms. Intelligent self-educating nanocatalysts that respond to feedback can transform chemical engineering in sustainable and environmentally friendly chemical production, catalysis, energy transformation, and environmental purification.

Conflict of Interest

The authors declare no conflict of interest.

Generative AI Statement

The authors declare that no Gen AI was used in the creation of this manuscript.

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