

AI-DRIVEN DESIGN, CHARACTERIZATION AND ANALYTICAL ASSESSMENT OF GREEN CATALYSTS FOR SUSTAINABLE CHEMISTRY

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Abstract

The integration of artificial intelligence (AI) and machine learning (ML) with green chemistry principles has revolutionized catalyst design, characterization, and performance assessment for sustainable chemical processes. This comprehensive review examines recent advances in AI-driven approaches for developing environmentally benign catalysts, encompassing computational methods including density functional theory (DFT), neural networks, random forests, and graph neural networks (GNNs). We analyze 30 high-impact studies demonstrating how AI accelerates catalyst discovery through data-driven screening, property prediction, and inverse design strategies. Key findings reveal that ML models achieve prediction accuracies exceeding $R^2 > 0.98$ for catalytic performance metrics, while AI-optimized green catalysts demonstrate conversion efficiencies up to 97% with enhanced selectivity and reduced environmental footprints. Advanced characterization techniques coupled with AI, including operando X-ray absorption spectroscopy (XAS) and high-throughput screening, enable real-time monitoring of catalyst dynamics at atomic resolution. Sustainability assessments indicate that AI-designed catalysts reduce greenhouse gas emissions by up to 40%, minimize waste generation, and promote circular economy principles through renewable feedstock utilization. This article synthesizes methodologies, performance benchmarks, and green metrics, providing a roadmap for next-generation sustainable catalysis driven by intelligent computational frameworks.

INTRODUCTION

The global imperative for sustainable chemical manufacturing has catalyzed a paradigm shift toward green chemistry principles, emphasizing waste minimization, energy efficiency, and the use of renewable resources (Brandão et al., 2024; Ye et al., 2019). Traditional catalyst development relies on iterative trial-and-error experimentation, which is time-consuming, resource-intensive, and often fails to explore the vast chemical space of potential

materials (Ying et al., 2025). The emergence of artificial intelligence (AI) and machine learning (ML) technologies offers transformative opportunities to accelerate catalyst discovery, optimize reaction conditions, and predict material properties with unprecedented accuracy (Fawzy et al., 2025; Integrating artificial intelligence with green chemistry, 2025).

AI-driven approaches integrate computational modeling, data analytics, and experimental validation to design catalysts that meet stringent

environmental criteria while maintaining high performance (Srivastava et al., 2025). Machine learning algorithms, including neural networks, random forests, gradient boosting, and graph neural networks (GNNs), enable the extraction of structure-property relationships from large datasets, facilitating inverse design strategies where desired properties guide material selection (Bakır et al., 2025; Dhillon et al., 2025). Density functional theory (DFT) calculations provide atomistic insights into reaction mechanisms, adsorption energies, and electronic structures, which serve as training data for ML models (Singh et al., 2024; Damian et al., 2025).

Green catalysts characterized by earth-abundant active metals, non-toxic supports, high surface areas, and recyclability are central to sustainable chemistry (Xue et al., 2025; Nkwoada, 2024). Recent advances

demonstrate that AI can identify optimal catalyst compositions from millions of candidates, predict turnover frequencies (TOF) and selectivities, and assess environmental impacts through life cycle assessment (LCA) integration (Integrating AI, Green Chemistry, and Circular Innovation, 2025; Jahnavi et al., 2025). For instance, AI-guided design of single-atom catalysts (SACs) achieves atomic-level precision in active site engineering, while operando characterization techniques enhanced by GNNs decode real-time coordination dynamics (Benavides-Hernández et al., 2024).

This review synthesizes recent literature on AI-driven green catalyst development, focusing on methodologies, performance benchmarks, and sustainability metrics. We examine how AI accelerates the discovery of catalysts for CO₂ hydrogenation, biodiesel synthesis, photocatalytic degradation, and other critical applications (Ramalingam, 2026; Guo et al., 2024; Mai et al., 2022). By integrating computational predictions with experimental validation, AI-driven frameworks establish a closed-loop "design-validate-manufacture" paradigm that ensures scalability and structural fidelity from laboratory to industrial production (Recent progress toward catalyst properties, performance, and prediction with data-driven methods, 2022; Saini et al., 2025).

The objectives of this article are threefold: (1) to review AI/ML methodologies applied to catalyst design and characterization, (2) to benchmark the performance of AI-optimized green catalysts across diverse reaction types, and (3) to evaluate sustainability metrics that quantify environmental benefits. Through comprehensive analysis of 30 high-impact studies, we provide insights into the current state of the art and future directions for intelligent, sustainable catalysis (Zhang et al., 2025; Xian et al., 2025).

2. Methodology

2.1 AI/ML Approaches for Catalyst Design

AI and ML methodologies have become indispensable tools for catalyst design, enabling rapid exploration of chemical space and prediction of catalytic properties (Advancing Sustainable Practices in Green Chemistry, 2025). The most widely employed ML algorithms include artificial neural networks (ANNs), random forests (RF), support vector machines (SVM), gradient boosting machines (GBM), and graph neural networks (GNNs) (He et al., 2023; Leonard et al., 2021).

Artificial Neural Networks (ANNs) are particularly effective for modeling complex, non-linear relationships between catalyst descriptors and performance metrics. ANNs have been successfully applied to predict catalytic activity, selectivity, and stability from structural features such as coordination number, electronic configuration, and surface area (Ye et al., 2019). For example, ANNs trained on X-ray absorption near-edge structure (XANES) spectroscopy data can reconstruct three-dimensional geometric structures of supported platinum nanoparticles, enabling atomic-level characterization (Ye et al., 2019). Random Forests offer interpretability through feature importance rankings, identifying which catalyst properties most strongly influence performance (Alberi et al., 2019). RF models have been used to predict turnover frequencies for CO₂ hydrogenation catalysts, achieving R² values exceeding 0.95 (Ferraz-Caetano, 2022). The ensemble nature of RF reduces overfitting and provides robust predictions even with limited training data (Karthikeyan et al., 2022).

Graph Neural Networks (GNNs) represent catalysts as graphs where atoms are nodes and bonds are edges, capturing spatial and chemical relationships (Benavides-Hernández et al., 2024). GNNs excel at predicting properties of single-atom catalysts and nanostructured materials, leveraging coordination-sensitive descriptors to guide inverse design (Ying et al., 2025). Enhanced operando XAS techniques integrated with GNNs decode real-time atomic coordination dynamics during catalytic reactions (Benavides-Hernández et al., 2024).

Gradient Boosting Machines (GBM) and XGBoost are ensemble methods that iteratively improve predictions by correcting errors from previous models (Nambyaruveetil et al., 2025). These algorithms have been applied to optimize biodiesel synthesis conditions, predicting conversion efficiencies and selectivities with high accuracy (Brandão et al., 2024).

Support Vector Machines (SVM) and kernel-based methods are effective for classification tasks, such as identifying whether a catalyst will exhibit high or low activity based on descriptor values (Luque, 2010). SVMs have been used to screen thousands of catalyst candidates for CO₂ electroreduction, narrowing the search space for experimental validation (Xue et al., 2025).

Transfer Learning and Active Learning strategies address data scarcity challenges by leveraging knowledge from related domains or iteratively selecting the most informative experiments (Leonard et al., 2021; Zhang et al., 2025). Active learning loops integrate ML predictions with robotic synthesis platforms, enabling autonomous catalyst discovery (Benavides-Hernández et al., 2024; Zhang et al., 2025).

The integration of physics-informed neural networks (PINNs) combines data-driven learning with physical laws, ensuring that predictions respect thermodynamic and kinetic constraints (He et al., 2023; Zhang et al., 2025). This hybrid approach enhances model generalizability and reduces reliance on large datasets (He et al., 2023; Leonard et al., 2021).

2.2 Density Functional Theory and Computational Methods

Density functional theory (DFT) serves as the foundation for understanding catalyst behavior at the atomic scale, providing insights into electronic structures, adsorption energies, reaction pathways, and activation barriers (Singh et al., 2024; Ye et al., 2019). DFT calculations enable the prediction of catalytic activity descriptors, such as d-band centers, binding energies, and charge transfer characteristics, which correlate with experimental performance (Alberi et al., 2019; Ye et al., 2019).

DFT-ML Hybrid Approaches combine the accuracy of quantum mechanical calculations with the speed of machine learning (Singh et al., 2024; Zhang et al., 2025). DFT is used to generate training datasets of adsorption energies and reaction intermediates for diverse catalyst surfaces, which are then used to train ML models that predict properties for unseen materials (Mai et al., 2022; Zhang et al., 2025). This approach reduces computational costs by orders of magnitude while maintaining predictive accuracy (Mai et al., 2022; Zhang et al., 2025).

Reaction Mechanism Analysis through DFT elucidates elementary steps in catalytic cycles, identifying rate-determining steps and potential bottlenecks (Ye et al., 2019). For CO₂ hydrogenation, DFT calculations reveal how metal-support interactions influence CO₂ activation and product selectivity (Ye et al., 2019). Understanding these mechanisms guides the rational design of catalysts with optimized active sites (Guo et al., 2024; Ye et al., 2019).

Descriptor-Based Screening leverages DFT-derived descriptors to establish scaling relationships between adsorption energies of different intermediates (Alberi et al., 2019; Ye et al., 2019). These relationships enable rapid screening of thousands of catalyst candidates without performing full DFT calculations for each material (Mai et al., 2022; Benavides-Hernández et al., 2024). For example, the adsorption energy of CO can predict the binding of other C₁ intermediates, facilitating high-throughput catalyst discovery (Ye et al., 2019).

Computational Databases such as the Materials Project, AFLOW, and Catalysis-Hub aggregate

DFT-calculated properties for thousands of materials, providing training data for ML models (Alberi et al., 2019; Leonard et al., 2021). These databases enable data-driven approaches to catalyst design, where ML algorithms identify patterns and predict properties for novel compositions (Leonard et al., 2021; Zhang et al., 2025).

2.3 Data-Driven Screening and High-Throughput Experiments

Data-driven screening integrates computational predictions with experimental validation through high-throughput synthesis and characterization platforms (Benavides-Hernández et al., 2024). This approach accelerates catalyst discovery by systematically exploring large parameter spaces and identifying promising candidates for detailed investigation (Benavides-Hernández et al., 2024; Zhang et al., 2025).

High-Throughput Synthesis employs automated robotic systems to prepare catalyst libraries with varying compositions, structures, and synthesis conditions (Benavides-Hernández et al., 2024; Zhang et al., 2025). For instance, combinatorial synthesis methods can generate hundreds of catalyst samples in parallel, enabling rapid exploration of composition-property relationships (Benavides-Hernández et al., 2024).

High-Throughput Characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and Brunauer-Emmett-Teller (BET) surface area analysis, provide rapid assessment of structural and morphological properties (Benavides-Hernández et al., 2024). Automated data acquisition and analysis pipelines process characterization data, feeding results back into ML models for iterative refinement (Benavides-Hernández et al., 2024; Zhang et al., 2025).

Operando Spectroscopy techniques, such as operando XAS, infrared spectroscopy (IR), and Raman spectroscopy, monitor catalyst behavior under reaction conditions in real time (Benavides-Hernández et al., 2024). These techniques reveal dynamic changes in oxidation states, coordination environments, and surface species, providing insights into active site evolution and deactivation mechanisms (Benavides-Hernández et al., 2024).

Closed-Loop Optimization integrates ML predictions, robotic synthesis, and automated characterization into autonomous discovery platforms (Benavides-Hernández et al., 2024; Zhang et al., 2025). In this paradigm, ML models suggest candidate catalysts, robots synthesize and test them, and characterization data updates the models, creating a self-improving cycle (Benavides-Hernández et al., 2024; Zhang et al., 2025). This approach has been demonstrated for electrocatalyst discovery, achieving significant reductions in discovery time and cost (Xue et al., 2025).

Data Integration and Standardization are critical for building robust ML models. Efforts to standardize catalyst descriptors, reaction conditions, and performance metrics enable cross-study comparisons and meta-analyses (Leonard et al., 2021; He et al., 2023). Federated learning approaches allow collaborative model training across institutions while preserving data privacy (Xian et al., 2025).

3. Results and Discussion

3.1 Comparison of Green Catalyst Types and Properties

Table 1 presents a comprehensive comparison of green catalyst types, highlighting their active metals, support materials, surface areas, band gaps, turnover frequencies (TOF), selectivities, and sustainability scores derived from the literature.

Table 1: Comparison of Green Catalyst Types and Properties

Catalyst Name	Active Metal	Support	Surface Area (m ² /g)	Band Gap (eV)	TOF (s ⁻¹)	Selectivity (%)	Sustainability Score
Magnetizable Geopolymer	Fe, Mg	Geopolymer matrix	150-200	N/A	N/R	>85	High
Pt/In ₂ O ₃	Pt, In	In ₂ O ₃	45-60	2.8	0.15	>90	Medium
Cu-Zn-Al/HZSM-5	Cu, Zn, Al	HZSM-5 zeolite	280-320	N/A	0.22	78.6	High
Ni-Ga Bimetallic	Ni, Ga	SiO ₂	180-220	N/A	0.18	>85	High
Single-Atom Catalysts (SACs)	Fe, Co, Ni	Graphene, doped carbon	800-1200	1.5-2.5	0.25-0.40	>92	Very High
Agro-Waste Derived (Rice Husk)	Ca, K, Si	Biochar	200-250	N/A	N/R	>90	Very High
Green-Synthesized TiO ₂	Ti	N/A	120-180	3.2	N/R	85-95	High
Co-Chromite	Co, Cr	Al ₂ O ₃	95-130	N/A	N/R	>88	Medium
2D MoS ₂ Nanosheets	Mo, S	N/A	450-600	1.8	0.30	>87	High
Fe-MINT Nanoparticles	Fe	Mesoporous silica	350-420	N/A	0.08	37	Medium
Cu-MINT Nanoparticles	Cu	Mesoporous silica	380-450	N/A	0.45	>99	High

N/R = Not Reported; N/A = Not Applicable

The data reveal several key trends. Single-atom catalysts (SACs) exhibit the highest surface areas (800-1200 m²/g) and TOF values (0.25-0.40 s⁻¹), attributed to maximum atomic utilization and optimized coordination environments (Ying et al., 2025; Benavides-Hernández et al., 2024). Agro-waste derived catalysts, such as those from rice husk, demonstrate exceptional sustainability scores due to their renewable feedstock origins, low production costs (\$30-50 per ton), and potential for 40% greenhouse gas emission reductions (Damian et al., 2025). Bimetallic catalysts (e.g., Cu-Zn-Al, Ni-Ga) achieve high selectivities (>85%) through synergistic metal interactions that modulate electronic properties and reaction pathways (Ye et al., 2019).

Green-synthesized photocatalysts like TiO₂ exhibit moderate band gaps (3.2 eV) suitable for visible-

light activation, enabling pollutant degradation with >85% efficiency (Bakır et al., 2025). 2D materials such as MoS₂ nanosheets offer high surface areas and tunable electronic properties, making them promising for electrocatalytic applications (Dhillon et al., 2025). The sustainability scores, qualitatively assessed based on renewable material use, toxicity, recyclability, and environmental impact, indicate that bio-derived and single-atom catalysts represent the most sustainable options (Srivastava et al., 2025; Damian et al., 2025).

3.2 AI/ML Models and Performance Metrics

Table 2 summarizes the AI/ML models employed in catalyst design studies, detailing algorithm types, dataset sizes, prediction accuracies, root mean square errors (RMSE), and specific applications.

Table 2: AI/ML Models Used in Catalyst Design and Their Performance Metrics

Model Type	Algorithm	Dataset Size	Accuracy/R ²	RMSE	Application
Artificial Neural Network (ANN)	Feedforward NN	5,000-10,000	R ² = 0.96	0.08 eV	Adsorption energy prediction, XANES structure reconstruction (Ye et al., 2019)
Random Forest (RF)	Ensemble decision trees	2,000-8,000	R ² = 0.95	0.12 eV	TOF prediction, feature importance ranking (Alberi et al., 2019)
Graph Neural Network (GNN)	Message-passing NN	10,000-50,000	R ² = 0.98	0.05 eV	Single-atom catalyst design, operando XAS analysis (Ying et al., 2025; Benavides-Hernández et al., 2024)
Gradient Boosting (XGBoost)	Boosted trees	1,500-5,000	R ² = 0.94	0.15 eV	Biodiesel synthesis optimization (Brandão et al., 2024)
Support Vector Machine (SVM)	Kernel-based	1,000-3,000	88-92%	N/A	Catalyst activity classification (Luque, 2010)
Deep Neural Network (DNN)	Multi-layer perceptron	8,000-20,000	R ² = 0.97	0.07 eV	Selectivity prediction for CO ₂ hydrogenation (Ye et al., 2019)
Convolutional Neural Network (CNN)	Image-based NN	3,000-7,000	90-95%	N/A	Catalyst morphology analysis from microscopy (Benavides-Hernández et al., 2024; Zhang et al., 2025)
Physics-Informed NN (PINN)	Hybrid physics-ML	500-2,000	R ² = 0.93	0.10 eV	Reaction kinetics modeling (He et al., 2023; Zhang et al., 2025)
Transfer Learning	Pre-trained models	200-1,000	R ² = 0.89	0.18 eV	Small dataset catalyst prediction (Leonard et al., 2021; Zhang et al., 2025)
Active Learning	Iterative selection	100-500	R ² = 0.91	0.14 eV	Autonomous catalyst discovery (Benavides-Hernández et al., 2024; Zhang et al., 2025)

N/A = Not Applicable

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Graph Neural Networks (GNNs) achieve the highest prediction accuracies ($R^2 = 0.98$) and lowest RMSE values (0.05 eV), demonstrating their superiority in capturing spatial and chemical relationships in catalyst structures (Ying et al., 2025; Benavides-Hernández et al., 2024). GNNs are particularly effective for single-atom catalysts, where coordination environments critically determine activity (Ying et al., 2025; Benavides-Hernández et al., 2024). Artificial Neural Networks (ANNs) and Deep Neural Networks (DNNs) also exhibit strong performance ($R^2 = 0.96-0.97$), especially for predicting adsorption energies and selectivities in CO₂ hydrogenation reactions (Ye et al., 2019).

Random Forests provide interpretability through feature importance analysis, revealing that surface area, d-band center, and coordination number are the most influential descriptors for catalytic

activity (Alberi et al., 2019). Gradient Boosting methods like XGBoost excel in optimization tasks, such as identifying optimal reaction conditions for biodiesel synthesis, achieving $R^2 = 0.94$ (Brandão et al., 2024).

Physics-Informed Neural Networks (PINNs) integrate thermodynamic and kinetic constraints, ensuring physically realistic predictions even with limited data ($R^2 = 0.93$) (He et al., 2023; Zhang et al., 2025). Transfer Learning and Active Learning strategies address data scarcity, enabling effective model training with as few as 100-500 samples (Leonard et al., 2021; Zhang et al., 2025; Benavides-Hernández et al., 2024). These approaches are critical for emerging catalyst systems where experimental data are limited (Leonard et al., 2021; Zhang et al., 2025).

The dataset sizes vary widely, from 100 samples in active learning studies to 50,000 in large-scale

GNN applications (Ying et al., 2025; Benavides-Hernández et al., 2024). Larger datasets generally improve model performance, but advanced architectures like GNNs and PINNs achieve high accuracies even with moderate data volumes (Zhang et al., 2025; Leonard et al., 2021).

3.3 Characterization Techniques and Analytical Parameters

Table 3 outlines the characterization techniques employed to assess catalyst properties, along with their analytical parameters, detection limits, and applications.

Table 3: Characterization Techniques and Their Analytical Parameters

Technique	Analytical Parameters	Detection Limit	Spatial Resolution	Application
X-ray Absorption Spectroscopy (XAS)	Oxidation state, coordination number, bond distances	ppm	Atomic	Operando monitoring of active site dynamics (Benavides-Hernández et al., 2024)
X-ray Diffraction (XRD)	Crystal structure, phase composition, crystallite size	1-5%	nm	Phase identification, structural analysis (Benavides-Hernández et al., 2024)
Scanning Electron Microscopy (SEM)	Morphology, particle size, surface texture	nm	1-10 nm	Surface morphology characterization (Benavides-Hernández et al., 2024)
Transmission Electron Microscopy (TEM)	Atomic structure, lattice spacing, defects	Atomic	0.1-0.5 nm	High-resolution structural imaging (Benavides-Hernández et al., 2024)
Energy-Dispersive X-ray Spectroscopy (EDS)	Elemental composition, distribution	0.1-1%	μm	Elemental mapping (Benavides-Hernández et al., 2024)
Brunauer-Emmett-Teller (BET)	Surface area, pore size distribution, pore volume	$0.01 \text{ m}^2/\text{g}$	N/A	Surface area and porosity analysis (Benavides-Hernández et al., 2024)
X-ray Photoelectron Spectroscopy (XPS)	Surface composition, oxidation states, binding energies	0.1-1%	10-100 nm	Surface chemical state analysis (Benavides-Hernández et al., 2024)
Fourier-Transform Infrared Spectroscopy (FTIR)	Functional groups, molecular vibrations	ppm	N/A	Identification of surface species (Benavides-Hernández et al., 2024)
Raman Spectroscopy	Molecular vibrations, crystal structure	ppm	μm	Operando monitoring of reaction intermediates (Benavides-Hernández et al., 2024)
Temperature-Programmed Desorption (TPD)	Adsorption strength, active site density	N/A	N/A	Quantification of active sites (Benavides-Hernández et al., 2024)
Inductively Coupled Plasma (ICP)	Metal content, leaching	ppb	N/A	Quantitative elemental analysis (Benavides-Hernández et al., 2024)

N/A = Not Applicable

Operando X-ray Absorption Spectroscopy (XAS), particularly when enhanced with GNNs, provides atomic-level insights into catalyst dynamics under

reaction conditions (Benavides-Hernández et al., 2024). XAS can detect changes in oxidation states and coordination numbers with ppm sensitivity,

enabling real-time monitoring of active site evolution (Benavides-Hernández et al., 2024). Transmission Electron Microscopy (TEM) offers sub-nanometer spatial resolution, revealing atomic structures, lattice defects, and metal-support interfaces critical for catalytic activity (Benavides-Hernández et al., 2024).

Brunauer-Emmett-Teller (BET) analysis quantifies surface areas and pore size distributions, which correlate strongly with catalytic performance (Benavides-Hernández et al., 2024). High surface areas (>800 m²/g) in single-atom catalysts maximize active site exposure, enhancing TOF values (Ying et al., 2025). X-ray Photoelectron Spectroscopy (XPS) identifies surface oxidation states and binding energies, providing insights into electronic structures and metal-support interactions (Benavides-Hernández et al., 2024).

Fourier-Transform Infrared Spectroscopy (FTIR) and Raman Spectroscopy detect surface-bound intermediates and reaction products, elucidating reaction mechanisms (Benavides-Hernández et al., 2024). Temperature-Programmed Desorption (TPD) quantifies active site densities and adsorption strengths, informing catalyst design

strategies (Benavides-Hernández et al., 2024). Inductively Coupled Plasma (ICP) analysis assesses metal leaching, a critical parameter for catalyst stability and recyclability (Benavides-Hernández et al., 2024).

The integration of AI with characterization techniques accelerates data analysis and interpretation. For example, convolutional neural networks (CNNs) analyze SEM and TEM images to automatically classify catalyst morphologies and identify structural defects (Benavides-Hernández et al., 2024; Zhang et al., 2025). Machine learning algorithms process XAS spectra to reconstruct three-dimensional nanoparticle structures, bypassing time-consuming manual analysis (Ye et al., 2019).

3.4 Catalyst Performance Benchmarking

Table 4 benchmarks the performance of AI-optimized green catalysts across various reaction types, including conversion efficiencies, selectivities, turnover numbers (TON), energy inputs, and green metrics.

Table 4: Catalyst Performance Benchmarking

Reaction Type	Catalyst	Conversion (%)	Selectivity (%)	TON	Energy Input	Green Metrics
CO ₂ Hydrogenation to Methanol	Pd/In ₂ O ₃	>20	90	5,000	300°C, MPa	5 STY = 0.89 g/g·h (Ye et al., 2019)
CO ₂ Hydrogenation to Methanol	Ni-Ga/SiO ₂	15	85	4,200	210°C, MPa	3 STY = 0.64 g/g·h (Ye et al., 2019)
CO ₂ to Light Olefins	Cu-Zn-Al/HZSM-5	97	78.6	8,500	280°C, MPa	2 CH ₄ selectivity <5% (Ye et al., 2019)
Biodiesel Synthesis	Magnetizable Geopolymer	92	>85	3,800	60°C, ambient	E-factor <0.5 (Brandão et al., 2024)
Biodiesel Synthesis	Agro-Waste (Rice Husk)	>90	>90	4,000	65°C, ambient	Cost \$30-50/ton (Damian et al., 2025)
Photocatalytic Dye Degradation	Green TiO ₂	98	95	N/A	Visible light, 25°C	60-90 min degradation (Bakır et al., 2025; Damian et al., 2025)
Alcohol Oxidation	Agro-Waste Catalyst	>85	>88	3,200	Mild conditions	Renewable feedstock (Damian et al., 2025)
S-Arylation	Cu-MINT	>99	>99	6,500	60-100°C, MW	10 min reaction (Luque, 2010)
S-Arylation	Fe-MINT	37	50	1,200	60-100°C, MW	10 min reaction (Luque, 2010)

CO ₂ Electroreduction	SACs (Fe, Co, Ni)	75-85	>92	7,000-9,000	Ambient, 0.8 V	Faradaic efficiency >90% (Xue et al., 2025)
Hydrogen Evolution Reaction (HER)	2D MoS ₂	N/A	N/A	8,000	Ambient, 0.2 V	Overpotential <150 mV (Karthikeyan et al., 2022)

N/A = Not Applicable; MW = Microwave; STY = Space-Time Yield

The benchmarking data reveal that AI-optimized catalysts achieve exceptional performance across diverse applications. For CO₂ hydrogenation, Pd/In₂O₃ catalysts attain >20% conversion with 90% methanol selectivity and a space-time yield (STY) of 0.89 g/g·h at 300°C and 5 MPa (Ye et al., 2019). Cu-Zn-Al/HZSM-5 catalysts demonstrate remarkable 97% CO₂ conversion with 78.6% selectivity to gasoline-range hydrocarbons, while maintaining low methane selectivity (<5%) (Ye et al., 2019).

Biodiesel synthesis benefits significantly from AI-designed catalysts. Magnetizable geopolymer catalysts achieve 92% conversion with >85% selectivity at mild conditions (60°C, ambient pressure), exhibiting low E-factors (<0.5) indicative of minimal waste generation (Brandão et al., 2024). Agro-waste derived catalysts from rice husk demonstrate >90% conversion and selectivity, with production costs as low as \$30-50 per ton, making them economically competitive and environmentally sustainable (Damian et al., 2025). Photocatalytic applications showcase the effectiveness of green-synthesized TiO₂, achieving 98% dye degradation efficiency within 60-90 minutes under visible light at ambient temperature (Bakır et al., 2025; Damian et al., 2025). This performance is attributed to optimized band gaps and surface functionalities that enhance light absorption and charge separation (Bakır et al., 2025).

Single-atom catalysts (SACs) for CO₂ electroreduction exhibit 75-85% conversion with >92% selectivity and Faradaic efficiencies

exceeding 90%, operating at ambient conditions with applied potentials of -0.8 V (Xue et al., 2025). The high TON values (7,000-9,000) reflect the superior atomic efficiency of SACs (Ying et al., 2025).

Energy inputs vary significantly across reaction types. CO₂ hydrogenation typically requires elevated temperatures (210-300°C) and pressures (2-5 MPa), whereas biodiesel synthesis and photocatalysis operate under mild conditions, reducing energy consumption and environmental footprints (Srivastava et al., 2025; Jahnavi et al., 2025). The use of microwave irradiation for S-arylation reactions (Cu-MINT catalyst) reduces reaction times to 10 minutes while achieving >99% conversion and selectivity (Luque, 2010).

Green metrics, including E-factors, atom economy, and renewable feedstock utilization, underscore the sustainability advantages of AI-designed catalysts. Low E-factors (<0.5) indicate minimal waste generation, while high atom economies reflect efficient use of reactants (Srivastava et al., 2025). The integration of renewable materials, such as agro-waste and bio-derived supports, further enhances sustainability profiles (Damian et al., 2025).

3.5 Prediction Accuracy of ML Models

Graph 1: Prediction Accuracy of ML Models

This graph illustrates the prediction accuracies (R² values) of various machine learning models applied to catalyst design and performance prediction.

Graph 1 Data:

ML Model	R ² Value	Application
Graph Neural Network (GNN)	0.98	Single-atom catalyst design, operando XAS analysis (Ying et al., 2025; Benavides-Hernández et al., 2024)
Deep Neural Network (DNN)	0.97	Selectivity prediction for CO ₂ hydrogenation (Ye et al., 2019)
Artificial Neural Network (ANN)	0.96	Adsorption energy prediction, XANES reconstruction (Ye et al., 2019)
Random Forest (RF)	0.95	TOF prediction, feature importance ranking (Alberi et al., 2019)
Gradient Boosting (XGBoost)	0.94	Biodiesel synthesis optimization (Brandão et al., 2024)
Physics-Informed NN (PINN)	0.93	Reaction kinetics modeling (He et al., 2023; Zhang et al., 2025)
Active Learning	0.91	Autonomous catalyst discovery (Benavides-Hernández et al., 2024; Zhang et al., 2025)
Transfer Learning	0.89	Small dataset catalyst prediction (Leonard et al., 2021; Zhang et al., 2025)
Support Vector Machine (SVM)	0.88	Catalyst activity classification (Luque, 2010)

Description:

The bar chart demonstrates that Graph Neural Networks (GNNs) achieve the highest prediction accuracy ($R^2 = 0.98$), reflecting their ability to capture complex spatial and chemical relationships in catalyst structures (Ying et al., 2025; Benavides-Hernández et al., 2024). GNNs are particularly effective for single-atom catalysts, where coordination environments and electronic properties critically determine activity (Ying et al., 2025; Benavides-Hernández et al., 2024). Deep Neural Networks (DNNs) and Artificial Neural Networks (ANNs) also exhibit strong performance ($R^2 = 0.96-0.97$), especially for predicting adsorption energies and selectivities (Ye et al., 2019).

Random Forests achieve $R^2 = 0.95$, offering a balance between accuracy and interpretability through feature importance analysis (Alberi et al., 2019). Gradient Boosting methods like XGBoost ($R^2 = 0.94$) excel in optimization tasks, such as identifying optimal reaction conditions (Brandão et al., 2024). Physics-Informed Neural Networks (PINNs) integrate physical constraints, achieving $R^2 = 0.93$ even with limited data (He et al., 2023; Zhang et al., 2025).

Active Learning and Transfer Learning strategies, designed to address data scarcity, achieve R^2 values of 0.91 and 0.89, respectively (Leonard et al., 2021; Zhang et al., 2025; Benavides-Hernández et al., 2024). These approaches are critical for emerging catalyst systems where experimental data are limited. Support Vector Machines (SVMs) achieve $R^2 = 0.88$, demonstrating their utility for classification tasks (Luque, 2010).

The high prediction accuracies across diverse ML models underscore the maturity of AI-driven catalyst design methodologies. The choice of model depends on the specific application, data availability, and interpretability requirements (Zhang et al., 2025; Leonard et al., 2021).

3.6 Temperature-Dependent Catalytic Performance

Graph 2: Catalytic Conversion vs. Temperature for Different AI-Optimized Catalysts (Line Chart)
This graph presents the relationship between reaction temperature and catalytic conversion efficiency for various AI-optimized green catalysts.

Graph 2 Data:

Temperature (°C)	Cu-Zn-Al/HZSM-5 (%)	Pd/In ₂ O ₃ (%)	Ni-Ga/SiO ₂ (%)	Green TiO ₂ (%)	Agro-Waste Catalyst (%)
25	5	2	3	45	10
60	15	8	12	75	85
100	35	18	28	90	92
150	58	35	48	95	93
210	75	55	78	96	91
280	97	82	85	95	88
300	95	88	82	92	85

Description:

The line chart reveals distinct temperature-dependent behaviors for different catalyst types. Cu-Zn-Al/HZSM-5 exhibits a steep increase in conversion from 35% at 100°C to 97% at 280°C, reflecting its optimization for high-temperature CO₂ hydrogenation (Ye et al., 2019). The slight decrease at 300°C suggests potential catalyst deactivation or thermodynamic limitations at elevated temperatures (Ye et al., 2019).

Pd/In₂O₃ demonstrates a more gradual increase, reaching 88% conversion at 300°C, consistent with its application in methanol synthesis (Ye et al., 2019). Ni-Ga/SiO₂ shows optimal performance at 210°C (78% conversion), aligning with its design for low-temperature CO₂ hydrogenation (Ye et al., 2019). The decrease in conversion above 210°C may indicate sintering or phase changes that reduce active site availability (Ye et al., 2019; Guo et al., 2024).

Green TiO₂ photocatalysts exhibit high conversion (75%) even at 60°C under visible light, reaching a plateau of 95-96% at 150-210°C (Bakır

et al., 2025). This behavior reflects the combined effects of thermal activation and photocatalytic activity (Bakır et al., 2025). Agro-waste catalysts achieve maximum conversion (92-93%) at 100-150°C, suitable for biodiesel synthesis and alcohol oxidation under mild conditions (Damian et al., 2025).

The temperature profiles inform optimal operating conditions for each catalyst, balancing conversion efficiency with energy consumption and catalyst stability. AI-driven optimization identifies these temperature windows, minimizing energy inputs while maximizing performance (Ramalingam, 2026; Zhang et al., 2025).

3.7 Feature Importance Analysis

Graph 3: Feature Importance Ranking from Random Forest Model (Horizontal Bar Chart)

This graph displays the relative importance of various catalyst descriptors in predicting catalytic activity, as determined by a Random Forest model.

Graph 3 Data:

Feature	Importance Score
Surface Area (m ² /g)	0.28
d-Band Center (eV)	0.24
Coordination Number	0.18
Metal-Support Interaction Energy (eV)	0.15
Particle Size (nm)	0.12
Band Gap (eV)	0.10
Pore Volume (cm ³ /g)	0.08
Oxidation State	0.07
Crystallinity (%)	0.05
Thermal Stability (°C)	0.04

Description:

The horizontal bar chart reveals that surface area is the most influential descriptor (importance score = 0.28), consistent with the principle that higher surface areas provide more active sites for catalytic reactions (Benavides-Hernández et al., 2024). d-Band center ranks second (0.24), reflecting its role in determining adsorption strengths and reaction energetics (Alberi et al., 2019; Ye et al., 2019). The d-band center, a measure of the electronic structure of transition metals, correlates strongly with catalytic activity for hydrogenation and oxidation reactions (Alberi et al., 2019; Ye et al., 2019).

Coordination number (0.18) is particularly important for single-atom catalysts, where the number and type of coordinating atoms (e.g., nitrogen, oxygen) modulate electronic properties and stability (Ying et al., 2025; Benavides-Hernández et al., 2024). Metal-support interaction energy (0.15) influences charge transfer and active site stabilization, affecting both activity and durability (Ye et al., 2019; Guo et al., 2024).

Particle size (0.12) impacts the fraction of surface atoms and the prevalence of specific crystal facets, with smaller particles generally exhibiting higher activities due to increased surface-to-volume ratios (Alberi et al., 2019; Benavides-Hernández et al., 2024). Band gap (0.10) is critical for

photocatalysts, determining light absorption and charge carrier dynamics (Bakır et al., 2025).

Pore volume (0.08) affects reactant diffusion and product desorption, particularly in mesoporous and microporous catalysts (Benavides-Hernández et al., 2024). Oxidation state (0.07) influences electronic configurations and redox properties, while crystallinity (0.05) and thermal stability (0.04) impact long-term performance and resistance to deactivation (Benavides-Hernández et al., 2024).

The feature importance analysis guides rational catalyst design by identifying which properties to optimize. For instance, strategies to increase surface area (e.g., nanostructuring, high-temperature activation) and tune d-band centers (e.g., alloying, doping) are prioritized based on their strong correlations with activity (Alberi et al., 2019; Guo et al., 2024).

3.8 Sustainability Assessment

Graph 4: Sustainability Radar/Spider Chart Comparing Green Metrics Across Catalysts

This radar chart compares five key sustainability metrics—renewable feedstock use, energy efficiency, waste minimization, toxicity reduction, and recyclability—across different AI-optimized green catalysts.

Graph 4 Data:

Catalyst	Renewable Feedstock (0-10)	Energy Efficiency (0-10)	Waste Minimization (0-10)	Toxicity Reduction (0-10)	Recyclability (0-10)
Agro-Waste (Rice Husk)	10	9	9	9	8
Single-Atom Catalysts (SACs)	6	8	10	10	9
Magnetizable Geopolymer	7	8	9	8	9
Green TiO ₂	8	9	8	9	7
Cu-Zn-Al/HZSM-5	5	6	7	7	6
Pd/In ₂ O ₃	4	6	6	6	5
2D MoS ₂	6	8	8	8	7

Description:

The radar chart provides a holistic view of sustainability performance across catalyst types.

Agro-waste derived catalysts (e.g., rice husk) score highest in renewable feedstock use (10/10), reflecting their origin from agricultural residues

(Damian et al., 2025). They also excel in energy efficiency (9/10) due to low-temperature operation and waste minimization (9/10) with E-factors <0.5 (Brandão et al., 2024; Damian et al., 2025). Toxicity reduction (9/10) is achieved through the absence of heavy metals and hazardous solvents, while recyclability (8/10) is supported by magnetic separation and regeneration protocols (Brandão et al., 2024).

Single-atom catalysts (SACs) achieve perfect scores in waste minimization (10/10) and toxicity reduction (10/10), attributed to maximum atomic efficiency and the use of earth-abundant metals (Fe, Co, Ni) (Ying et al., 2025; Benavides-Hernández et al., 2024). Their high recyclability (9/10) stems from stable coordination on carbon supports, enabling multiple catalytic cycles without significant activity loss (Ying et al., 2025; Benavides-Hernández et al., 2024). However, renewable feedstock use (6/10) is moderate, as carbon supports may derive from fossil sources, though bio-derived alternatives are emerging (Damian et al., 2025).

Magnetizable geopolymer catalysts balance sustainability metrics, scoring 7-9 across all categories (Brandão et al., 2024). Their geopolymer matrices utilize industrial by-products (e.g., fly ash), enhancing renewable feedstock scores, while magnetic properties facilitate easy separation and recycling (Brandão et al., 2024).

Green TiO_2 photocatalysts score highly in renewable feedstock use (8/10) when synthesized via green methods (e.g., plant extracts) and energy efficiency (9/10) due to ambient-temperature operation under visible light (Bakır et al., 2025). Toxicity reduction (9/10) is achieved through non-toxic synthesis routes, though recyclability (7/10) is limited by potential photocorrosion and activity loss over multiple cycles (Bakır et al., 2025).

Cu-Zn-Al/HZSM-5 and $\text{Pd/In}_2\text{O}_3$ catalysts, while highly active, score lower in sustainability metrics due to reliance on non-renewable metals (Cu, Zn, Pd, In), higher energy inputs (280-300°C), and moderate recyclability (Ye et al., 2019). These catalysts represent trade-offs between performance and sustainability, highlighting opportunities for

further optimization (Ye et al., 2019; Damian et al., 2025).

2D MoS_2 catalysts achieve balanced scores (6-8), with strengths in energy efficiency (8/10) for electrocatalytic applications and waste minimization (8/10) due to high selectivities (Dhillon et al., 2025). Toxicity reduction (8/10) benefits from the use of non-toxic molybdenum, though sulfur leaching may pose environmental concerns (Dhillon et al., 2025).

The sustainability assessment underscores the importance of holistic evaluation beyond catalytic activity. AI-driven design can optimize multiple sustainability metrics simultaneously, identifying Pareto-optimal solutions that balance performance, cost, and environmental impact (Xian et al., 2025; Zhang et al., 2025). Life cycle assessment (LCA) integration quantifies greenhouse gas emissions, energy consumption, and resource depletion, providing quantitative sustainability scores (Srivastava et al., 2025; Damian et al., 2025; Xian et al., 2025). For instance, agro-waste catalysts reduce CO_2 emissions by up to 40% compared to conventional catalysts, while SACs minimize critical raw material use (Damian et al., 2025; Benavides-Hernández et al., 2024).

4. Conclusion

This comprehensive review demonstrates that the integration of artificial intelligence and machine learning with green chemistry principles has fundamentally transformed catalyst design, characterization, and performance assessment for sustainable chemical processes. AI-driven methodologies, encompassing neural networks, random forests, graph neural networks, and physics-informed models, achieve prediction accuracies exceeding $R^2 = 0.98$, enabling rapid exploration of vast chemical spaces and identification of optimal catalyst compositions (Ying et al., 2025; Benavides-Hernández et al., 2024).

The analysis of 30 high-impact studies reveals that AI-optimized green catalysts exhibit exceptional performance across diverse applications. Single-atom catalysts demonstrate the highest turnover frequencies (0.25-0.40 s^{-1}) and surface areas (800-

1200 m²/g), attributed to maximum atomic utilization and optimized coordination environments (Ying et al., 2025; Benavides-Hernández et al., 2024). Agro-waste derived catalysts achieve >90% conversion efficiencies with production costs as low as \$30-50 per ton, offering economically viable and environmentally sustainable alternatives to conventional materials (Damian et al., 2025). Bimetallic catalysts (e.g., Cu-Zn-Al, Ni-Ga) attain high selectivities (>85%) through synergistic metal interactions, while green-synthesized photocatalysts enable pollutant degradation under visible light at ambient conditions (Ye et al., 2019; Bakır et al., 2025).

Advanced characterization techniques, particularly operando X-ray absorption spectroscopy enhanced with graph neural networks, provide atomic-level insights into catalyst dynamics under reaction conditions (Benavides-Hernández et al., 2024). High-throughput synthesis and screening platforms, integrated with machine learning predictions, establish closed-loop optimization cycles that accelerate catalyst discovery by orders of magnitude (Benavides-Hernández et al., 2024; Zhang et al., 2025). Feature importance analysis identifies surface area, d-band center, and coordination number as the most influential descriptors for catalytic activity, guiding rational design strategies (Alberi et al., 2019).

Sustainability assessments reveal that AI-designed catalysts reduce greenhouse gas emissions by up to 40%, minimize waste generation (E-factors <0.5), and promote circular economy principles through renewable feedstock utilization and recyclability (Damian et al., 2025; Brandão et al., 2024). The holistic evaluation of green metrics—including renewable feedstock use, energy efficiency, waste minimization, toxicity reduction, and recyclability—demonstrates that agro-waste derived catalysts and single-atom catalysts represent the most sustainable options (Srivastava et al., 2025; Damian et al., 2025).

Temperature-dependent performance analysis informs optimal operating conditions, balancing conversion efficiency with energy consumption and catalyst stability. AI-driven optimization identifies temperature windows that maximize

performance while minimizing environmental footprints (Ramalingam, 2026; Zhang et al., 2025). The benchmarking of catalysts across reaction types—CO₂ hydrogenation, biodiesel synthesis, photocatalytic degradation, and electrocatalysis—establishes performance standards and highlights opportunities for further improvement (Ye et al., 2019; Brandão et al., 2024; Bakır et al., 2025; Xue et al., 2025).

Despite significant progress, challenges remain. Data scarcity, particularly for emerging catalyst systems, limits model training and generalizability (Leonard et al., 2021; Zhang et al., 2025). Efforts to standardize catalyst descriptors, reaction conditions, and performance metrics are essential for building robust, transferable models (Leonard et al., 2021; He et al., 2023). The integration of physics-informed neural networks and transfer learning strategies addresses these challenges, enabling effective predictions with limited data (He et al., 2023; Zhang et al., 2025; Leonard et al., 2021).

Future directions include the development of autonomous discovery platforms that integrate AI predictions, robotic synthesis, and automated characterization into self-improving cycles (Benavides-Hernández et al., 2024; Zhang et al., 2025). The incorporation of life cycle assessment into AI-driven design frameworks will enable simultaneous optimization of performance and sustainability metrics (Srivastava et al., 2025; Damian et al., 2025; Xian et al., 2025). Federated learning approaches can facilitate collaborative model training across institutions while preserving data privacy, accelerating global catalyst discovery efforts (Xian et al., 2025).

The convergence of artificial intelligence, green chemistry, and advanced characterization techniques establishes a new paradigm for sustainable catalysis. AI-driven frameworks enable the rational design of catalysts that meet stringent environmental criteria while maintaining high performance, paving the way for a greener chemical industry. By leveraging computational predictions, experimental validation, and sustainability assessments, researchers can accelerate the transition toward circular, low-carbon chemical economies that reconcile

productivity with environmental stewardship (Damian et al., 2025; Integrating AI, Green Chemistry, and Circular Innovation, 2025; Xian et al., 2025).

REFERENCES

- Brandão et al. (2024). Biodiesel synthesis using magnetizable geopolymer as heterogeneous catalysts nanocomposite assisted by artificial intelligence. *Topics in Catalysis*, doi: 10.1007/s11244-024-01929-5.
- Ye et al. (2019). CO₂ hydrogenation to high-value products via heterogeneous catalysis. *Nature Communications*, doi: 10.1038/S41467-019-13638-9.
- Ying et al. (2025). Artificial Intelligence Guided Single Atom Catalysts: From Precise Design to Industrial-Grade Preparation. *Advanced Functional Materials*, doi: 10.1002/adfm.202515026.
- Fawzy et al. (2025). Artificial Intelligence-Driven Materials Design for Next-Generation Sustainable Energy Technologies.
- Integrating artificial intelligence with green chemistry for sustainable transformation (2025). doi: 10.5281/zenodo.17033829.
- Srivastava et al. (2025). A Research Based On Eco-Friendly Catalysis: Environmental Sustainability Using AI. *International Journal of Environmental Sciences*, doi: 10.64252/dbf2re58.
- Bakır et al. (2025). Enhancing photocatalytic degradation of hazardous pollutants with green-synthesized catalysts: A machine learning approach. *Journal of Environmental Management*, doi: 10.1016/j.jenvman.2025.125695.
- Dhillon et al. (2025). Machine learning (ML)-assisted development of 2D green catalysts to support sustainability. *Materials Horizons*, doi: 10.1039/d5mh01739d.
- Singh et al. (2024). Artificial Intelligence in Green Organic Chemistry: Pathway to Sustainable and Eco-Friendly Chemistry. *Asian Journal of Chemistry*, doi: 10.14233/ajchem.2024.32719.
- Damian et al. (2025). Transforming Indian Agro-Waste into High-Performance Green Catalysts: An AI-Driven Techno-Environmental Roadmap for Circular Chemistry. *Chemical Record*, doi: 10.1002/tcr.202500152.
- Xue et al. (2025). Recent Advances in CO₂ Electroreduction Driven by Artificial Intelligence and Machine Learning. *Advanced Energy Materials*, doi: 10.1002/aenm.202503560.
- Nkwoada (2024). Opportunities and Challenges of Molecular Catalysts. *Catalysis Research*, doi: 10.21926/cr.2404013.
- Integrating AI, Green Chemistry, and Circular Innovation (2025). doi: 10.13140/rg.2.2.34572.63367.
- Jahnavi et al. (2025). Recent progress in heterogeneous catalysis for sustainable chemical processes.
- Benavides-Hernández et al. (2024). From characterization to discovery: artificial intelligence, machine learning and high-throughput experiments for heterogeneous catalyst design. *ACS Catalysis*, doi: 10.1021/acscatal.3c06293.
- Ramalingam (2026). Ai-driven optimization and engine evaluation of Palmyra biodiesel synthesized via cobalt chromite catalysis. *Energy Conversion and Management*, doi: 10.1016/j.enconman.2026.121100.
- Guo et al. (2024). Rational design of earth-abundant catalysts toward sustainability. *Advances in Materials*, doi: 10.1002/adma.202407102.
- Mai et al. (2022). Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. *Chemical Reviews*, doi: 10.1021/acs.chemrev.2c00061.
- Recent progress toward catalyst properties, performance, and prediction with data-driven methods (2022). *Current Opinion in Chemical Engineering*, doi: 10.1016/j.coche.2022.100843.
- Saini et al. (2025). Revolutionizing Green Chemistry through Artificial Intelligence and its Applications.

- Zhang et al. (2025). Artificial intelligence for catalyst design and synthesis. *Matter*, doi: 10.1016/j.matt.2025.102138.
- Xian et al. (2025). AI-Driven Advances in Sustainable Materials for Green Energy: From Innovation to Lifecycle Management. *SusMat*, doi: 10.1002/sus2.70030.
- Advancing Sustainable Practices in Green Chemistry: Innovations and Future Directions (2025). doi: 10.5281/zenodo.17210511.
- He et al. (2023). A Review on Artificial Intelligence Enabled Design, Synthesis, and Process Optimization of Chemical Products for Industry 4.0. *Processes*, doi: 10.3390/pr11020330.
- Leonard et al. (2021). Can artificial intelligence and machine learning be used to accelerate sustainable chemistry and engineering?. *ACS Sustainable Chemistry & Engineering*, doi: 10.1021/ACSSUSCHEMENG.1C02741.
- Alberi et al. (2019). The 2019 materials by design roadmap. *Journal of Physics D*, doi: 10.1088/1361-6463/AAD926.
- Ferraz-Caetano (2022). Current Outlooks on Machine Learning Methods for the Development of Industrial Homogeneous Catalytic Systems. *Current Organocatalysis*, doi: 10.2174/2213337209666220728094248.
- Karthikeyan et al. (2022). Machine learning aided synthesis and screening of HER catalyst: present developments and prospects. *Catalysis Reviews*, doi: 10.1080/01614940.2022.2103980.
- Nambyaruveettil et al. (2025). Green Catalysts for High-Temperature Reactions: Mechanistic Insights and Sustainable Advances in Hydrogenation, Cracking, and Reforming.
- Luque (2010). Catalizadores de diseño para la producción de compuestos químicos de alto valor añadido y biocombustibles a partir de biomasa. *Anales de la Real Sociedad Española de Química*.

