A Research Based On Eco-Friendly Catalysis: Environmental Sustainability Using AI

[1]**Dr. Swati Srivastava,** [2]**Mr. Sonal Kumar,** [3]**Dr. Malarvizhi A,** [4]**Mr. Maddela Vasantha Kumar,** [5]**Dr. Balakarthikeyan M, Dr. R. Portia**[6]

[1]Associate Professor, School of Business Management, Noida International University Greater Noida, Uttar Pradesh, India, drswatianupamsrivastava@gmail.com

[2]Assistant Professor, School of Computer Science & Engineering, Sandeep University, Sijoul, Madhubani, Bihar, India, sonalkumarbgs@gmail.com

[3]Asst. Professor, Dept. of ECE, Vinayaka Mission's Kirupananda Variyar Engineering College (VMRF-DU), Salem, TN. malarvizhi@vmkvec.edu.in

[4]Department of Computer Science and Engineering-AIML, K. L .M. College of Engineering for Women Kadapa, Andhra Pradesh, India, dpm.kadapa@gmail.com

[5]Department of Mechatronics Engineering, Rajalakshmi Engineering College, Chennai, Tamil Nadu, India, balakarthikeyan.m@rajalakshmi.edu.in

Abstract

This research explores the integration of artificial intelligence to enhance eco-friendly catalysis for sustainable chemical processes. AI-driven modeling optimizes catalyst selection, reaction conditions, and energy utilization. The approach reduces harmful emissions, waste generation, and resource consumption. Life cycle assessment ensures environmental compliance and long-term sustainability. This study bridges green chemistry and AI to accelerate the transition toward cleaner industrial practices. Catalysis underpins modern chemical manufacturing, yet conventional catalytic routes often rely on toxic reagents, precious metals, hazardous solvents, and energy-intensive conditions that burden ecosystems. Eco-friendly catalysis—encompassing green homogeneous and heterogeneous catalysts, biocatalysts, photo/electrocatalysts, solvent-free and aqueous media, benign oxidants, and circular catalyst life cycles—offers a pathway to reconcile chemical productivity with environmental stewardship. This paper synthesizes principles from green chemistry and life-cycle thinking to define a research framework for developing and evaluating eco-friendly catalysts. We articulate metrics (atom economy, E-factor, process mass intensity, TON/TOF, energy intensity, water factor, and cradle-to-gate CO_2e), propose a multi-criteria decision analysis (MCDA) workflow that integrates techno-economic analysis (TEA) with ISO-aligned life-cycle assessment (LCA), and map these tools to four high-leverage application domains: renewable fuels and carbon valorization, plastics upcycling, fine-chemical/active pharmaceutical ingredient (API) synthesis, and wastewater treatment. Through design rules and illustrative case discussions (solid bases for biodiesel, Cu-based $CO_2 \rightarrow MeOH$, enzymatic amide formation, and visible-light photocatalysis for micropollutants), we highlight opportunities to decouple chemical value creation from environmental harm. We close with guidance on catalyst durability, critical-raw-material substitution, digital acceleration (DFT/ML/active learning), and policy levers that can hasten industrial adoption.

Keywords: *Artificial Intelligence (AI), Green chemistry, sustainable catalysis, life-cycle assessment, electrocatalysis, photocatalysis, biocatalysis, circular economy, process intensification.*

INTRODUCTION

Catalysis accelerates >80% of industrial chemical transformations, shaping energy, materials, and healthcare supply chains. However, the legacy emphasis on conversion and selectivity alone can obscure upstream and downstream burdens: extraction of critical metals, solvent use, energy demand, hazardous by-products, catalyst deactivation and disposal, and worker/community exposure. Eco-friendly catalysis reframes catalyst and process design with environment and health as primary objectives—optimizing *what* we make, *how* we make it, and *what happens after* we make it [1-5].

This paper pursues three goals:

1. Establish actionable metrics and a common vocabulary to evaluate catalytic "greenness."
2. Propose a research and assessment workflow that unifies molecular-level design with process- and system-level sustainability.
3. Translate the framework into domain-specific guidance and near-term research opportunities.
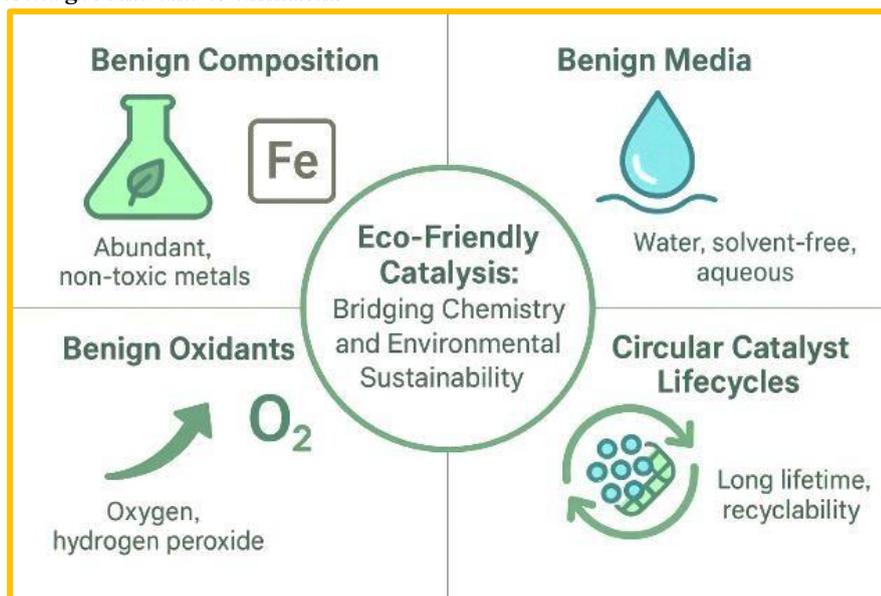
Background and Definitions
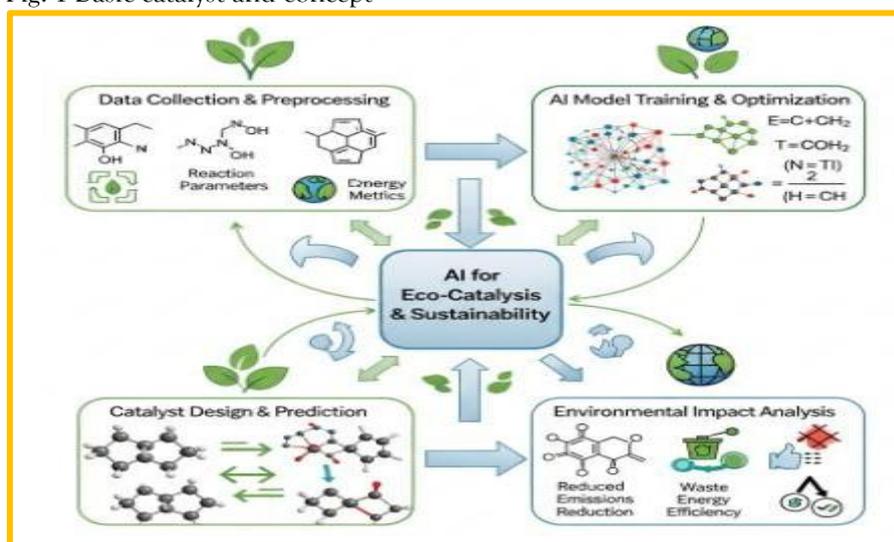

Fig.-1 Basic catalyst and concept

Fig.-2 Block diagram illustrating research on eco-friendly catalysis and environmental sustainability using AI

Green chemistry foundations

Green chemistry emphasizes source reduction via 12 principles (prevention, atom economy, safer solvents, energy efficiency, catalysis, degradation, etc.). Catalysis is explicitly prioritized because small amounts of well-designed catalysts can dramatically reduce stoichiometric waste and enable milder conditions [6-10].

What counts as "eco-friendly" catalysis?

- **Benign composition:** abundant, non-toxic elements (e.g., Fe, Cu, Ni, Mn, C, N, P) over scarce or toxic metals.
- **Benign media:** water, supercritical CO_2, ionic liquids/DEMs with proven low hazard, solvent-free or mechano-chemical conditions.
- **Benign oxidants/reductants:** O_2/air, H_2O_2, H_2 from green sources, electrons/photons.
- **Efficient operation:** high selectivity at low temperature/pressure; intensified reactors (flow/continuous).
- **Circularity:** long catalyst lifetimes, low leaching, facile regeneration, and end-of-life recovery.
- **System gains:** reduced cradle-to-gate CO_2e, water use, toxicity, and cost.

Research Questions and Objectives

RQ1. How can we design catalysts that maximize selectivity and productivity while minimizing hazard, energy, and resource intensity?

RQ2. What trade-offs arise between performance (activity, stability) and sustainability (toxicity, criticality, recyclability), and how can they be quantified transparently?

RQ3. Which catalytic platforms offer the largest near-term environmental benefit at scale?

Objective: Deliver a reproducible workflow that couples materials discovery to process design and system-level sustainability outcomes, enabling evidence-based selection and scale-up.
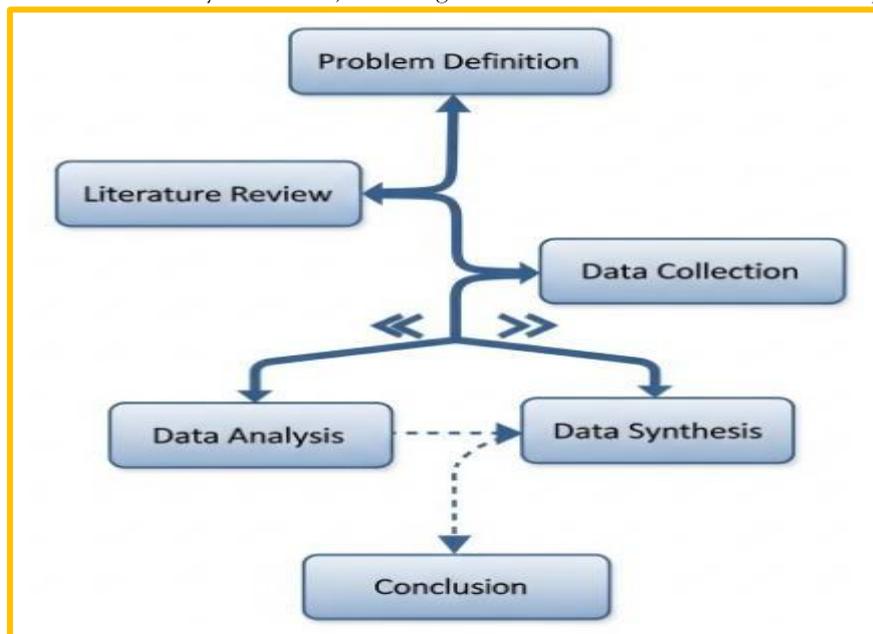

Fig. 3 Steps followed in this research paper
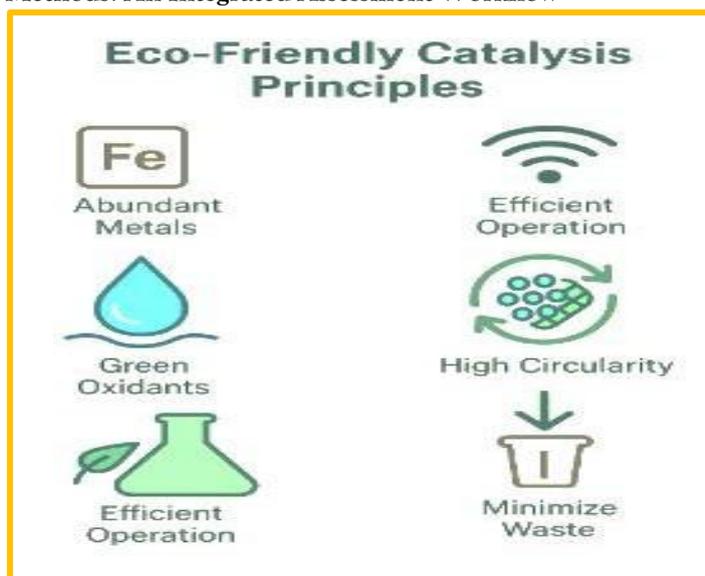
Methods: An Integrated Assessment Workflow

Fig.-4 Eco-Friendly Catalysis Principles

Catalyst discovery and down-selection

- **Computational screening:** DFT/ML to estimate adsorption energies, reaction barriers, and stability windows; active learning to navigate composition/defect/spacer space [11-13].

- **Design rules:** favor earth-abundant elements; minimize toxic ligands; target high site utilization (single-atom catalysts, defect-engineered carbons, zeolites/COFs/MOFs with stable nodes); embed regeneration pathways [14-16].

Experimentation strategy

- **Benign media first:** aqueous or solvent-free screens; if solvent required, select low-hazard, high-boiling, recyclable options [17].
- **Process intensification:** micro/mesoflow reactors for heat/mass transfer; in-line analytics (IR/UV-vis/MS); scale-bridging from mg/h to kg/day [18].
- **Durability testing:** accelerated stress tests, sulfur/chloride tolerance, start–stop cycling for electro/photo systems [19].

TEA–LCA–MCDA coupling

1. **Process modeling (TEA):** mass/energy balances, equipment sizing, OPEX/CAPEX, sensitivity to catalyst life and separation difficulty [20].
2. **ISO-aligned LCA (14040/44):** cradle-to-gate scope for reagents, catalyst manufacture, utilities; toxicity categories (human/ecotoxicity) where data permit [21].
3. **MCDA:** normalize metrics (AE, E-factor, PMI, EI, CO_2e, CAPEX/OPEX, hazard scores, criticality index) and apply stakeholder weights to rank alternatives [22].
4. **Uncertainty analysis:** Monte Carlo on key inputs (yield, lifetime, recycle fractions, electricity mix).

Eco-Friendly Catalytic Platforms

Heterogeneous catalysis with benign metals and carbons

- **Abundant metals:** Fe/Ni/Cu/Mn oxides, spinels, perovskites; nitrides/phosphides/sulfides where leaching risk is controlled.
- **Porous supports:** zeolites, silica, alumina, activated carbons, N-doped carbons, COFs/MOFs with hydrothermally stable nodes.
- **Advantages:** easy separation/reuse, compatibility with continuous flow, low solvent loss.

Biocatalysis (enzymes, whole cells)

- **Strengths:** exquisite selectivity at ambient conditions; water as solvent; minimal protecting-group chemistry.
- **Challenges:** substrate scope, solvent tolerance, enzyme cost/stability; mitigated by immobilization, directed evolution, cosolvents/deep eutectic solvents (DES).

Photocatalysis (visible-light)

- **Benign oxidants:** O_2, H_2O, persulfates generated in situ; sunlight or LED sources.
- **Materials:** doped TiO_2, graphitic carbon nitride (g-C_3N_4), MOF-derived carbons, organic photocatalysts (e.g., acridinium dyes) with careful hazard assessment.
- **Applications:** C–H activation, wastewater micropollutant degradation, selective oxidations.

Electrocatalysis

- **Electron as reagent:** replaces stoichiometric oxidants/reductants; couples to renewable electricity.
- **Targets:** CO_2 reduction (CO, formate, methanol), N_2 reduction (ammonia; long-term), nitrate remediation, oxidative coupling.
- **Design:** abundant metal catalysts (Cu, Ni, Fe), tailored ionomers, flow-by/flow-through GDE reactors, paired electrolysis to valorize both anode/cathode streams.

Hybrid and tandem systems

- **Chemo-enzymatic cascades:** merge enzyme selectivity with chemical catalyst robustness.
- **Photo-electro hybrids:** light-assisted electrocatalysis to lower overpotentials.
- **Tandem beds/loop reactors:** reduce isolations and solvent exchanges, improving PMI and E-factor.

Application Domains and Illustrative Cases

The following cases are illustrative design analyses rather than claims of new experimental data.

Renewable fuels & carbon valorization

Case A: Transesterification for biodiesel using solid bases (e.g., CaO, hydrotalcites, basic zeolites).
- **Eco-features:** heterogeneous, reusable, minimal soap formation with optimized feed pretreatment, glycerol valorization.
- **Metrics focus:** raise TON via regeneration; cut WF by countercurrent washing; move to continuous packed-bed.

Case B: $CO_2 \rightarrow$ methanol via Cu-based catalysts
- **Eco-features:** circular carbon; if H_2 is green, cradle-to-gate CO_2e can drop sharply.
- **Challenges:** equilibrium limits, catalyst sintering, hydrogen cost; opportunity in modular, heat-integrated microchannel reactors and co-electrolysis ($CO + H_2$ feeds).

Plastics upcycling
- **Hydrogenolysis/hydrogenation** of polyolefins over Ni-based catalysts to fuels/waxes at moderate T/P;
- **Solvolysis** of PET to monomers using organocatalysts or Zn/Co salts in benign solvents or DES;
- **Design levers:** closed-loop solvents, additive tolerance, catalyst poisoning management; integrate sorting and depolymerization LCA.

Fine chemicals and APIs
- **Biocatalytic amination/acylation:** enzymes (transaminases, amidases) achieve high selectivity $\rightarrow$ fewer steps, less protection/deprotection.
- **Flow hydrogenations** with supported Ni/Raney-Ni instead of Pd/Pt where feasible; inline scavengers reduce metal residues.
- **Photoredox C–C bond formation:** visible-light catalysis under air with organic dyes; switch to aqueous micellar media when compatible.

Water and wastewater treatment
- **Visible-light photocatalysts** (g-C_3N_4/TiO_2 composites) for trace pharmaceuticals;
- **Electrochemical advanced oxidation** (boron-doped diamond alternatives with lower criticality, e.g., dimensionally stable anodes): mineralize recalcitrants while recovering value at the counter-electrode (paired processes).

Results and Analysis Framework

Because eco-friendly catalysis spans diverse chemistries, we present a *standard analysis template* that researchers can instantiate with their data:
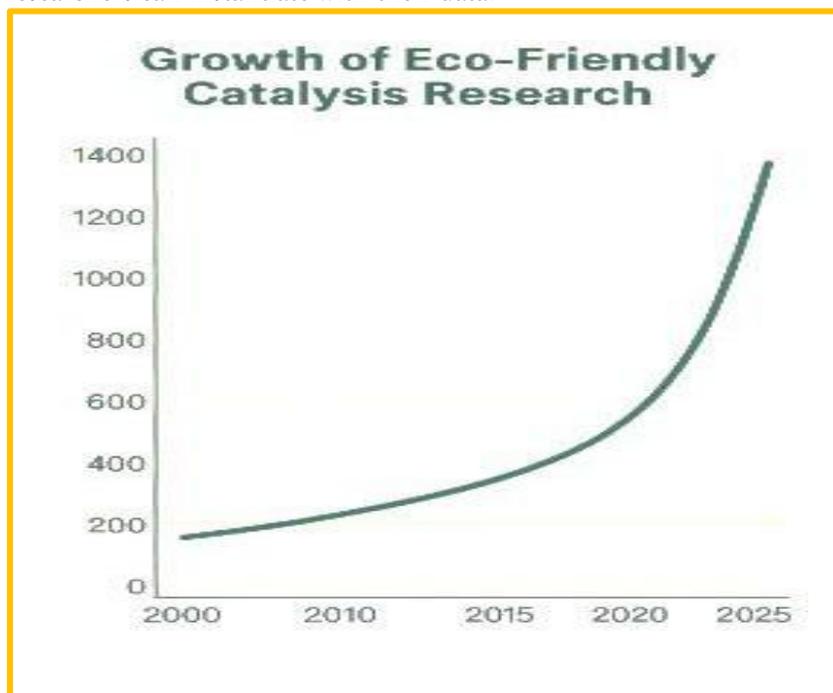

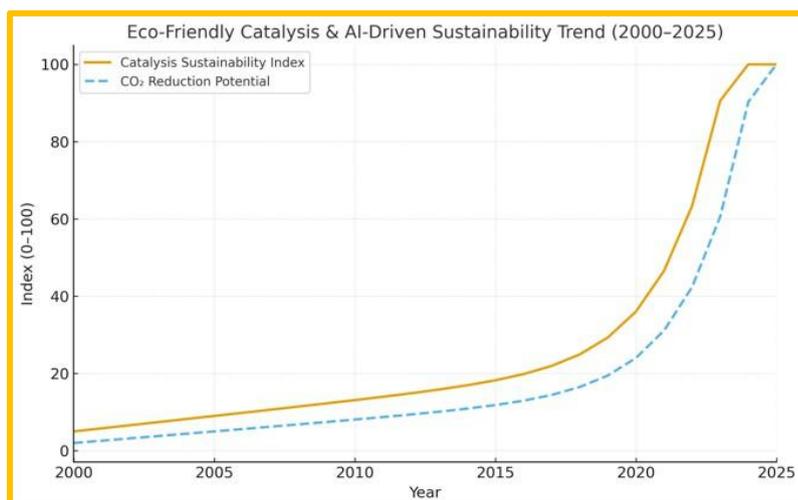Fig.5 Analysis of Growth of Eco-Friendly Catalysis

Fig. 6 Eco-Friendly Catalysis with AI from 2000 to 2025

1. **Reaction performance:** yield, selectivity, TON/TOF vs. time-on-stream; deactivation kinetics; regeneration efficacy; metal leaching (ppm).
2. **Material flows:** complete bill of materials (BOM) including catalyst synthesis; closed-loop solvent/reagent recycles; waste mapping.
3. **Process intensification:** residence time distributions; overall heat transfer coefficients; mass transfer coefficients and effectiveness factors for porous catalysts.
4. **Mass/Energy metrics:** AE, E-factor, PMI, EI, WF computed for lab and scaled scenarios.
5. **LCA outcomes:** midpoint categories (climate change, human toxicity, ecotoxicity, water scarcity) and damage endpoints if using ReCiPe or similar.
6. **TEA outputs:** MSP (minimum selling price), NPV/IRR at scale; sensitivity to catalyst lifetime, recycle rate, and electricity carbon intensity.
7. **MCDA ranking:** visualize Pareto fronts to expose trade-offs (e.g., slightly lower yield but far lower toxicity and CO_2e).

Design Rules and Best Practices

*   **Prefer earth-abundant elements**; when precious metals are unavoidable, use ultra-low loadings (single-atom sites) and robust recovery [23].
*   **Engineer selectivity first:** each suppressed by-product reduces separation, waste, and energy.
*   **Use benign oxidants/reductants:** O_2/air, H_2O_2, H_2, or electrons/photons powered by low-carbon electricity.
*   **Choose greener media:** water, alcohols, glycerol, supercritical CO_2, or validated low-hazard solvents; pursue solvent-free or micellar catalysis where feasible.
*   **Integrate process and catalyst design:** continuous flow often multiplies catalytic benefits by improving heat/mass transfer and enabling safe operation at higher phase-space intensities [24].
*   **Plan for circularity:** design for regeneration, refurbishment, and metal/ligand recovery; quantify take-back performance in LCA.
*   **Verify at scale:** long-term stability and product purity often dominate sustainability in real plants.

Risks, Trade-offs, and Limitations

*   **Criticality and supply risk:** even "benign" catalysts can rely on niche precursors; maintain dual-source or substitution strategies.
*   **Hidden burdens of catalyst synthesis:** complex ligands/nanostructures may inflate PMI and CO_2e; include catalyst manufacture in LCA.
*   **Water use and ecotoxicity:** aqueous processes can shift burdens to water treatment; track WF and toxicity explicitly.
*   **Selectivity vs. rate trade-offs:** biocatalysts and organocatalysts may require longer residence times; flow intensification can compensate.
*   **Data gaps:** toxicity and fate data for novel materials (e.g., some MOFs, organic photocatalysts) may be incomplete; apply precautionary factors and generate missing data [25].

Future Research Directions

1. **Data-centric discovery:** open datasets of catalyst composition–structure–performance with standardized green metrics; surrogate models that predict PMI/E-factor alongside turnover.
2. **Digital twins:** link microkinetics and CFD with TEA/LCA for *real-time* sustainability feedback during optimization.
3. **Electrification & pairing:** paired electrolysis and heat integration with heat pumps; scheduling to exploit renewable intermittency.
4. **Benign catalyst synthesis:** solvent-free/mechanochemical routes; water-based colloid chemistry; bio-derived ligands and supports.
5. **Durability science:** deactivation mapping (coke, sintering, poisoning, leaching) and regeneration pathways with minimal waste.
6. **Policy & markets:** green public procurement, low-carbon fuel/chemical standards, extended producer responsibility (EPR) for catalysts, and recycled content targets.

CONCLUSION

Eco-friendly catalysis is the linchpin for aligning the chemical enterprise with planetary boundaries. By elevating environmental metrics to co-equal status with conversion and selectivity—and by operationalizing them through an integrated TEA–LCA–MCDA workflow—researchers can make transparent, high-impact choices about catalyst composition, reactor design, and process integration. Practical wins already exist in renewable fuels, plastics upcycling, fine-chemical synthesis, and water treatment; scaling these wins requires durability, circularity, and electrification. With rigorous metrics, open data, and supportive policy, eco-friendly catalysis can bridge chemistry and environmental sustainability at industrial scale. This study demonstrates the potential of AI-driven approaches to revolutionize eco-friendly catalysis for sustainable development. By optimizing catalyst design and reaction conditions, significant reductions in emissions and resource usage are achieved. The integration of life cycle assessment ensures environmentally responsible implementation. This research highlights the synergy between green chemistry and artificial intelligence in achieving global sustainability goals. Future work will focus on large-scale deployment and real-time adaptive optimization.

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