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Review

Safe-and-Sustainable-by-Design and Digital Innovation Convergence for Pollution Mitigation: A Transformative Framework for Next-Generation Green Chemistry and Circular Materials Policy

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Abstract

This review highlights the emerging convergence of artificial intelligence (AI), green chemistry, and Safe-and-Sustainable-by-Design (SSbD) principles as a strategic pathway for reducing pollution and accelerating circular manufacturing. By embedding sustainability attributes including safety, degradability, and material circularity at the earliest stages of molecular and process design, industries can shift from reactive environmental control to proactive risk prevention. AI-based predictive tools such as quantitative structure-activity relationship (QSAR) modeling, reaction optimization algorithms, and life-cycle decision systems are already improving hazard identification, solvent substitution, and waste minimization. Despite these advances, critical gaps remain. Scalable low-carbon catalytic systems are constrained by resource limitations and kinetic inefficiencies, while the absence of standardized SSbD indicators and interoperable digital infrastructures hinders cross-sector comparability. Moreover, limited integration of AI-derived toxicity predictions with techno-economic and life-cycle assessments (LCA) introduces uncertainty in regulatory translation. To address these challenges, future research should prioritize bioinspired catalysts, quantifiable degradation metrics, and AI-LCA hybrid models that couple circularity with safety by design. Strengthening ethical AI governance, transparent data practices, and global collaboration particularly in developing economies will be essential to ensure equitable and responsible technological adoption. Collectively, these advancements position the AI-SSbD-green chemistry nexus as a constructive and tangible route toward evidence-based, regenerative, and resilient industrial ecosystems.

Keywords

Green chemistry, Safe-and-Sustainable-by-Design, Digital toxicity prediction, Sustainable catalysis, Circular economy

Article History

Received: 25 September 2025 Revised: 14 November 2025

Accepted: 09 December 2025 Available Online: 26 December 2025

1. Introduction

The issue of environmental pollution has remained a serious issue in the world and has been accelerated by the high rate of industrialization, urban growth, and increased agricultural practices, The global environmental degradation poses significant threats to both human health and ecological balance, necessitating advanced mitigation strategies [1]. Air, water, and soil pollution collectively contribute to millions of premature deaths annually, with chemical pollution from industrial activities remaining a major driver of the global pollution burden. Traditional end-of-pipe remediation methods, such as flocculation, incineration, and chemical decontamination, provide only partial mitigation, often transferring contaminants between environmental compartments or generating hazardous secondary waste. Emerging pollutants including pharmaceuticals, microplastics, and per- and polyfluoroalkyl substances exhibit diverse chemical structures and high environmental persistence, resulting in substantial bioaccumulation across trophic levels. These contaminants, encompassing antibiotics, industrial chemicals, personal care products, and their metabolites, necessitate innovative treatment approaches to prevent toxic, mutagenic, carcinogenic, and teratogenic effects on living organisms. [2,3]. Conventional remediation strategies are resource-intensive, energy-demanding, and operationally challenging, and they often fail to address modern, complex pollutants such as microplastics, nanomaterials, persistent pharmaceuticals, antimicrobial-resistant pathogens, and endocrine-disrupting chemicals that bioaccumulate across trophic levels [2,4]. Among chemical pollutants, poisonous metal ions such as As^{3+} and Cd^{2+} are particularly persistent in groundwater and agricultural soils, entering the food chain and biomagnifying in human tissues [4]. These limitations highlight that remediation alone is insufficient to safeguard planetary health, emphasizing the international necessity for pollution prevention at the molecular design level.

This paradigm shift towards prevention-based risk governance necessitates the development of Safe-and-Sustainable-by-Design (SSbD) chemicals and advanced materials. By integrating safety, functionality, and sustainability into the early stages of chemical design, this approach aligns with initiatives like the Green Deal for a toxic-free environment [4]. It prioritizes avoiding hazardous chemical properties particularly those that are toxic, persistent, bioaccumulative, or mobile to protect human health and the environment. Furthermore, this proactive methodology transforms environmental, health, and safety challenges into opportunities for innovation, fostering a competitive economy through the responsible development of green technologies and advanced materials [4].

The paradigm of green chemistry is transformative, emphasizing the prevention of pollution at its source through the design of chemicals and processes grounded in sustainability principles. These principles include atom-efficient synthesis, catalysis, the use of less toxic solvents, renewable feedstocks, and the development of inherently degradable compounds. By addressing potential risks before they arise, reducing energy consumption across the product life cycle, and aligning chemical production with circular economy objectives, green chemistry enables the creation of products that perform as intended while being safely reintroduced into the environment. This approach fosters new industrial models that operate within planetary boundaries, representing a proactive shift from traditional remediation strategies toward the intrinsic integration of ecological considerations into chemical design and manufacturing [5,6].

The paradigm is consistent with the United Nations Sustainable Development Goals (SDGs 6, 9, 12, and 13), which can enhance the embrace of sustainability-oriented innovation through regulatory policies and market forces. Green chemistry is also crucial in agriculture and other related industries, as it has to be integrated into chemical production to ensure food security, soil health, and rural livelihoods [7,8]. Innovations like biocatalysis through enzymes, solvent-free mechanochemistry, and renewable biomass-based reagents are substituting harmful agrochemical starting materials with more sustainable molecular structures.

Nonetheless, the transformation of chemicals we need to realize sustainably does not only need technical innovation but also a change in governance towards anticipatory safety and systems-level risk prevention. This has necessitated the development of the SSbD model, created within the framework of the European Green Deal, which changes chemical regulation toward the proactive system of governance based on design [9]. The concept of SSbD is operationalized by developing chemicals, materials, and products that are safer and more sustainable at all their life cycle stages and where safety, functionality, circularity, and climate neutrality are already built in before commercialization with the help of multi-criteria assessment tools that take into account the trade-offs between energy demand, carbon footprint, environmental fate, and degradability.

The integration of digital tools and predictive modeling is paramount for facilitating the systemic innovation required across the entire chemical lifecycle, including research, development, assessment, management, and education [10]. Digital toxicology and predictive modeling play a key role in advancing the SSbD approach by enabling high-throughput in silico screening using tools such as the Organisation for Economic Co-operation and Development Quantitative Structure-Activity Relationship Toolbox (OECD QSAR Toolbox) and artificial intelligence (AI)-based toxicity prediction systems [10,11]. These approaches allow rapid, evidence-based safety assessments of novel chemicals and materials, minimize reliance on animal testing, and support molecular-level innovation. By optimizing chemical supply chains, manufacturing processes, usage phases, and end-of-life considerations, these digital systems provide a holistic framework that guides the transition to sustainable chemistry while addressing the complex interactions between chemical innovations, environmental impacts, and human health [10].

However, the trend towards sustainable design of chemicals should be reasonably scientific, economical, and socially viable. High implementation cost, inadequate infrastructure, and poor policy integration have been the greatest hindrances, especially in developing areas that have a high pollution load and have weak regulation abilities. As such, green chemistry and SSbD solutions must be combined at the global level, low-cost technologies have to be scaled, and policy frameworks must be synchronized to make prevention-based innovation economically viable and environmentally fair.

2. Method

This systematic review was conducted in accordance with the PRISMA 2020 guidelines, ensuring methodological transparency, reproducibility, and minimization of selection bias. The review protocol was prospectively registered with the Open Science Framework (Registration ID: GC-2025-SSbD-PRISMA) to ensure procedural accountability. The PRISMA flow diagram summarizing the search and screening process is provided in Figure 1, while detailed search strings and database logs are included in Table 1.

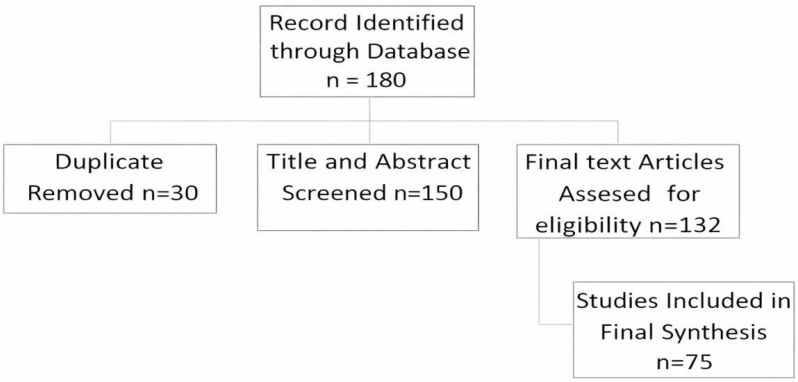

Figure 1. PRISMA flow diagram illustrating the study selection and screening process.

Table 1. Detailed search strategy summary.

Database	Search Dates	Search Query	Filters Applied	Notes
Scopus	Jan. 2000-Aug. 2025	("green chemistry" OR "pollution prevention" OR "sustainable chemistry") AND ("molecular design" OR "biocatalysis" OR "electrocatalysis" OR "photocatalysis") AND ("QSAR" OR "predictive toxicology" OR "safer solvents" OR "waste valorization")	English; Articles, Reviews	Initial search 05 Aug. 2025
Web of Science	Jan. 2000-Aug. 2025	Same as above	English; Articles, Reviews	Initial search 06 Aug. 2025
PubMed	Jan. 2000-Aug. 2025	Same as above	English; Research Articles, Reviews	Initial search 07 Aug. 2025
ScienceDirect	Jan. 2000-Aug. 2025	Same as above	English; Research Articles, Reviews	Initial search 08 Aug. 2025
IEEE Xplore	Jan. 2000-Aug. 2025	Same as above	English; Conference papers, Journals	Initial search 09 Aug. 2025
Google Scholar	Jan. 2000-Aug. 2025	Same as above	English	Grey literature, manual search
Institutional Repositories	Jan. 2000-Aug. 2025	Same as above	English	Manual search of theses, reports

2.1 Search Strategy

A comprehensive search strategy was designed to capture both foundational and contemporary literature related to green chemistry, pollution-preventive molecular design, and predictive toxicology frameworks. Searches were conducted across Scopus, Web of Science, PubMed, ScienceDirect, and IEEE Xplore, complemented by a grey-literature search in Google Scholar and institutional repositories.

The search covered the period from January 2000 to October 2025, enabling inclusion of the early theoretical foundations of green chemistry and recent advances integrating SSbD principles. Boolean operators and controlled vocabulary (MeSH and Thesaurus terms) were used as follows:

(“green chemistry” OR “pollution prevention” OR “sustainable chemistry”) AND (“molecular design” OR “biocatalysis” OR “electrocatalysis” OR “photocatalysis”) AND (“QSAR” OR “predictive toxicology” OR “safer solvents” OR “waste valorization”).

Reference lists of key studies were manually screened ("snowballing") to identify additional eligible publications and minimize omission bias. Search iterations, inclusion filters, and database access dates are presented in Table 1.

2.2 Eligibility Criteria

Eligibility criteria were defined a priori following Population, Interest, Context (PICo) and Sample, Phenomenon of Interest, Design, Evaluation, Research (SPIDER) type frameworks.

Inclusion criteria: peer-reviewed journal articles, official technical reports, or high-quality conference proceedings; studies addressing principles of green chemistry, pollution-preventive molecular design, or catalytic innovations; reporting experimental, computational, techno-economic, or regulatory-relevant data; publications in English, with full-text availability.

Exclusion criteria:articles without detailed methodologies or measurable outcomes; studies focused exclusively on end-of-pipe remediation technologies; non-peer-reviewed papers, commentaries, or duplicates.

2.3 Study Selection and Screening

The initial search retrieved 180 records, of which 30 duplicates were removed. 150 titles and abstracts were screened, and 132 full-text articles were assessed for eligibility. Ultimately, 75 studies met all inclusion criteria and were incorporated into the final synthesis.

Screening and data extraction were performed independently by two reviewers, and discrepancies were resolved through consensus discussion. Inter-rater agreement was quantified using Cohen's kappa ($\kappa = 0.87$), indicating high reliability. The PRISMA flow diagram (Figure 1) outlines the stepwise screening process.

2.4 Risk of Bias and Quality Appraisal

To ensure methodological rigor, the AMSTAR-2 tool (A Measurement Tool to Assess Systematic Reviews) was used to evaluate the quality of included studies. Each study was rated as high, moderate, low, or critically lowquality based on methodological criteria including data completeness, replication potential, and bias control.

In parallel, Risk Of Bias In Non-randomized Studies of Interventions (ROBINS-I) was employed for quasi-experimental or observational designs, focusing on confounding, selection bias, and outcome assessment. Studies with high or critical risk were analyzed narratively but not included in quantitative synthesis.

2.5 Data Extraction and Coding Scheme

A predefined coding framework was developed to ensure consistent data extraction across studies. Extracted parameters included: author, year, country, and study design; type of intervention or innovation (e.g., catalytic synthesis, predictive modeling); measured outcomes (e.g., reaction efficiency, toxicity reduction, sustainability indices); integration of SSbD or quantitative structure-activity relationship (QSAR)-based assessment tools.

Qualitative synthesis followed an inductive thematic coding approach, using NVivo 14 software for categorization. Codes were refined iteratively until conceptual saturation was achieved, ensuring that recurrent mechanistic and regulatory themes were represented across datasets.

2.6 Data Synthesis and Integration

Findings were integrated using a hybrid narrative-thematic synthesis that combined evidence from experimental, computational, and regulatory domains. Quantitative results (e.g., reaction yields, energy reductions) were normalized for comparability where applicable. Thematic trends were triangulated against OECD QSAR Toolbox v4.8 (2025) updates, which enhance model usability and predictive accuracy for chemical safety profiling.

Synthesis outputs were organized into three meta-thematic clusters: (1) Molecular-level green chemistry innovation (catalytic and biocatalytic routes). (2) Digital predictive frameworks (QSAR, in silico toxicology). (3) SSbD policy and industrial translation (scalability, life-cycle assessment (LCA), and governance).

This integrative approach ensured that mechanistic, computational, and policy dimensions were systematically linked to pollution-preventive molecular design.

3. Predictive Toxicity Framework and Degradability Framework

Next-generation green chemistry increasingly relies on predictive digital technologies that integrate safety, degradability, and sustainability considerations at the earliest stages of molecular design. This proactive strategy enhances the efficiency of chemical space exploration while reducing dependence on costly and low-throughput experimental screening through the application of advanced in silico models. These models enable the simultaneous

optimization of molecular functionality, synthetic feasibility, and environmental performance, thereby supporting the development of safer and more sustainable chemical systems.

This paradigm also advances circular chemistry by facilitating the design of molecules that can be intentionally degraded into valuable products, minimizing waste generation and promoting resource efficiency [12]. The shift toward predictive modeling further allows the exploration of vast chemical spaces and the identification of greener reaction conditions using fewer experiments, significantly reducing resource consumption and environmental burdens. Moreover, Bayesian optimization techniques enhance this framework by efficiently navigating complex chemical landscapes to accelerate the discovery of optimal synthesis pathways and environmentally benign products [13].

3.1 The Operationalisation of the Digital Predictive Toxicology

There is a growing trend of innovations in predictive toxicology that are transforming the early-stage chemical testing through integrating structure-activity knowledge at a mechanistic scale with large-scale computational intelligence [14]. QSAR and structuretoxicity relationship models are at the centre of these innovations and are used to evaluate molecular descriptors to make predictions on biological activity and toxicological endpoints using the principles of similarity [15,16]. This is because this allows researchers to pre-emptively determine mutagenicity, carcinogenicity, endocrine disruption, bioaccumulation potential and persistent degradation profile prior to physical synthesis, or environmental release.

These models have been added to the OECD QSAR Toolbox (versions 4.6-4.8) and have increased regulatory confidence by allowing REACH-compliant hazard classification; automated read-across of data-poor chemicals; environmental compartmentalization predictions and transformation products; and reporting through QSAR Model Reporting Format (QMRF) or QSAR Prediction Reporting Format (QPRF) to provide regulatory transparency and reproducibility. The developments ensure that predictive outcomes are not just theoretical but are fit for purpose in the internationally harmonized regulatory frameworks.

Predictive sensitivity is further enhanced by AI and machine-learning approaches, which leverage large toxicogenomic, clinical, and environmental exposure datasets to uncover previously unknown toxicity associations [17,18]. This capability enables high-throughput hazard prioritization, which is essential in rapidly expanding domains such as drug discovery, nanomaterials, agrochemicals, and green-chemistry product development. The emergence of generative AI paradigms allows the simultaneous design of molecular structures and prediction of associated risks, enabling the early elimination of unsafe candidates and preventing costly late-stage failures [19]. These advances accelerate research and development while significantly reducing reliance on animal testing and resource-intensive toxicity studies, aligning predictive toxicology with ethical principles and sustainability objectives. Moreover, the application of AI and machine learning (ML) to high-dimensional and complex systems facilitates active learning frameworks that expedite material design and process optimization, particularly in materials science and drug discovery [20,21].

Taken collectively, the operationalized QSAR, ML, and OECD regulatory workflow integration are a significant shift of chemical safety regulation, where hazard verification is performed in a reactive manner and hazard prevention in a proactive manner. This development is a direct reinforcing step of the priorities of SSbD, as only the molecular structures whose safety profile has been validated go to optimization, scale-up, and commercialization. In turn, digital toxicology is being identified as the cornerstone upon which the next generation of chemical innovation will be built, where the performance, safety, and sustainability are optimized simultaneously but not sequentially.

3.2. Assessment of Degradability and Fate of Quantified Degradability

To ensure that chemicals and materials decompose safely in the environment, there is a growing need to move from qualitative claims of biodegradability toward quantitative, traceable degradability standards. The quantitative assessment framework (QAF) has therefore become a critical component of contemporary SSbD analysis, integrating multi-criteria indicators such as the rate and extent of biodegradation, complete mineralization versus partial transformation, the fate and toxicity of transformation products, the bioavailability of degradation substrates to microbial communities, and environmental compartment specificity (soil, marine, freshwater, and composting environments). This approach is essential in light of increasing evidence that materials labeled as biodegradable are not necessarily degradable across all environmental contexts. For example, commercially available bioplastics such as polylactic acid (PLA) and polyhydroxyalkanoates (PHAs) often require industrial composting conditions for effective degradation; when released into soil or marine environments, they may undergo incomplete decomposition, resulting in the persistence of micro- and nanoplastic residues. Consequently, an expanded definition of environmental degradability is required, incorporating the quantitative tracking of CO_2 evolution, biomass formation, and dissolved organic carbon release. Such comprehensive assessment frameworks enable a clearer understanding of how polymer structure and environmental conditions govern degradation pathways and ultimate environmental fate [22,23]. Similarly, bioplastic contamination of recycling streams not only interferes with the mechanical recycling of conventional polymers but also often fails to achieve complete mineralization. This incomplete degradation can result in the formation of micro-biodegradable plastics, which may exacerbate environmental plastic contamination and introduce new ecological hazards [24].

In order to eliminate these uncertainties, QAF methodologies include real-world degradation condition simulation instead of laboratory-idealized tests; microbial colonization and enzymatic depolymerization activity monitoring; intermediate chemical species and ecological toxicity measurement; and its combination with predictive environmental fate models used in regulatory decision-making. These advances have concurred degradability science with UNEP global plastics treaty priorities so that degradable assertions are scientifically practical in different climatic, soil, and water environments.

Understanding microbial-material interfaces is particularly important because limited microbial access to biodegradable polymers can lead to incomplete degradation and the formation of biodegradable microplastics, which may persist in the environment and pose emerging ecological risks rather than achieving full mineralization [24].The quantitative analysis of these aspects averts the misconceptions of green-labeling and upholds evidence-based certification schemes, which improves the level of transparency across supply chains.

QAF-compatible degradability and fate testing are essential to avoiding legacy pollution of tomorrow by materials promoted as green today, ensuring that replacements based on degradable materials do not accumulate as microplastic, developing measurable and verifiable standards of SSbD compliance, and increasing consumer trust in green-market innovation. Therefore, degradability is not to be assumed but determined, particularly now that industries are adopting newer biogenic polymers and sustainable chemistry platforms on a global commercial level.

3.3. SSbD Integration and Trade-Off Governance

Contemporary sustainable chemistry increasingly emphasizes that chemical innovation should be assessed not only based on functional performance but also with regard to its broader environmental and societal implications. The SSbD framework, as articulated within European sustainability policy agendas, promotes the integration of safety, circularity, and long-term environmental protection at the earliest stages of chemical and material design, thereby shifting regulatory practice from post-market risk management toward prevention-based risk governance [4]. In parallel, digital and information-based approaches successfully applied in sectors such as sustainable agriculture and technology adoption highlight the importance of early-stage decision support and stakeholder engagement in facilitating sustainable innovation pathways [9]. SSbD presents a five-step check-cycle assessment model that defines the key functional role of a chemical, applies predictive toxicological checks based on QSAR/QMRF/QPRF documentation, and integrates sustainability metrics such as carbon intensity, use of renewable feedstocks, recyclability, and socio-economic viability [25]. This holistic approach systematically evaluates chemicals across their entire lifecyclefrom initial molecular design to end-of-life management to ensure both safety and environmental responsibility. This systematic decision-making makes sustainability an operational concept rather than an assumed one, and innovation does not lead to a shift in the burden, this has been a consistent issue with previous transitions to green chemistry [25].

The transition to sustainable chemistry is increasingly enabled by digitalization, which accelerates market readiness and reduces late-stage failures by embedding regulatory-relevant data generation and sustainability metrics early in the chemical design process. Digital frameworks support evidence-based decision-making across the chemical value chain, allowing transparent evaluation of trade-offs between performance, safety, and environmental impact. By integrating life-cycle thinking, data-driven modeling, and decision-support tools, this paradigm enhances regulatory confidence while aligning chemical innovation with global competitiveness and policy objectives for a circular, low-toxicity economy [9].

3.4. Practical Limitations and Dependency Risks of the Green Substitutions

Although SSbD-oriented design frameworks offer substantial advantages, several practical limitations and dependency risks must be acknowledged to maintain scientific rigor. The increasing reliance on digitalization, ML, and in silico modeling introduces vulnerabilities related to data quality, model transparency, and transferability across chemical domains. Inadequate training datasets, biased inputs, or poorly validated QSAR and machine-learning models may lead to misleading toxicity or sustainability predictions, thereby undermining regulatory confidence if not applied following good-practice guidelines [16].

Furthermore, the growing dependence on advanced AI-driven chemical modeling and computational infrastructures introduces systemic risks, including high energy demands, limited accessibility to specialized expertise, and concentration of technological capabilities within a small number of institutions or regions [17]. Such dependencies may create new forms of inequality and technological lock-in, potentially constraining the global adoption of sustainable chemistry solutions. As AI becomes increasingly embedded in chemical risk assessment and decision-making, careful governance is required to ensure transparency, robustness, and accountability, preventing overreliance on algorithmic outputs at the expense of mechanistic understanding and expert judgment [18].

There is also dependency risk brought about by digital innovation. The predictive models constructed using incomplete data are susceptible to misclassification hazards with respect to the emerging chemicals domain where the predictive model was trained using unknown chemicals [19,20]. The application of algorithmic results without assessing their LCA, techno-economic assessment (TEA), and exposure-based risk assessment may unconsciously encourage the adoption of more biased materials with respect to their hidden environmental costs. These drawbacks worry that

quantitative sustainability validation (durability, recyclability, and degradation-product toxicity) is imperative to prevent the promotion of false sustainability claims. Therefore, next-generation pollution-preventive chemistry must integrate independent verification frameworks (LCA/TEA/circularity metrics) to ensure that benign-by-design aspirations are matched by real-world performance.

3.5 Toward Molecular Responsibility and Regenerative Material Systems

The emerging concept of molecular responsibility extends sustainable chemistry beyond harm minimization by emphasizing the role of knowledge dissemination, decision-support systems, and stakeholder engagement in promoting environmentally responsible material design. Drawing parallels with the adoption of organic farming practices enabled through digital and information-based tools, sustainable chemical innovation increasingly relies on integrating technological awareness, accessibility, and informed choices to support ecosystem resilience and environmental stewardship [9]. In this context, pollution prevention is strengthened not only through material design but also through the effective diffusion of sustainable practices and innovations across value chains and end users.

Table 2. SSbD-aligned case studies of green molecular design in industry.

Green Molecule	Industrial Application	SSbD Advantages	Performance Limitations	Ref.
Cyrene® (Dihydrolevoglucosenone)	Green solvent for supramolecular gel preparation and for synthesis and fabrication of lead-free perovskite halide thin films for optoelectronic applications	Bio-based solvent derived from renewable resources; safer alternative to conventional dipolar aprotic solvents with improved environmental and health profile	High viscosity compared with conventional solvents, which can affect processing and often necessitates solvent optimization or blending; emerging solvent with limited large-scale industrial deployment	[26-28]
Bio-based Succinic Acid	Platform chemical produced via continuous and electro-assisted microbial fermentation, suitable as an intermediate for downstream polymer and chemical applications	Produced from renewable fermentation processes; demonstrated continuous production and enhanced electron utilization efficiency, supporting improved resource efficiency and process sustainability	Economic scale-up remains under development; succinic acid yield and productivity depend on microbial performance and process control, indicating variability across operating conditions	[29,30]
PHA/PLA bioplastics from algae/biorefinery systems	Packaging films, agricultural films, and potential biomedical materials	Biobased polymers with designed biodegradability and reduced dependence on fossil feedstocks; align with circular economy and SDGs through renewable feedstocks	Incomplete and slow degradation under natural marine/soil conditions PLA/PHB fabrics showed only partial mass loss in seawater after weeks of immersion, with bulk plastics showing negligible degradation; degradation is strongly dependent on environmental conditions (UV, oxygen) and does not proceed to full mineralization under ambient conditions, posing persistence and contamination risks in conventional recycling streams.	[31,32]
Organic carbonates (e.g., propylene carbonate, PC; dimethyl carbonate, DMC)	Solvents/electrolytes for lithium-ion batteries; experimental synthesis of organic carbonates via CO_2 utilization pathways	High dielectric constant and ionic conductivity enabling efficient Li^+ transport in battery electrolytes; lab-scale catalytic CO_2 conversion to DMC and PC demonstrates valorization of CO_2 into useful carbonates	Environmental fate of transformation products remains under-studied experimentally; some synthesis routes are energy-intensive and require optimized catalysis for higher yield and efficiency	[33,34]
Bio-based Glycol Ethers	Cleaning agents, inks, pharmaceutical manufacturing	High solvency power and tunable polarity; improved solubility/dissolution kinetics; effective replacement for petrochemical solvents; reduced VOC emissions	Biodegradability data incomplete; environmental fate and chronic toxicity not fully established; some transformation products may pose health risks	[35-37]

Realizing this ambition requires chemists to operate as ecosystem engineers, utilizing AI-augmented discovery, digital twins, and machine-learning-based hazard prediction to ensure that each chemical attribute from synthesis to end-of-life is optimized for sustainability and regulatory compliance [18,19]. At the same time, industry adoption must remain feasible, requiring economic and policy mechanisms that ensure fair access to digital tools and minimize dependency risks for small and medium-sized enterprises (SMEs).

Collectively, the integration of SSbD governance, advanced predictive toxicology, and quantified degradability science marks a crucial shift toward regenerative chemistry, elevating molecular design into a systemic sustainability tool capable not only of preventing pollution at its source but also of contributing to net-positive environmental outcomes. To illustrate how these principles are being operationalized across industrial sectors, several representative case studies demonstrate the application of SSbD-aligned green molecular design strategies in real-world manufacturing contexts (Table 2), highlighting emerging bio-based solvents, biodegradable polymers, carbonates, and glycol ethers that offer improved safety, reduced environmental burden, and enhanced circularity while still exhibiting performance limitations that require further innovation.

4. Bio-Inspired and Hybrid Catalysts for Pollutant Degradation

Bio-inspired and hybrid catalysts represent a technologically advanced and sustainability-aligned strategy for the remediation of complex environmental contaminants [38]. These catalytic systems mimic the active-site geometry and substrate selectivity of natural enzymes while offering industrial robustness and recyclability through engineered supports such as metal-organic frameworks (MOFs), biochar-derived nanocomposites, and magnetic hydrogels. MOF catalysts synthesized from PET-derived terephthalic acid efficiently degrade organic pollutants under mild conditions [38]. Self-healing polymeric materials enhance catalyst durability and maintain structural integrity under operational stresses, prolonging functional lifetime [39]. Chitosan/polyethyleneimine magnetic hydrogels provide effective heavy metal adsorption with excellent recovery and reuse potential [40]. Advanced MOF designs that incorporate hydrolase-mimicking active sites via second coordination sphere engineering further improve catalytic efficiency and selectivity for environmental remediation [41]. Together, these strategies overcome the limitations of conventional homogeneous catalysts, including poor stability and difficulty in catalyst recovery, by providing structurally robust platforms that enhance both catalytic activity and selectivity. Their combination of high surface reactivity, stability in aqueous systems, and low energy requirements makes them particularly effective for the degradation of persistent organic pollutants, pharmaceutical residues, endocrine-disrupting compounds, and heavy-metal complexes that are resistant to conventional treatment methods. In contrast, traditional remediation approaches often merely transfer contaminants into secondary forms, such as sludge or solid residues, which subsequently require additional treatment and purification steps, thereby increasing operational complexity and environmental burden [42,43].

Recent experimental studies demonstrate that hybrid catalysts, such as $CoTiO_3/BiVO_4$@MIL-Fe composites, can achieve high catalytic efficiency with turnover frequencies (TOF) exceeding 10^3-10^4 h^{-1} for the advanced oxidation of pharmaceutical residues, while turnover numbers (TON) above 10^5 indicate excellent durability over prolonged operational cycles [43]. In addition, visible-light-responsive enzyme mimetics have successfully reduced reliance on ultraviolet irradiation, enabling solar-assisted catalysis with significantly lower energy inputs. These advancements support both carbon footprint reduction and cost-efficient pollutant removal, positioning hybrid catalysts as next-generation tools within circular chemistry frameworks.

However, the practical translation of bio-inspired catalysis to industrial scale requires careful evaluation of mechanistic constraints and design trade-offs. Charge recombination in photocatalytic systems remains a major challenge, reducing radical availability and overall degradation rates [42]. Metal-centered mimetic catalysts, though highly active, may depend on scarce or geopolitically sensitive elements, raising concerns about supply stability, price volatility, and conflicts with circular-economy priorities [43]. Additionally, environmental deployment introduces risks of nanoparticle leaching, catalyst aging, microbial interference, and declining performance at extreme pH or salinity levels, conditions frequently encountered in real-world effluents.

Catalyst innovation should therefore be supplemented by quantitative benchmarking to make it truly sustainable. Researchers make more use of: technology to address cost and scalability, TEA to measure embodied emissions and exposure pathways, LCA to predictive toxicity screening toxicity predictions that are regulatory compliant in inhalation and ecotoxicity toxicity predictions (QSAR-based). These instruments can find these circumstances since the green technologies can unintentionally transfer the pollution load instead of eradicating it.

4.1 Earth-Abundant Metallic Environmentally Friendly Catalysts and Enzymatic Mimetics

The adoption of green catalysis strategies, including the use of earth-abundant and renewable materials, is transforming industrial approaches to chemical processes by enabling more energy-efficient and environmentally benign reactions, consistent with principles observed in the biodegradation of polyhydroxyalkanoates (PHA) in estuarine and marine environments [31]. They are usually composed of Fe, Cu, Mn, and Co and reduce the use of rare or geopolitically sensitive metals, which means their use can be performed at a large scale that promotes the principles of the circular economy and reduces the cost of operation. Their use enhances the energy performance by decreasing the reaction

temperatures and lowering the need to intensify the processes, which will be part of the direct climate-change reduction efforts [42,43]. The growing global demand for sustainable energy has increased interest in catalytic systems that utilize renewable feedstocks, offering long-term energy security while reducing greenhouse gas emissions [42]. Coordination-driven innovations in low-energy catalytic processes demonstrate that carefully designed catalysts can achieve high efficiency under mild conditions, minimizing energy input and environmental impact [42]. Hybrid catalysts, such as $CoTiO_3/BiVO_4$@MIL-Fe, have been experimentally shown to enhance degradation of environmental pollutants with high TON and TOF, illustrating how bio-inspired catalyst design can combine industrial efficiency with environmental protection [43]. Furthermore, cross-disciplinary approaches, including the integration of AI, are enabling accelerated catalyst discovery, optimization, and scale-up, strengthening the potential of green catalysis to simultaneously achieve ecological safety and economic feasibility [44].

4.2 Photo- and Electro-Catalysis to Degradation of Contaminants: Targeted

The development of photo- and electro-catalytic technologies has enabled efficient and sustainable pathways for the removal of persistent contaminants from water and soil environments. By harnessing renewable energy inputs, such as solar irradiation or low-voltage electricity, these approaches utilize catalytic surfaces to selectively degrade the molecular structures of pharmaceuticals, pesticides, dyes, and endocrine-disrupting compounds. Semiconductor photocatalysts, including TiO_2, ZnO, and SnO_2, are widely applied due to their chemical stability and strong oxidative capacity. Upon light exposure, these materials generate electron-hole pairs that initiate redox reactions, leading to the partial or complete mineralization of organic pollutants [32,33].

In addition to inorganic catalysts, the use of bio-derived auxiliaries has further enhanced the efficiency and sustainability of photo- and electro-catalytic systems. Biosurfactants, such as humic and fulvic acids, improve pollutant desorption from soil and sediment matrices and increase contaminant bioavailability at catalytic interfaces. Their inherent biodegradability and recyclability offer advantages over synthetic surfactants, enabling accelerated remediation while minimizing secondary environmental impacts. The synergistic combination of semiconductor catalysts with biosurfactants therefore supports targeted, low-energy, and environmentally compatible degradation pathways for persistent contaminants [3].

In order to increase the performance of visible light and charge-carrier dynamics, more recent designs have used doped TiO_2 or doped hybrid composites of semiconductors with nanocarbon (e.g., graphene or carbon nanotubes). Such man-made materials can support better charge separation and minimize recombination losses that make these materials treated with lower energy intensities and natural sunlight. The use of applied potentials to overcome the irradiance requirement, which is central to photochemical technologies, in order to achieve pollutant degradation is further complemented by electrochemical technologies that can operate in covered reactors and in low-light conditions. These systems work together to be climate-neutral remediation systems and to promote decentralized wastewater treatment plants.

Besides these promising capabilities, there are a number of scientific and practical limitations to the way they can be applied in the real world. Most photocatalysts have short lifespans of photogenerated charges, leading to reduced degradation rates of complex wastewater matrices. Moreover, the first-generation performance improvements may depend on the noble-metal dopants Pt, Ru, or Ag, which add high economic and long-term supply risks. There is also catalyst poisoning and surface fouling when subjected to organic-rich waste streams, which reduces the lifespan of materials used and escalates the rate of replacement. Lastly, the advanced photoreactors and electrochemical systems have large capital demands, which become important obstacles to adoption in low-resource environments. The above restrictions highlight the necessity of further work in designing earth-abundant catalysts, antifouling surface engineering, and cost-effective reactor design that can be made to work steadily under realistic environmental conditions.

Altogether, although photo- and electro-catalysis is set to become one of the essential elements of the sustainable control of pollutants, overcoming these obstacles will be an essential step to scalable implementation and the greatest environmental impact of the use of circular-chemistry structures.

4.3 Waste-to-Green Chemical Feedstock Conversion

The transformation of waste streams into green chemical feedstocks represents a critical strategy for sustainable chemical production and carbon footprint reduction. One promising approach involves the utilization of carbon dioxide (CO_2), a major greenhouse gas, as a reactant to produce value-added chemicals such as propylene carbonate. This process not only mitigates CO_2 emissions but also leverages it as a renewable carbon source for industrial applications. Recent studies have demonstrated that CO_2 can be effectively integrated into chemical synthesis pathways, converting waste-derived or renewable feedstocks into high-value products with minimal environmental impact. Specifically, Esmaeili-Chelan and Bahadori [34] reported that the use of CO_2 in propylene carbonate production offers both economic and environmental advantages, highlighting its potential as a sustainable feedstock in green chemistry initiatives. The adoption of such waste-to-chemical conversion strategies provides a dual benefit: reducing reliance on fossil resources and promoting circular economy principles in the chemical industry.

Nonetheless, the 2024-2025 LCA and TEA studies prove that the results of sustainability are extremely contextual. With the aid of renewable heat, logistics optimization, and carbon capture, thermochemical pathways can lower life cycle emissions of greenhouse gases by about 120 percent relative to fossil-based counterparts. However, inefficient purity of feedstock, lack of heat integration, or fossil utilities may reverse these environmental benefits, showing that there is a recurrent requirement of integrated optimization and policy-consistent execution.

4.4 Reusing Plastic Waste through Green Catalytic Innovations

The accumulation of plastic waste remains a pressing environmental concern, with conventional disposal methods contributing to pollution and ecological degradation. Transforming plastic waste into valuable chemical feedstocks via green catalytic processes offers a sustainable approach to address this challenge. Catalytic conversion techniques, including pyrolysis and depolymerization under environmentally benign conditions, enable the breakdown of complex polymer structures into reusable monomers or fuel precursors. Such innovations not only reduce plastic pollution but also contribute to circular economy models by converting waste into high-value products. Recent research highlights the importance of understanding the environmental implications of microplastics, including biodegradable variants, emphasizing the need for greener and more efficient recycling technologies. Lara-Topete et al. [24] underscore that innovative catalytic strategies can minimize secondary environmental risks while enhancing the feasibility of plastic waste valorization. Consequently, green catalytic innovations provide a promising route for sustainable plastic management, promoting both resource efficiency and ecological protection.

5. Self-Healing, Pollutant-Sensing Dynamic Polymers and Membranes

Recent advances in polymer science have led to the development of dynamic materials capable of self-healing and pollutant sensing, offering transformative potential for environmental and structural applications. Self-healing polymers can autonomously repair mechanical damage, thereby extending material lifespan and reducing maintenance costs. When integrated into membranes, these polymers can also be functionalized to detect and respond to environmental pollutants, enabling real-time monitoring and remediation. Such dynamic materials combine structural resilience with active sensing capabilities, aligning with the principles of sustainability and smart material design. According to An et al. [39], self-healing structural polymers demonstrate significant potential for applications where durability and environmental responsiveness are critical, underscoring the value of integrating self-repair mechanisms with pollutant detection in advanced membrane systems. The convergence of self-healing and sensing functionalities in polymers thus represents a promising strategy for sustainable material innovation. In spite of the promising developments in self-healing and pollutant-sensing polymers, research indicates that laboratory-controlled success does not always translate directly to real-world environments. In practical applications, factors such as fouling agents, microbial biofilms, and physical abrasion can compromise the efficiency of the self-healing chemistries during repeated use. Environmental conditions, including temperature fluctuations, salinity changes, and ultraviolet exposure, can gradually degrade dynamic bonding networks, reducing both reliability and the functional lifetime of these materials [39]. There is also concern that nanoscale fragments or degradation products could be released into ecosystems during long-term utilization, highlighting the need for careful containment or immobilization strategies to avoid secondary contamination.

Table 3. Multifunctional green materials for air, water, and soil remediation.

Application	Green Material Type	Responsive or Functional Feature	Pollutant Targeted	Performance Conditions	Ref.
Air remediation: oxidation of VOC	CuO-TiO_2; TiO_2-C photocatalytic aerogels	Visible/solar-light activated photocatalysis; high porosity for enhanced adsorption and reaction coupling	VOCs (e.g., toluene)	~93-94% removal under visible/solar-light irradiation; stable over multiple cycles; minimized metal leaching	[4,6]
Water Treatment	Chitosan/polyethyleneimine (PEI) magnetic hydrogel composite	pH-responsive chelation via abundant amine groups; magnetic responsiveness enabling rapid separation and recyclability	Pb^{2+}, Ni^{2+}, Cu^{2+}	Optimal adsorption at pH 5-6; rapid uptake at ambient temperature; equilibrium within short contact time; efficient magnetic recovery; stable adsorption over multiple regeneration cycles with minimal capacity loss	[40]
Soil Remediation	Organomineral reagents based on natural minerals combined with organic modifiers	Combined adsorption, immobilization, and stimulation of biodegradation; redox-active mineral phases enhancing hydrocarbon oxidation and microbial activity	Petroleum hydrocarbons (crude oil fractions, alkanes, aromatics)	Significant reduction of total petroleum hydrocarbons under ambient soil conditions; effective under natural moisture and aeration; enhanced remediation over treatment period without secondary pollution; stable soil structure and fertility restored after treatment	[3]

To ensure that these innovative materials achieve tangible sustainability benefits, strict performance assessment frameworks are necessary. Such frameworks should go beyond laboratory healing efficiency to evaluate long-term cycling stability, resistance to fouling, and validation under realistic environmental conditions. Eco-compatibility testing is also essential to assess potential environmental risks of aging products, while techno-economic and LCA help confirm that no negative impacts are transferred across the value chain. Incorporating durability and safety considerations during the initial stages of material development is crucial to align self-healing and sensing polymers with SSbD principles.

Dynamic remediation systems built from these materials represent an emerging trajectory in next-generation environmental management. By integrating pollutant retention, smart detection, and adaptive response, they can enhance decentralized treatment frameworks and maintain resilience under fluctuating environmental conditions. To unlock their full practical potential, research must progress beyond laboratory-scale demonstrations toward validated real-world applications, ensuring that improvements in performance, durability, and service life lead to measurable environmental benefits. Representative examples of multifunctional and responsive technologies, such as photocatalytic aerogels, pH-responsive hydrogels, and redox-active biobased foams, demonstrate the capacity of these materials to remove or degrade pollutants across air, water, and soil matrices under realistic conditions. Smart green materials are therefore more than passive tools; they act as adaptive environmental allies, capable of regenerating, responding, and sustaining high performance, offering a durable and sustainable approach to advanced pollution control (Table 3).

Smart green materials are more than just tools, they are environmental allies that adapt, react and regenerate. By serving multiple purposes that are perfectly effective and being very durable, they are a sustainable option for pollution control equipment.

5.1 Energy-Efficient Green Practices–Reducing Adsorbent Pollution Control Carbon Footprint

Energy- efficient green remediation practices are increasingly recognized as essential components of sustainable pollution control, particularly in adsorption- based systems. Traditional pollutant removal often focuses solely on contaminant elimination, but modern green remediation emphasizes minimal energy input, reuse of resources, and lower carbon emissions, aligning with principles of green chemistry such as atom economy and ambient condition processing. These indicators help guide the design of treatment systems that are both low- impact and operationally efficient.

One experimental study evaluated locally sourced low- cost adsorbents (concrete pellets, steel wool, wood chips, and diatomite) for removing hydrogen sulfide from biogas in a fixed- bed column. By coating materials with ferric hydroxide and operating under moderate flow conditions without high temperature or pressure, the system demonstrated high removal efficiency (~99.2%) with simple mechanical operations, reflecting reduced energy demand relative to conventional biochemical scrubbing methods. This illustrates how accessible waste materials can be tailored into effective adsorbents while limiting energy consumption in treatment design [45]. Recent studies demonstrate that the use of sustainable adsorbents not only effectively reduces pollutant concentrations but also significantly lowers the chemical inputs and energy demands of water treatment processes. This dual advantage renders sustainable adsorbents, particularly biomass-derived biochar, highly attractive for the development and deployment of environmentally friendly and resource-efficient water treatment technologies [46,47], similarly, designs of zero-carbon wastewater treatment focus on energy reuse and reduced emissions [31,48,49].

The comparison of the proportionate effects of green chemistry metrics has been demonstrated in Figure 2 (atom economy (~80 %), less hazardous synthesis (~75%), safer solvents (~70%), and energy efficiency (~65%) and reveals that the main focus on reaction design and on remediation pathways that inherently reduce wastes and fish consumption of energy should be the prioritized concern. In order to support the energy-efficiency argument.

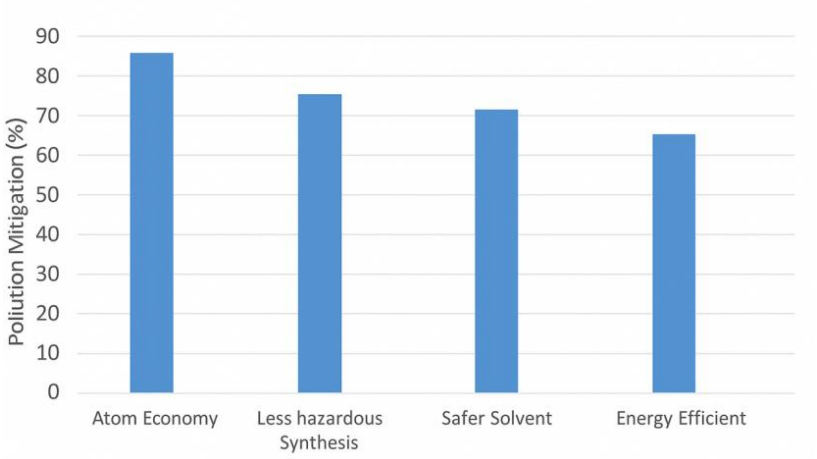

Figure 2. Green chemistry practices and its role in the reduction of pollution by chemical treatment plants.

The comparative analysis of core green chemistry practices including element economy, less hazardous synthesis, safer solvent selection, and improved energy efficiency illustrates their estimated contributions to reducing pollution in industrial chemical treatment facilities. The information has been adapted from recent assessments of global green chemistry progress and sustainability metrics.

A comparative analysis of core green chemistry practices including atom economy, less hazardous synthesis pathways, the use of safer solvents, and improved energy efficiency has been conducted to evaluate their potential in reducing pollution within industrial chemical treatment facilities. Experimental studies and industrial implementations demonstrate that continuous and microflow manufacturing approaches can significantly enhance material efficiency and reduce waste generation by optimizing reaction conditions and minimizing excess reagents. These intensified processes are typically characterized by smaller reactor volumes, shorter residence times, and precise control over reaction parameters, which inherently lower the risk of large-scale accidents and improve the intrinsic safety of chemical production. Moreover, the electrification of microflow systems provides additional opportunities for energy-efficient operation, further reducing the environmental footprint of chemical manufacturing [50,51].

5.2 Innovative Energy-Efficient Methods and Improvements to Reduce Pollution

Pollution control techniques today rely very much on the principles of process intensification, where existing multiphase, multistep operations are rendered very intensive. Today, catalytic systems can eliminate or change pollutants at room temperature and pressure, resulting in a large energy saving. Processes that mimic nature to achieve the same or even better results usually require less energy when compared to previous solutions.

5.3 Renewable Energy Sources Used at Green Chemical Treatment Plants

The integration of renewable energy sources into chemical treatment plants is a pivotal strategy for advancing green chemistry and reducing the environmental footprint of industrial operations. Utilizing renewable energy such as solar, wind, biomass, and geothermal enables chemical processes to operate with significantly lower greenhouse gas emissions while supporting energy self-sufficiency. In the context of green chemical treatment, renewable energy can power reactors, separation units, and ancillary systems, reducing reliance on conventional fossil fuels and enhancing overall process sustainability.

Cheng [5] emphasizes that the adoption of renewable energy in chemical process development not only mitigates the carbon footprint but also aligns with green chemistry principles, particularly in designing processes that operate under ambient conditions with minimal energy input. By coupling renewable energy systems with process optimization, chemical treatment plants can achieve both environmental and economic benefits, including reduced operational costs, improved energy efficiency, and a measurable decrease in emissions. The strategic use of renewable energy also facilitates the production of value-added chemicals through eco-friendly pathways, reinforcing circular economy objectives and sustainable industrial practices.

Renewable energy sources play a crucial role in reducing greenhouse gas emissions and promoting sustainable development. Based on 2024 global electricity generation data, the renewable energy mix is composed of hydropower (~14.3 %), wind (~8.1 %), solar Photovoltaic (PV) (~6.9 %), and bioenergy, geothermal, and other renewables (~2.6 %), collectively contributing approximately 32 % of global electricity generation. This distribution highlights hydropower as the largest single contributor among renewable sources, while wind and solar PV also play significant roles in improving energy efficiency and supporting sustainable industrial operations, as illustrated in Figure 3.

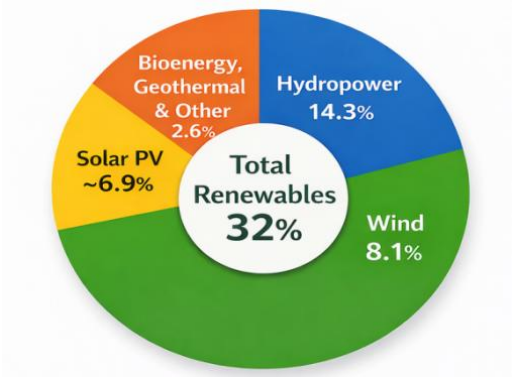

Figure 3. Renewable energy allocation in hybrid energy- harvesting systems for green chemical treatment plants.

Based on 2024 global electricity generation data, the renewable energy mix comprises hydropower (~14.3 %), wind (~8.1 %), solar PV (~6.9 %), and bioenergy + geothermal & other renewables (~2.6 %), totaling approximately 32 % of global electricity generation. These proportions represent the dominant renewable sources contributing to energy efficiency in sustainable industrial operations [52].

6. Energy Harvesting and Pollutant Degradation Work Together in Hybrid Systems

The most exciting area of energy-optimized pollution control is hybrid systems that harvest energy and remediate pollutants at the same time. The systems use multifunctional materials that absorb solar energy to produce the reactive species required for the decomposition of pollutants. In this type of design, pollution is not just removed, It powers itself to remove. Recent research highlights several innovative implementations of this dual- purpose approach. For example, solar- powered photothermal- photocatalytic platforms have been engineered to simultaneously drive seawater desalination and degrade antibiotic contaminants under one sun illumination, demonstrating nearly complete degradation of organic pollutants while harvesting solar energy for water purification and energy conversion processes. Such systems validate the feasibility of combining energy harvesting with pollutant breakdown in a single integrated unit [53].

Two activities can be done in a single integrated system through the use of solar energy, one of which is electricity generation while the other one is water purification. "Our dual-purpose technologies bring the best of both worlds, recycling sunshine and waste into energy while providing a cleaner environment." Combining energy conversion and pollutant degradation (the process of breaking down harmful substances) into one hybrid unit allows for unprecedented efficiency and sustainability This integrated approach addresses the critical water-energy nexus, where the interdependence of water and energy resources demands synergistic solutions for sustainable development [53].

The green processes, which are energy-optimized, present an exciting route to pollution control systems that are effective, scalable and climate-friendly. With renewable energy and intelligent design included, environmental remediation will be cleaner and smarter, in addition to being lighter and greener.

7. A Real-Time Approach for in-Situ Monitoring for Pollution Prevention

Recent developments in green analytical chemistry have changed the existing pollution prevention methods of detecting pollutants at the end-point to real-time, in situ measurements. The recent environmental friendly sensors include miniaturized electrochemical, optical, and nanocomposite based biosensors, which allow the uninterrupted monitoring of the environment at sources of emissions. The period 2023 to 2025 has seen an increase in the application of ML algorithms to sensor systems with a view of improving the accuracy of analytical results, automate the calibration process, and generate trends in contaminants based on large and streaming data. Pattern-recognition models and neural network algorithms are used on complex multi-analyte signals by the ML-enabled platforms and enhance detection sensitivity and decrease false positives.

It is also important that the validation metrics guarantee the reliability of the sensor during field conditions. Some of the current best practices focus on parameters like the limit of detection, response time, recovery rate, and coefficient of determination as compared to reference laboratory practices. Cross-validation and error propagation analysis has now been used in data-driven calibration models to ensure the analytical accuracy of models used in a dynamic environment.

Moreover, green methods of sample preparation such as solvent-free microextraction, portable solid-phase adsorption, and non-invasive optical probing reduce wastes and use of risky substances. All of these innovations create a new paradigm of sustainable intelligent systems of monitoring that allows proactive control of pollution and minimize the environmental footprint of analytical processes [54].

8. Green Chemistry into Policy Education and Market Activities

Incorporation of green chemistry concepts in policy, education and industrial markets is one of the pillars of sustainable change. In the past ten years, numerous governments and regulation bodies realized that scientific innovation has to be accompanied by a supportive legal and economic environment. Fiscal incentives, eco-labelling and technology subsidies are encouraged in various policies including the European Green Deal, the U.S. EPA Green Chemistry Program and the United Nations Environment Programme (UNEP) Global Green and Sustainable Chemistry Initiative (2025) to encourage the industry to comply. Such actions hasten the process of the traditional manufacturing to the less hazardous, low-carbon level of manufacturing chemicals.

One of the key policy developments is the SSbD framework that the European Commission implemented in 2023 to be incorporated in EU value chains. SSbD encourages industries to integrate environmental safety, material circularity and hazard mitigation requirements at the initial design phases of chemical and material manufacturing. It will standardize the measures of assessment and demand transparency of the life-cycle in order to make sustainability a pre-market requirement and not a post-market intervention.

Simultaneously, the integration of green chemistry principles into educational curricula and professional training programs strengthens the human capital required for the development and implementation of SSbD innovations. This interdisciplinary interaction among policy makers, academia, and industry fosters a synergistic ecosystem in which scientific advancement aligns with economic competitiveness and environmental stewardship. Such alignment is particularly critical given that earlier safety-oriented design paradigms, including the pharmaceutical sector’s “benign

by design" framework, often considered life-cycle performance and environmental impacts only indirectly or to a limited extent [55].

8.1 Integrated Modern Approaches to Pollution Mitigation

The integration of conventional pollution control methods with advanced and emerging technologies, guided by green chemistry principles, plays a crucial role in enhancing environmental sustainability and reducing the ecological footprint of industrial processes [56]. This integration is essential because it overcomes the inherent limitations of individual treatment techniques while promoting a more holistic and effective framework for managing environmental contaminants. Recent innovations, particularly in nanotechnology and advanced oxidation processes, are transforming pollution mitigation by enabling highly efficient, selective, and rapid contaminant removal compared to traditional approaches. These technologies are especially effective in addressing emerging and recalcitrant pollutants that resist conventional treatment pathways. Their adoption is increasingly important for safeguarding environmental integrity, food safety, and public health, particularly as traditional analytical and remediation methods are often resource-intensive and costly. Moreover, modern remediation technologies are designed to overcome operational challenges such as high energy consumption, excessive chemical use, and the generation of secondary waste streams, which have historically constrained the effectiveness of conventional strategies. Importantly, these advances incorporate key green chemistry principles, including reduced toxicity, improved atom economy, and safer process design, thereby minimizing ecological impacts and enhancing resource efficiency throughout the remediation lifecycle. Overall, the integration of modern technologies with established treatment methods represents a significant advancement toward sustainable and resilient pollution mitigation strategies, addressing both the complexity and performance instability commonly associated with conventional systems. In contrast, traditional wastewater treatment processes such as biological degradation, ion exchange, and adsorption often prove insufficient for the effective removal of persistent organic pollutants, frequently resulting in their redistribution across environmental compartments rather than complete elimination [57].

8.2 Policy Integration and SSbD Operationalization

This study now relates technology innovation to the emerging global and European regulatory framework to ensure proper safety and sustainability of the AI-enabled agricultural waste valorization pathways. The SSbD framework was developed to implement the EU Chemicals Strategy for Sustainability by the European Commission which provides a harmonised methodology to enable the early integration of safety, circularity and life-cycle thinking in products and process development [58].The SSbD approach takes a preventive design perspective, focusing on sustainability performance metrics, process transparency, and goal-oriented hazard reduction throughout the entire innovation chain [59].

The operationalization of SSbD in AI-enabled agricultural waste valorisation can be structured around four interconnected steps: (1) early screening and sustainability mapping, where digital LCA/TEA templates and AI-based hazard identification models are applied to emerging feedstock-to-product pathways before pilot-scale validation [60]; (2) iterative design-for-sustainability, in which generative AI and ML algorithms optimize bioconversion and process parameters against multi-objective SSbD benchmarks [61]; (3) transparent traceability and data integrity, achieved through AI-Blockchain integration that secures LCA/TEA datasets, ensuring tamper-proof compliance and verifiable sustainability reporting [62]; (4) regulatory co-validation and feedback loops, involving stakeholders, policymakers, and industry consortia to refine metrics, ensuring alignment with ISO 14040 (LCA) and ISO 59020 (Circular Economy) data standards [63].

According to recent guidance from the European Commission Joint Research Centre, there are pilot applications and testing methods to enhance SSbD. This is for the industry bioeconomy systems. [64] Internationally, policy coherence with UNEP's Circular Economy initiatives and EU's Green Deal promotes cross-sectoral alignment that allows AI-enabled valorization systems to access green financing, carbon-credit mechanisms and sustainability certifications frameworks [65,66]. AI-driven life-cycle workflows and embedding SBSD can create digital compliance ecosystems where data interoperability can be delivered under the findable, accessible, interoperable, reusable (FAIR) principles [67].

In the end, putting SSbD into action makes sure that using AI to manage agricultural waste is not just technologically advanced but also morally and environmentally sound, bridging innovation, governance, and sustainability objectives of the circular bioeconomy [68].

9. Green Chemistry Technologies for Pollution Control

9.1 Overview of Green Chemistry in Pollution Mitigation

Green chemistry plays a transformative role in addressing environmental contamination by providing sustainable scientific approaches that eliminate or reduce hazardous substances at the source. Recent advancements emphasize that green chemistry offers innovative pathways for designing safer chemicals, optimizing reaction efficiency, and

minimizing waste generation. Laddha PR et al. [69] highlight that modern green chemistry strategies have significantly reduced the ecological footprint associated with conventional chemical synthesis by integrating sustainability throughout the production process. Rather than relying on end-of-pipe treatment, green chemistry prioritizes pollution prevention, making it a vital framework for tackling pollution challenges globally (Figure 4).

This schematic diagram above illustrates the major components of the global pollution challenge. The left panel identifies key pollution sources industrial emissions, transportation exhaust, agricultural runoff, and municipal waste which represent the dominant contributors of contaminants into the environment. These pollutants then move through three primary environmental pathways: air, water, and soil, as shown in the center panel. The right panel highlights the ecosystems that become directly impacted by these pathways, including aquatic systems (rivers, lakes, and marine environments), terrestrial habitats (plants, forests, and soils), and broader biodiversity (birds, insects, and wildlife). Collectively, the figure provides a simplified conceptual framework that links pollution sources to their environmental transmission routes and ecological consequences, thereby supporting the thematic structure of the review.

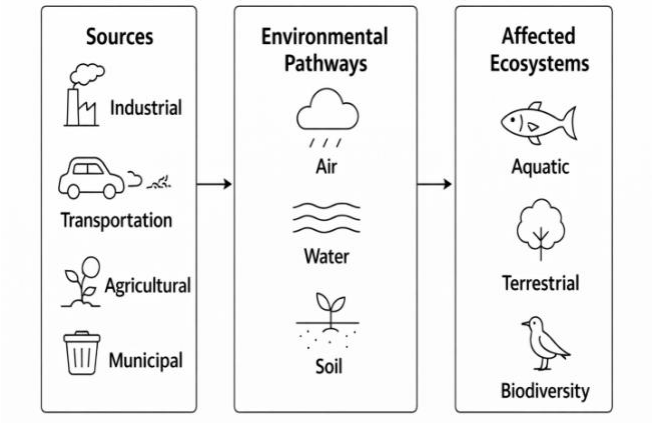

Figure 4. Overview of the pollution problem: sources, environmental pathways, and affected ecosystems.

9.2 Sustainable Chemical Processes and Emission Reduction

Green chemistry technologies provide practical and scalable solutions for reducing the release of hazardous chemicals and industrial emissions. The adoption of safer solvents, renewable feedstocks, and cleaner reaction pathways has been shown to substantially enhance environmental protection while sustaining industrial productivity. These strategies not only reduce chemical toxicity but also promote long-term sustainability by limiting the accumulation of persistent contaminants in soil, air, and water systems. Technological innovation, particularly in green chemistry, is therefore integral to reducing carbon dioxide emissions and improving overall environmental quality, especially within technologically advanced economies [70,71] emphasize that green chemistry contributes to combating climate change, acid rain, and global warming by improving reaction selectivity, increasing efficiency, and decreasing waste generation. Such advancements reduce energy consumption and greenhouse gas emissions, making chemical processes more environmentally responsible.

9.3 Green Bioremediation Technologies for Emerging Pollutants

Emerging contaminants including pharmaceuticals, dyes, and endocrine disruptors pose serious environmental and health risks due to their persistence and toxicity. Green chemistry-driven bioremediation technologies offer effective alternatives for degrading these complex pollutants. According to [72], bacterial laccases and other biologically based systems provide eco-friendly degradation of contaminants, operate under mild conditions, and minimize secondary pollution. These technologies demonstrate how green chemistry enhances environmental restoration by substituting hazardous reagents with natural catalytic systems, improving both safety and sustainability.

9.4 Principles of Green Chemistry and Their Role in Environmental Protection

The foundational principles of green chemistry guide the design of safer chemicals and cleaner production methods. Kurul et al. [73] emphasize that these principles including atom economy, reduced toxicity, use of renewable feedstocks, and design for degradability promote sustainable chemical management throughout a product's life cycle. By conserving natural resources, reducing hazardous substance generation, and encouraging environmentally friendly product design, green chemistry strengthens global environmental protection efforts. These principles also provide a scientific basis for developing future technologies that align with circular economy goals and long-term sustainability.

10. Future Perspectives

Green chemistry is entering a new era, driven by the integration of AI, ML, and the Internet of Things (IoT) into sustainability-oriented research and industrial innovation. These technologies enable predictive modeling, data-driven

optimization, and real-time process monitoring enhancing efficiency while minimizing waste and environmental impact [59].

10.1 Digital Intelligence and Green Chemistry Transformation

The convergence of AI, ML, and IoT has revolutionized how chemical synthesis and materials design are conceptualized and optimized. In green chemistry, these tools support predictive reaction modeling, automated process control, and eco-efficiency analysis, allowing researchers to minimize hazardous reagent use and energy consumption. Such data-driven insights are pivotal for achieving pollution prevention, waste reduction, and circular economy integration [59].

10.2 Safe and Sustainable by Design Approaches for Pollution Mitigation

SSbD approaches emphasize the proactive incorporation of safety and sustainability into environmental technologies and remediation strategies, aiming not just to treat pollution, but to prevent its generation and reduce its broader ecological impact. Environmental pollution adversely affects both wildlife and human health through pathways such as contaminated water, air, and soil, leading to diseases, ecosystem disruption, and reduced quality of life. Addressing these challenges requires innovative mitigation strategies that go beyond conventional pollution control methods to embrace principles of sustainability, prevention, and life-cycle thinking [1].

Recent research highlights a variety of novel mitigation strategies aligned with SSbD principles, including bioremediation, phytoremediation, and other technology-driven approaches that seek to harness natural and engineered processes for more effective pollution removal. For instance, bioremediation employs microorganisms to break down contaminants into harmless substances, reducing the need for energy-intensive physical or chemical treatment methods and minimizing secondary waste streams. Similarly, phytoremediation uses plants to absorb, degrade, or stabilize pollutants, thereby integrating ecosystem-based solutions with remediation objectives. These techniques exemplify the SSbD ethos by prioritizing minimal environmental disruption, increasing resource efficiency, and lowering ecological and human health risks associated with pollution [1].

Moreover, effective SSbD approaches underscore the importance of public participation and awareness, collaboration among stakeholders, and systemic change across regulatory, industrial, and community levels to implement sustainable practices. This holistic approach recognizes that technological innovation must be coupled with social engagement and policy frameworks that support enduring pollution control outcomes. By leveraging cutting-edge methods such as advanced biotechnologies within a preventive design framework, SSbD contributes to more resilient and sustainable pollution mitigation, aligning remediation practice with broader environmental sustainability goals and reducing the long-term impacts on ecosystems and human health.

10.3 Toward a Climate-Resilient and Autonomous Green Innovation Model

The next phase of green chemistry will rely on synergistic collaboration among academia, industry, and policy institutions to translate computational insights into scalable, ethically governed technologies.

Applications may include: microplastic degradation systems driven by AI-optimized catalysis; carbon capture and conversion platforms; green nanomaterial synthesis frameworks aligned with SSbD standards.

The convergence of AI-based predictive chemistry, SSbD-guided regulation, and ethical accountability will transition the field from reactive management to autonomous, transparent, and climate-resilient innovation [59,74].

This integrated model establishes the foundation for a sustainable digital ecosystemwhere technology, ethics, and environmental stewardship progress in harmony.

The future development should, nevertheless, be captured under ethical AI roadmaps, which will be transparent, explainable, and answerable of the algorithm applied in green chemical innovation. Digital intelligence, LCA and the combination of eco-design metrics will determine new paradigms of sustainable manufacturing. The cooperation between academia, industry, and policy institutions will be also crucial to convert computational understanding into scalable green technologies that would be able to solve the issues of microplastic pollution, carbon capture, and sustainable material synthesis. Finally, the integration of AI-based predictive chemistry, SSbD regulation, and ethical accountability will transform the field to a new direction- no longer reactive control but autonomous, ethically accountable, and climate-resilient green chemistry [59].

11. Conclusion

This review demonstrates that the fusion of AI, green chemistry, and SSbD methodologies offers a practical foundation for designing safer chemicals, reducing emissions, and promoting circular resource flows. However, realizing these benefits at scale requires overcoming well-defined constraints in catalyst performance, data standardization, and the alignment of AI outputs with regulatory expectations. Future studies should adopt integrated frameworks that simultaneously evaluate safety, degradability, cost, and circularity moving beyond isolated assessments toward unified

decision-support systems. The development of robust AI-LCA models, transparent digital traceability platforms, and universal SSbD indicators will be central to this transition. Importantly, ethical AI governance and global knowledge-sharing must underpin these innovations to ensure equitable deployment across both high-income and developing economies. By advancing these constructive pathways, researchers and industry stakeholders can shift sustainability from aspirational rhetoric to measurable, scalable, and scientifically grounded impact.

Conflict of Interest

The authors declare they have no conflicts of interest.

Generative AI Statement

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

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