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Artificial Intelligence in Chemistry for Future Sustainability: An In-Depth Scientific Review

Shyamalkant K. Biswas[1]

[1]Department of Chemistry, R.D. College of Science, Aheri, India

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Abstract: Artificial Intelligence (AI) is rapidly transforming chemical sciences by enabling data-driven molecular discovery, reaction prediction, and process optimization. Simultaneously, global sustainability challenges such as climate change, pollution, and energy scarcity require innovative chemical solutions with minimal environmental impact. The integration of AI with chemistry offers a powerful framework for achieving sustainable development through green molecular design, energy-efficient catalysis, optimized industrial processes, and enhanced environmental monitoring. This review critically examines recent advances in AI-driven chemistry and evaluates their role in promoting future sustainability, while highlighting challenges related to data quality, interpretability, energy consumption, and ethical governance [1–5].

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I. INTRODUCTION

Chemistry is central to modern civilization, influencing sectors ranging from pharmaceuticals and agriculture to energy and materials. However, conventional chemical processes are often resource-intensive and environmentally damaging, contributing to greenhouse gas emissions, hazardous waste, and ecosystem degradation [11,13]. Sustainable chemistry seeks to address these issues through safer chemicals, energy-efficient reactions, and circular material flows.

Artificial Intelligence (AI), encompassing machine learning (ML), deep learning (DL), and data-centric modeling, has emerged as a transformative tool in chemical research [2,18]. AI systems can process vast chemical datasets, uncover hidden patterns, and accelerate discovery cycles beyond human capabilities. When aligned with the principles of green chemistry, AI enables predictive and preventive approaches rather than corrective ones [16,17].

II. FUNDAMENTALS OF AI IN CHEMICAL SCIENCES

- *Machine Learning Techniques*

Machine learning algorithms establish relationships between molecular descriptors and target properties such as toxicity, solubility, or catalytic activity [3,20]. Commonly used techniques include random forests, support vector machines, and gradient boosting models [51].

- *Deep Learning and Neural Networks*

Deep learning models excel in handling high-dimensional chemical data, including spectra, images, and molecular graphs [19]. Graph Neural Networks (GNNs) are particularly effective in chemistry because they directly encode atomic connectivity and bonding environments [37,38].

- *Generative Models*

Generative AI models such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) can design novel molecules optimized for sustainability metrics such as low toxicity, biodegradability, and atom economy [5,14,17].

III. AI-DRIVEN MOLECULAR DESIGN FOR SUSTAINABILITY

AI enables inverse molecular design, where desired environmental and functional properties are specified first and suitable molecules are generated computationally [17]. This paradigm shift significantly reduces experimental trial-and-error. AI-designed molecules have been proposed for: Green solvents [16], Safer pharmaceuticals [19], Sustainable agrochemicals [11] Generative chemistry frameworks allow the rapid screening of millions of candidate structures, accelerating sustainable innovation while minimizing chemical waste [4,5].

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IV. AI IN CATALYSIS AND SUSTAINABLE ENERGY CHEMISTRY

Catalysts are essential for sustainable chemical transformations because they reduce energy requirements and increase selectivity [21,25]. AI models predict catalyst activity, stability, and deactivation mechanisms, significantly shortening discovery timelines [22,28]. AI-guided research has advanced: Hydrogen evolution catalysts [23,26] CO_2 reduction systems [24,29] Photocatalysts for solar fuel generation [27] These developments are critical for decarbonizing chemical industries and supporting renewable energy transitions [10,23].

V. REACTION PREDICTION AND GREEN SYNTHESIS PLANNING

Deep learning models such as transformer architectures accurately predict reaction outcomes, yields, and side products [31,32]. These tools reduce failed reactions and unnecessary reagent consumption. AI-based retrosynthesis planners propose synthetic routes that prioritize:

Fewer reaction steps Benign reagents Lower solvent and energy usage [6,35,38] Such approaches align directly with the 12 principles of green chemistry and significantly reduce environmental footprints [16,18].

VI. AI IN PROCESS OPTIMIZATION AND CHEMICAL MANUFACTURING

AI is increasingly integrated into chemical engineering through digital twins, surrogate models, and real-time optimization systems [42–44]. These technologies enhance energy efficiency, safety, and waste minimization in large-scale production. Smart chemical plants utilize AI for: Predictive maintenance [46], Process control and optimization [41,45] , Emission reduction strategies [47], These advancements contribute to sustainable industrial development and Industry 4.0 frameworks [48].

VII. ENVIRONMENTAL MONITORING AND REMEDIATION

AI systems analyze chemical sensor data, satellite imagery, and environmental measurements to detect pollutants and predict their dispersion [49,52]. Machine learning models support water quality monitoring, soil contamination assessment, and atmospheric chemistry modeling [53–55]. AI-driven environmental chemistry enhances decision-making in pollution control and climate mitigation strategies [50,56].

VIII. LIFE CYCLE ASSESSMENT AND CIRCULAR CHEMISTRY

Life Cycle Assessment (LCA) evaluates environmental impacts across a product's entire lifecycle. AI improves LCA by handling large, heterogeneous datasets and predicting impacts at early design stages [50,56]. This capability supports circular chemistry approaches, enabling:

Material reuse and recycling, Waste-to-resource pathways, Sustainable supply chain optimization [48,57]

IX. CHALLENGES AND ETHICAL CONSIDERATIONS

Despite its promise, AI-driven chemistry faces several challenges: Data bias and scarcity limit model generalization [58]. Black-box models hinder interpretability and regulatory acceptance [57]. High computational energy demands may offset sustainability gains [10].

Ethical and dual-use concerns require responsible governance [49,59]. Addressing these issues is critical for long-term adoption and societal trust.

X. FUTURE PERSPECTIVES

Future research will focus on: Autonomous laboratories combining AI and robotics [33,34], Hybrid quantum-AI chemical simulations [28], Explainable and energy-efficient AI models [57,60], Policy-aligned AI frameworks supporting UN Sustainable Development Goals [61], Education and interdisciplinary collaboration will be essential for training chemists capable of responsibly leveraging AI technologies [60].

XI. CONCLUSIONS

The convergence of AI and chemistry represents a paradigm shift toward sustainable scientific practice. From molecular design to industrial manufacturing and environmental protection, AI offers powerful tools to minimize environmental impact while accelerating innovation. However, realizing this potential requires careful attention to ethical, computational, and data-centric challenges. With responsible implementation, chemistry AI can play a pivotal role in shaping a sustainable future [1–61].

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