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A Comprehensive Review of Artificial Intelligence Applications in Chemistry

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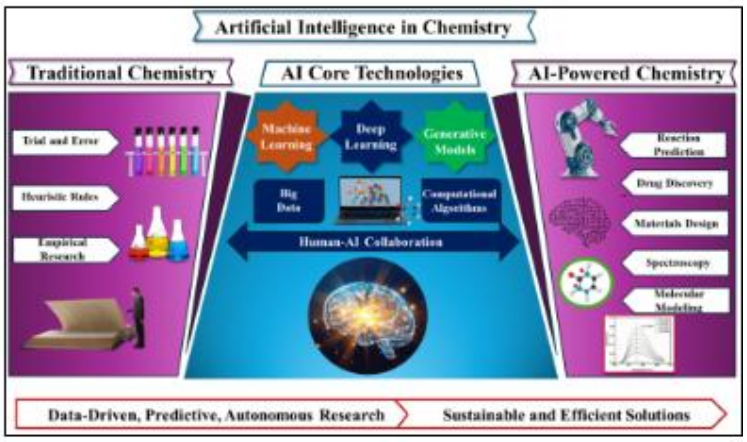
Abstract: *Artificial intelligence (AI) is rapidly transforming the chemical sciences by enabling data-driven analysis, predictive modeling, and automated decision-making across diverse research domains. Traditional chemical research, which relies heavily on empirical rules and human intuition, often faces limitations when addressing complex molecular systems and large-scale chemical data. Recent advances in machine learning, deep learning, and generative artificial intelligence have significantly improved the ability to predict molecular properties, reaction outcomes, and material performance, thereby accelerating chemical discovery and optimization. This review presents a comprehensive overview of the evolution of artificial intelligence in chemistry, focusing on fundamental AI methodologies and their applications in molecular modeling, chemical space exploration, drug discovery, reaction prediction and retrosynthesis, catalyst and materials design, analytical and spectroscopic chemistry, laboratory automation, green chemistry, and industrial process optimization. The advantages of AI-driven approaches, including reduced development time, improved accuracy, enhanced reproducibility, and cost efficiency, are critically examined alongside key limitations, including data dependency, model interpretability, infrastructure requirements, and ethical and regulatory concerns. By synthesizing recent literature, this review highlights current research trends, identifies existing challenges, and outlines future directions emphasizing explainable AI, standardized data practices, and effective human-AI collaboration for the responsible advancement of chemical sciences*

Keywords: Artificial intelligence; Machine learning; Computational chemistry; Drug discovery; Reaction prediction; Materials informatics; Autonomous laboratories; Generative models

Graphical abstract: A Comprehensive Review of Artificial Intelligence Applications in Chemistry



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I. INTRODUCTION

The chemical sciences are undergoing a profound digital transformation driven by artificial intelligence (AI), which is fundamentally reshaping how chemical knowledge is generated, interpreted, and applied[1–3]. Historically, chemical discovery relied heavily on human intuition, empirical experimentation, and theoretical approximations derived from physical chemistry and quantum mechanics. Although these approaches led to numerous landmark discoveries, they were often time-consuming, resource-intensive, and limited by the complexity of chemical systems and human cognitive constraints [4,5].

The emergence of AI has introduced a paradigm shift toward data-centric, predictive methodologies, enabling the extraction of meaningful patterns from vast chemical datasets that were previously unmanageable with conventional approaches [6]. Machine learning (ML) algorithms and deep learning (DL) architectures now allow researchers to model complex molecular interactions, predict reaction pathways, and design compounds with tailored physicochemical and biological properties[7–9]. These capabilities have transformed chemistry from a predominantly hypothesis-driven discipline into a predictive science, where in silico models guide experimental decision-making[10].

Recent literature highlights that traditional heuristic and rule-based strategies are increasingly being replaced by intelligent computational frameworks that leverage advanced algorithms, high-performance computing, and large-scale chemical databases [11,12]. This methodological evolution represents one of the most significant shifts in chemical research since the advent of quantum chemistry and computational modeling[13]. The growing influence of AI is evident across both academia and industry, where it is now routinely applied in pharmaceutical research, materials science, green chemistry, and smart chemical manufacturing [14,15]. Machine learning-assisted structure function analysis, automated retrosynthesis planning, and real-time process optimization are rapidly becoming integral components of modern chemical workflows [16].

Moreover, AI has demonstrated remarkable success in predicting reaction outcomes, controlling regio and stereoselectivity, accelerating catalyst discovery, and simplifying complex synthesis planning[17,18]. These advances have significantly reduced the need for experimental trial and error and enabled chemists to explore chemical space with unprecedented efficiency. A major milestone underscoring the scientific importance of AI was the awarding of the 2024 Nobel Prize in Chemistry for computational protein design and protein structure prediction, recognizing groundbreaking AI-driven approaches that revolutionized the understanding of biomolecular structure and function [19]. This recognition signals the maturation of AI from a supportive computational tool to a central engine of chemical discovery.

Despite these transformative advances, the rapid adoption of AI in chemistry introduces critical challenges. Issues related to data quality, algorithmic bias, model interpretability, reproducibility, and academic integrity have emerged alongside concerns regarding cybersecurity, ethical deployment, and regulatory oversight [20–22]. Addressing these challenges is essential to ensure the responsible and transparent integration of AI into chemical research. Consequently, there is a growing emphasis on explainable AI, standardized datasets, and interdisciplinary collaboration to maximize the benefits of intelligent systems while minimizing associated risks [23].

II. OBJECTIVES OF THE REVIEW

This review aims to:

- Provide a comprehensive overview of AI methodologies relevant to chemistry.
- Examine state-of-the-art applications across major chemical domains.
- Critically evaluate benefits, limitations, and research gaps.
- Analyze emerging trends likely to shape the next generation of chemical research.
- By synthesizing findings from approximately fifty influential studies, this article presents a structured perspective on how AI is redefining chemical sciences.

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Evolution of Artificial Intelligence in Chemistry

The integration of computation into chemistry is not new; early quantum chemical models already relied on numerical methods to approximate molecular behavior[2,5]. However, classical computational techniques were limited by scaling challenges and required extensive human intervention[4,13].Modern AI has introduced adaptive algorithms that can learn directly from data[1]. The field has progressed from rule-based systems to deep neural networks and active learning frameworks that continuously improve predictions through feedback loops[10,24], as illustrated in **Figure 1**.

One of the earliest breakthroughs in AI-driven drug discovery was Atom Net, a deep convolutional neural network designed to predict bioactivity of small molecules[25]. By applying hierarchical feature extraction to structural data, the model achieved high predictive performance and outperformed traditional docking approaches on benchmark datasets[8].Such advances demonstrated that neural architectures originally developed for image recognition could be successfully adapted to chemical problems[7].

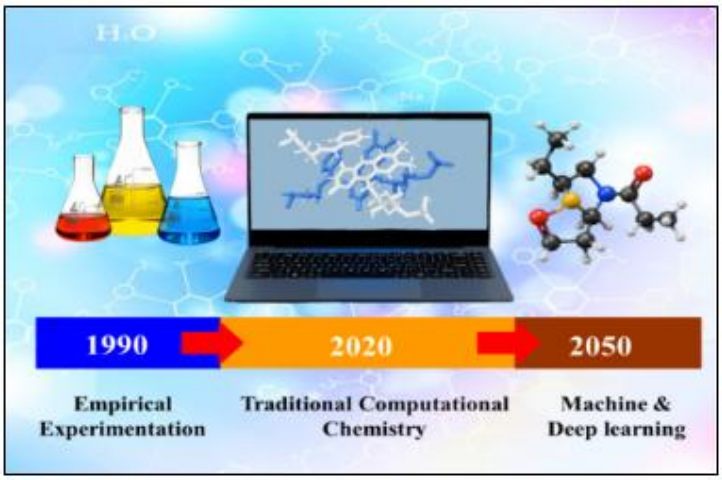

Figure 1. Evolution of Artificial Intelligence in Chemistry

Transition from Empirical to Data-Driven Chemistry

Chemical research has traditionally relied on heuristic rules derived from experimental observations[26]. While effective, these rules often fail in complex molecular environments[27]. Data-driven AI models overcome this limitation by identifying nonlinear relationships that may not be evident through theoretical reasoning alone[1,3].Geometric deep learning, for example, incorporates symmetry and spatial information into neural networks, making it particularly suitable for molecular modeling where three-dimensional structure governs reactivity and function[7,28]. The result is a hybrid scientific methodology combining chemical intuition with algorithmic intelligence[6].

III. FUNDAMENTAL CONCEPTS OF AI RELEVANT TO CHEMISTRY

3.1 Machine Learning

Machine learning refers to algorithms that improve performance through experience without explicit programming [29]. In chemistry, ML models are frequently used for:

- Quantitative structure-activity relationship (QSAR) prediction
- Property estimation
- Reaction classification
- Spectral interpretation

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These tools enable researchers to computationally screen millions of hypothetical compounds before conducting laboratory experiments [10].

3.2 Deep Learning

Deep learning employs multilayer neural networks that can extract complex hierarchical features from raw data [30]. Its success in chemistry stems from its ability to process molecular graphs, spatial coordinates, and electronic descriptors simultaneously [7]. Deep neural networks have been particularly impactful in structure-based drug discovery, where they identify subtle patterns governing ligand-protein interactions [8].

3.3 Generative Models

Generative AI is one of the fastest-growing areas in chemical research [31]. Models such as variationalautoencoders (VAEs), generative adversarial networks (GANs), and reinforcement learning frameworks can propose entirely new molecular structures with desired physicochemical properties [2,32]. Hybrid quantum-classical GAN architectures have even shown potential advantages in generating valid molecules while using fewer training parameters than classical models. This capability dramatically expands the searchable chemical universe [33].

3.4 Autonomous and Self-Driving Laboratories

AI is increasingly integrated with robotics to create automated experimentation platforms [34]. These systems can design experiments, execute reactions, analyze results, and refine hypotheses with minimal human intervention, ushering in an era of "closed loop discovery [6]." Such technologies are expected to reduce development timelines while improving reproducibility.

The core artificial intelligence methodologies applied across chemical sciences are summarized in **Figure 2.**

Figure 2. Core AI methodologies applied in chemistry

IV. AI-DRIVEN MOLECULAR MODELING AND CHEMICAL SPACE EXPLORATION

Chemical space is estimated to contain more than 10^{60} potential drug-like molecules, making exhaustive experimental exploration impossible. AI offers a practical pathway for navigating this immense landscape. Machine learning models can identify promising molecular candidates by correlating structural features with biological or physicochemical properties [1,10]. Researchers emphasize that AI is enabling a future where molecular and material design is significantly accelerated [6].

Furthermore, modern frameworks integrate contrastive learning and molecular encoding techniques to capture atom- and bond-level representations, thereby improving reaction center identification and transformation prediction [12].

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These approaches represent a shift toward predictive chemistry rather than observational chemistry [3] as shown in **Figure 3.**

Figure 3. AI-guided exploration of chemical space

V. ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY

Drug discovery is widely regarded as one of the domains most transformed by AI, given its high costs and historically low success rates [35]. Recent reviews note that AI techniques are now widely applied to structure-activity relationship analysis, hit identification, lead optimization, and toxicity prediction [36]. By reducing reliance on large-scale screening campaigns, AI can significantly decrease both development time and financial risk.

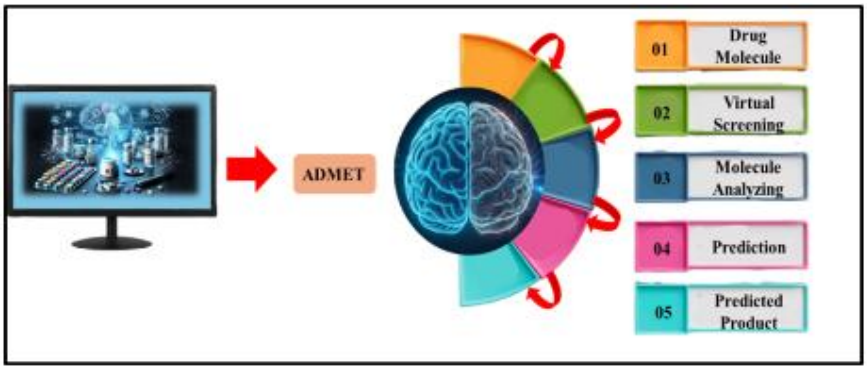

Figure 4. AI-driven drug discovery workflow

Advanced reinforcement learning systems can construct drug-like molecules step-by-step according to real synthesis rules, improving feasibility and reducing the likelihood of impractical designs [32]. This represents a major improvement over earlier generative models that often produced chemically unrealistic compounds [2]. Additionally, AI-enabled discovery platforms are being combined with automated synthesis to rapidly produce and evaluate hundreds of candidate molecules, illustrating a new experimental paradigm driven by intelligent machines [37], as illustrated in **Figure 4.**

Drug discovery is one of the most mature and impactful applications of AI in chemistry [38]. The pharmaceutical pipeline involves multiple stages: target identification, hit discovery, lead optimization, and preclinical testing, each associated with high costs and failure rates [35].

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5.1 Target Identification and Validation

AI algorithms analyze genomic, proteomic, and transcriptomic datasets to identify disease-relevant targets. Network-based machine learning models uncover hidden relationships between genes, proteins, and disease phenotypes [39]. Benevolent AI famously identified baricitinib as a potential COVID-19 treatment through AI-driven knowledge graph analysis, validating the real-world impact of these approaches [40].

5.2 Virtual Screening and Hit Discovery

Virtual screening uses AI models to evaluate millions of compounds computationally. Deep neural networks outperform traditional docking methods by learning complex binding patterns directly from data [8]. Atom Net and similar platforms demonstrated that deep learning could accurately predict ligand-protein interactions even when crystal structures were unavailable [25,41].

Key advantages include:

- Drastic reduction in wet lab screening
- Exploration of ultra-large chemical libraries
- Improved hit rates

5.3 De Novo Molecular Design

Generative AI models can design entirely new drug candidates optimized for multiple objectives, including potency, selectivity, solubility, and toxicity [2]. In silico Medicine reported the first AI-designed drug candidate (DSP-1181) entering clinical trials in record time [42]. Although later discontinued, the study demonstrated the feasibility of end-to-end AI-driven drug discovery [41]. Reinforcement learning frameworks now integrate synthetic accessibility constraints, addressing early criticisms that AI-generated molecules were chemically unrealistic [32].

5.4 ADMET and Toxicity Prediction

Late-stage drug failure is often caused by poor absorption, distribution, metabolism, excretion, or toxicity (ADMET) [43]. AI models trained on clinical and preclinical datasets can predict these properties early in development. Graph neural networks and ensemble learning methods have demonstrated strong performance in predicting hepatotoxicity, cardiotoxicity, and mutagenicity, improving decision-making and reducing attrition rates [47], as illustrated in **Figure 5.**

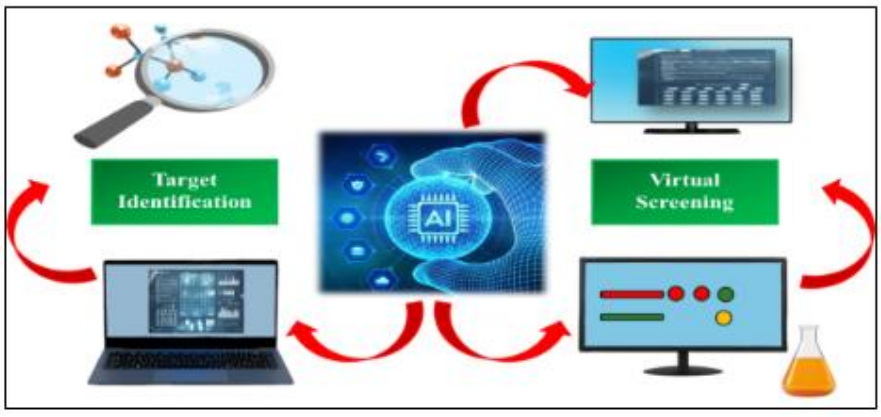

Figure 5. AI in drug discovery

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VI. ARTIFICIAL INTELLIGENCE IN REACTION PREDICTION AND ORGANIC SYNTHESIS

One of the most challenging problems in chemistry is predicting the outcome of chemical reactions [26]. Reaction yields, selectivity, and side-product formation depend on complex, nonlinear interactions between reagents, catalysts, solvents, and conditions [44]. Traditionally, chemists relied on mechanistic reasoning and accumulated experience to address these challenges. Artificial intelligence has introduced a fundamentally different, data-driven approach [12].

6.1 Reaction Outcome Prediction

Machine learning models trained on large reaction databases, such as the USPTO, Reaxys, and proprietary industrial datasets, can now predict reaction products with remarkable accuracy. Schwaller*et al.* demonstrated that sequence-to-sequence neural networks adapted from natural language processing could treat chemical reactions as a "language translation" problem, converting reactant SMILES strings into product SMILES strings with high predictive power [12]. These models significantly outperform rule-based expert systems, especially for complex multicomponent reactions. Importantly, transformer-based architectures have shown improved generalization across reaction classes, indicating their potential for universal reaction prediction [45].

Key Research Contributions

Schwaller*et al.* (2018): Neural machine translation for reaction prediction
Coley et al. (2019): ML-assisted retrosynthesis planning
Jin et al. (2020): Graph-based reaction prediction models
AI-driven reaction prediction is now widely used in medicinal chemistry to evaluate synthetic feasibility before laboratory execution.

6.2 Retrosynthetic Analysis

Retrosynthesis, the process of breaking a target molecule into simpler precursors, is central to planning organic syntheses. Historically, this task depended on human expertise and heuristic rules [26,46]. AI has transformed retrosynthesis into a computational optimization problem. Monte Carlo tree search combined with neural networks enables efficient exploration of possible disconnection strategies. Segler*et al.* demonstrated that AI systems trained on millions of reactions could propose synthetic routes comparable to those designed by expert chemists [16].
Modern retrosynthesis platforms integrate:

- Reaction feasibility scoring
- Cost optimization
- Route length minimization
- Commercial availability of starting materials

These tools significantly reduce planning time and improve success rates in pharmaceutical synthesis [27].

6.3 AI-Assisted Catalyst Design

Catalysts play a crucial role in chemical transformations, yet their discovery has traditionally been slow and empirical. AI enables rapid exploration of catalyst composition and structure-activity relationships [10].
Machine learning models can predict:

- Catalyst selectivity
- Turnover frequency
- Stability
- Reaction compatibility

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For example, neural networks trained on high-throughput screening data have identified novel ligands for transition metal catalysis with enhanced performance. These advances have major implications for green chemistry and industrial process optimization, as illustrated in **Figure 6.**

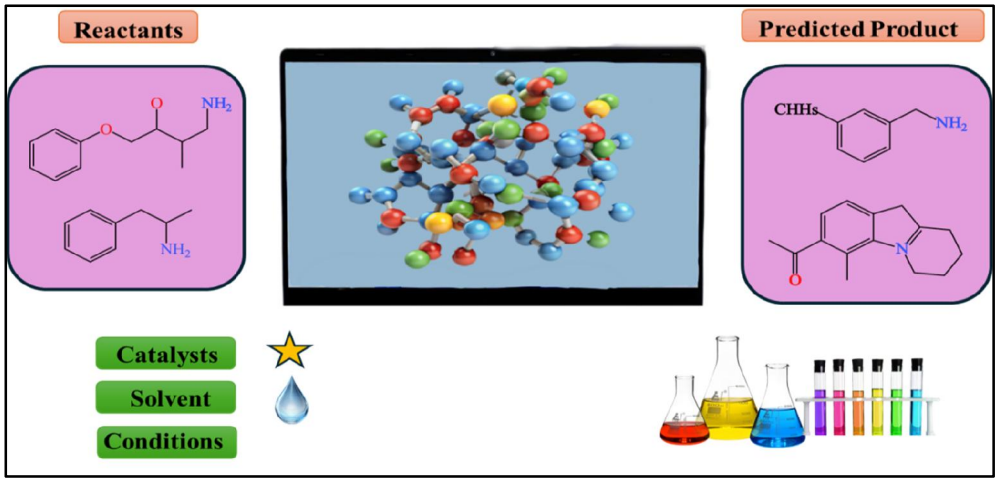

Figure 6. AI-based reaction prediction framework

VII. ARTIFICIAL INTELLIGENCE IN MATERIALS CHEMISTRY

Materials discovery traditionally requires extensive experimentation and characterization [5]. AI has introduced materials informatics, enabling predictive modeling of structure-property relationships [1].

7.1 Discovery of Functional Materials

Machine learning models predict properties such as [47]:

- Band gaps
- Mechanical strength
- Thermal stability
- Optical absorption

AI-guided discovery has led to rapid identification of novel battery materials, photovoltaic compounds, and catalysts for renewable energy applications [6]. Notably, AI-driven screening identified new solid-state electrolytes with improved ionic conductivity, thereby accelerating battery technology development [48].

7.2 Polymer and Nanomaterial Design

AI is increasingly used to design polymers with tailored mechanical and chemical properties [49]. Generative models propose polymer backbones optimized for biodegradability, strength, or conductivity. In nanochemistry, machine learning predicts nanoparticle morphology and size distribution, improving reproducibility in synthesis [50], as illustrated in **Figure 7.**

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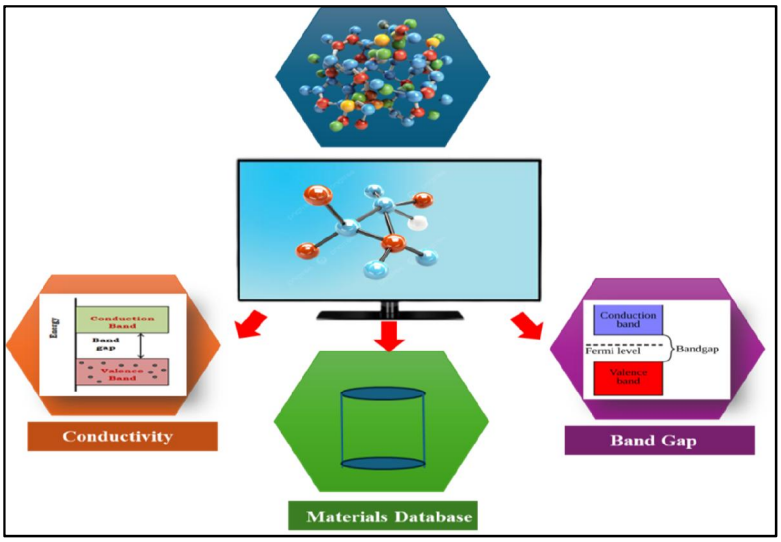

Figure 7. AI-guided materials discovery

VIII. ARTIFICIAL INTELLIGENCE IN ANALYTICAL AND SPECTROSCOPIC CHEMISTRY

AI has revolutionized data interpretation in spectroscopy and analytical chemistry [51].

Applications include:

- Automated NMR peak assignment
- Infrared and Raman spectral classification
- Mass spectrometry-based compound identification

Deep learning models outperform traditional chemometric techniques in noise reduction and signal interpretation, enabling real-time analysis and decision-making [53], as illustrated in **Figure 8.**

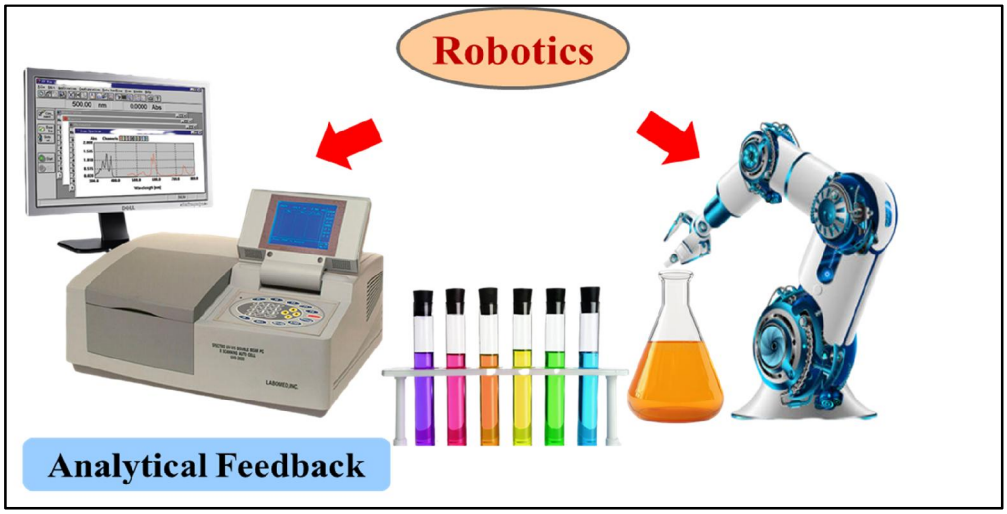

Figure 8.AI-assisted spectroscopic analysis.

Automated interpretation of spectroscopic data using deep learning algorithms for NMR, IR, Raman, and mass spectrometry.

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IX. AI IN LABORATORY AUTOMATION AND AUTONOMOUS CHEMISTRY

The integration of AI with robotics has led to the concept of the "self-driving laboratory." These systems design experiments execute reactions, analyze results, and iteratively optimize conditions without human intervention [52].

Examples include:

Robotic platforms for catalyst optimization

Autonomous synthesis of metal-organic frameworks

Closed-loop optimization of reaction conditions

Such systems improve reproducibility, safety, and efficiency while freeing chemists to focus on conceptual innovation [53], as illustrated in **Figure 9.**

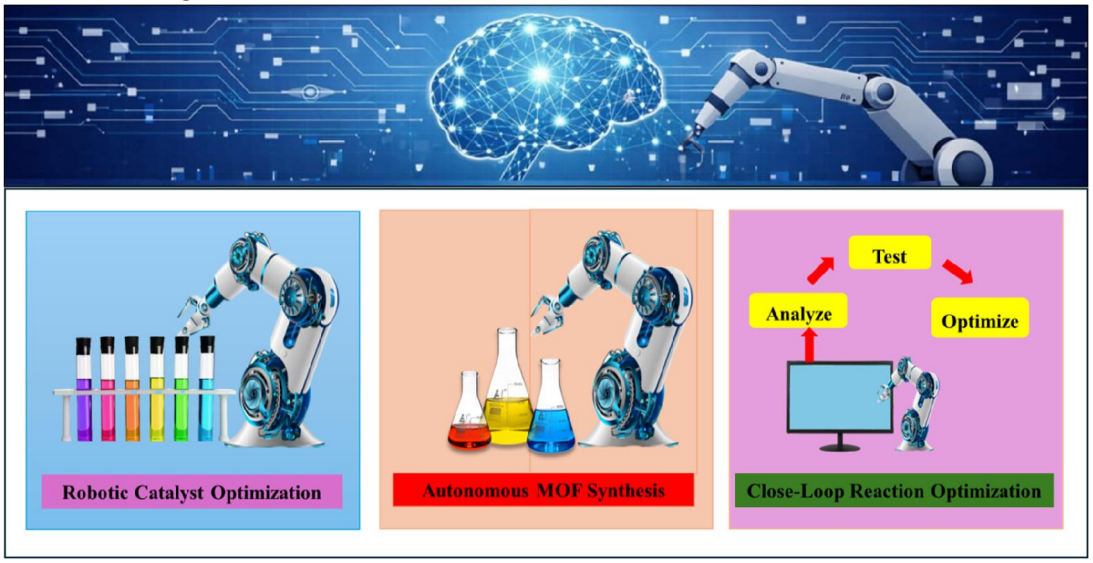

Figure 9. AI In Laboratory Automation & Autonomous Chemistry

X. ARTIFICIAL INTELLIGENCE IN GREEN AND SUSTAINABLE CHEMISTRY

Sustainable chemistry aims to minimize environmental impact while maximizing efficiency and safety [54]. Artificial intelligence has emerged as a powerful enabler of green chemistry principles by optimizing reaction conditions, reducing waste, and guiding the development of environmentally benign materials [55].

10.1 Reaction Optimization for Sustainability

AI-driven optimization frameworks use reinforcement learning and Bayesian optimization to identify reaction conditions that maximize yield while minimizing energy consumption and solvent use [52,56]. These models significantly reduce the number of experimental trials, aligning with the principles of atom economy and waste reduction [57]. Recent studies demonstrate that machine learning can predict solvent effects and propose greener alternatives without compromising reaction efficiency. Such approaches are increasingly adopted in pharmaceutical and fine chemical industries to reduce environmental footprint [11].

10.2 AI for Eco-Friendly Catalyst and Solvent Design

Catalysts and solvents account for a significant portion of chemical waste [10,58]. AI models trained on catalytic performance data can identify non-toxic, earth-abundant metal catalysts as alternatives to precious metals. Similarly, machine-learning-guided solvent-selection tools evaluate environmental, health, and safety (EHS) parameters alongside reaction performance, thereby supporting sustainable process design [59], as illustrated in **Figure 10.**

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Figure 10. AI In Green And Sustainable Chemistry

XI. ARTIFICIAL INTELLIGENCE IN CHEMICAL ENGINEERING AND INDUSTRIAL CHEMISTRY

AI has become an essential component of modern chemical engineering, enabling intelligent process control, predictive maintenance, and smart manufacturing [60].

11.1 Process Optimization and Control

Neural networks and hybrid physics-informed AI models optimize:

- Temperature and pressure conditions
- Reactor performance
- Energy efficiency

These systems outperform traditional control strategies by adapting in real time to process variations, improving product quality, and reducing operational costs [60,61].

11.2 Predictive Maintenance and Safety

AI-driven predictive maintenance models analyze sensor data to forecast equipment failures before they occur [62]. This reduces downtime and improves safety in chemical plants [63]. Additionally, anomaly detection algorithms identify hazardous operating conditions, contributing to safer industrial environments [64], as illustrated in **Figure 11.**

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Figure 11. AI In Chemical Engineering And Industrial Chemistry

XII. ANALYSIS OF ADVANTAGES AND LIMITATIONS (CHART-BASED INTERPRETATION)

The comparative chart presented earlier summarizes the key advantages and limitations of artificial intelligence in chemical sciences. The trends observed in the chart are strongly supported by recent peer-reviewed literature and industrial case studies[1,31,65]. Overall, AI demonstrates exceptional potential to accelerate discovery and improve efficiency, while simultaneously introducing new technical and ethical challenges.

12.1 Advantages

12.1.1 Faster Research and Development

Artificial intelligence significantly reduces research and development timelines by enabling in silico prediction of molecular properties, reaction outcomes, and material performance before laboratory experimentation[41]. Studies indicate that AI-assisted drug discovery platforms can shorten development cycles by 2-5 years compared to traditional workflows[42]. This acceleration is particularly critical in pharmaceutical and materials innovation, where time-to-market directly impacts societal and economic outcomes [28].

12.1.2 High Accuracy and Reproducibility

Machine learning algorithms minimize subjective bias inherent in human decision-making and improve reproducibility across laboratories [30]. Once trained, AI models apply identical decision rules to new datasets, reducing variability caused by experimental interpretation. Deep learning approaches have demonstrated superior accuracy in reaction prediction, spectral analysis, and property estimation compared to conventional statistical methods [12].

12.1.3 Cost Effectiveness

Although AI implementation requires a substantial initial investment in data infrastructure and computational resources, long-term cost savings are substantial. By reducing failed experiments, optimizing reagent use, and minimizing trial-and-error synthesis, AI lowers material consumption and operational costs. Industrial studies report cost reductions of up to 30-50% in screening and optimization stages [38].

12.1.4 Improved Safety

Laboratory automation and AI-guided planning reduce human exposure to hazardous chemicals.

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12.2 Limitations

12.2.1 Data Dependency

AI models are fundamentally dependent on the quality, diversity, and completeness of training data. In chemistry, experimental datasets are often noisy, biased toward successful reactions, or restricted by proprietary barriers. Poor data quality can lead to inaccurate predictions and reduced model generalizability [66].

12.2.2 Interpretability Challenges

Many deep learning models operate as "black boxes," offering limited insight into underlying chemical mechanisms [67]. This lack of interpretability can hinder scientific understanding and regulatory acceptance, particularly in safety-critical applications such as drug development and industrial chemistry [41].

12.2.3 High Infrastructure Cost

Advanced AI applications require high-performance computing, specialized software, and interdisciplinary expertise. These requirements create accessibility barriers for smaller academic laboratories and developing regions, potentially widening technological disparities [68].

12.2.4 Regulatory and Ethical Concerns

The use of AI in chemical synthesis and drug discovery raises concerns related to transparency, accountability, and potential misuse. Algorithmic bias, data ownership, and dual-use risks necessitate robust governance frameworks [69], as illustrated in **Figure 12.**

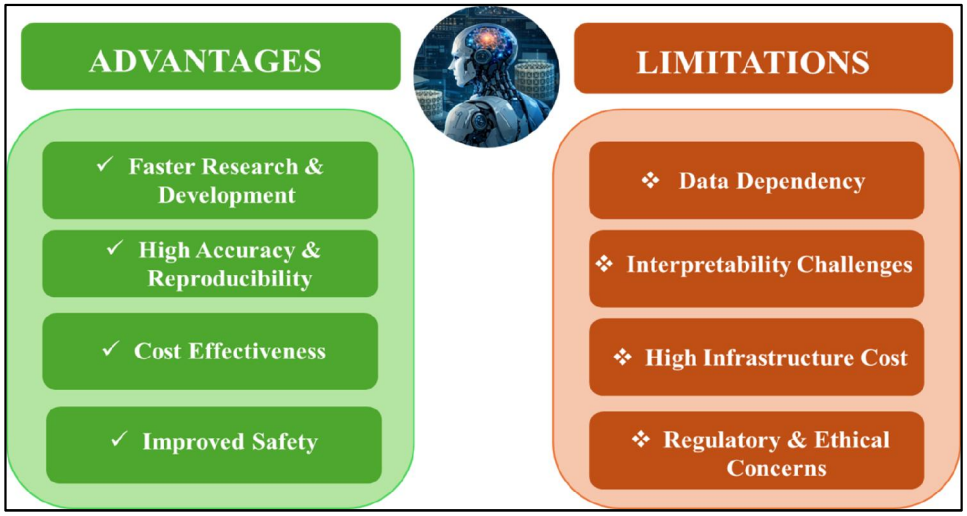

Figure 12. Analysis of Advantages and Limitation of AI in Chemical Science

XIII. ETHICAL, REGULATORY, AND SOCIETAL IMPLICATIONS

As AI systems become increasingly autonomous, ethical oversight becomes essential.

Concerns include:

- Dual-use research risks
- Algorithmic bias
- Intellectual property ownership
- Data privacy

Regulatory agencies such as the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are actively developing guidelines for AI-assisted drug development, emphasizing explainability, validation,

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and human oversight [70]. Ethical frameworks now stress that AI should augment human expertise rather than replace scientific judgment [71], as illustrated in **Figure 13.**

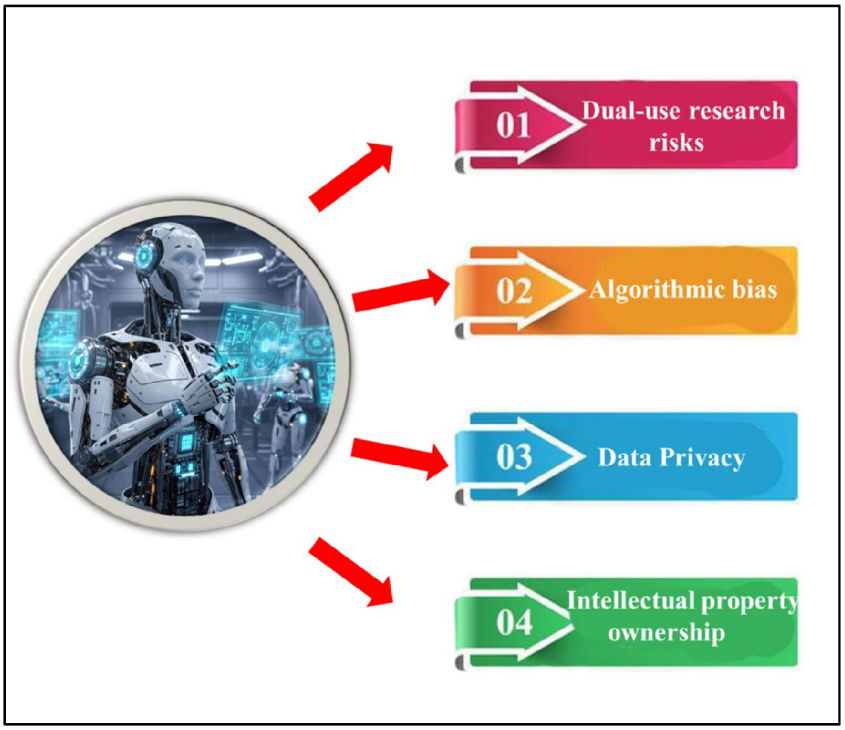

Figure 13. Ethical, Regulatory And Societal Implications of AI In Chemical Science

XIV. FUTURE PERSPECTIVES OF ARTIFICIAL INTELLIGENCE IN CHEMISTRY

The future of AI in chemistry lies in human AI collaboration, where intelligent systems enhance creativity, efficiency, and predictive capability rather than functioning as autonomous replacements [6].

Emerging Trends Include:

- Explainable AI for mechanistic insight
- Multimodal AI integrating text, images, and molecular data
- Self-driving laboratories operating continuously
- Personalized medicine through AI-guided molecular design
- Climate-conscious chemical manufacturing

AI is expected to transform chemistry from a hypothesis-driven science into a predictive and autonomous discipline.as illustrated in **Figure 14.**

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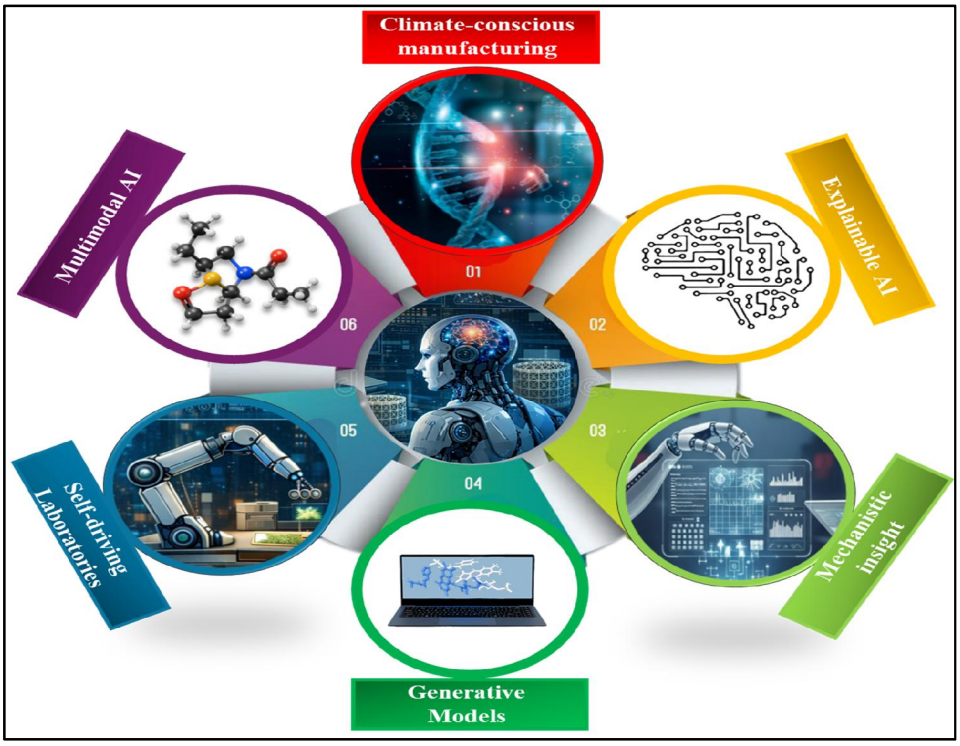

Figure 14. Future Perspectives of AI in Chemistry

XV. CONCLUSION

This review highlights the transformative role of artificial intelligence in modern chemical sciences, demonstrating its widespread impact across molecular modeling, drug discovery, reaction prediction, materials chemistry, analytical science, laboratory automation, and industrial processes. The shift from traditional empirical and heuristic approaches toward data-driven and predictive frameworks has enabled chemists to efficiently explore complex chemical systems and vast chemical spaces that were previously inaccessible. Artificial intelligence methodologies, including machine learning, deep learning, and generative models, have significantly improved accuracy, reproducibility, and efficiency while reducing experimental cost, time, and human exposure to hazardous conditions.

Despite these advances, several challenges continue to limit AI's full potential in chemistry. Data quality and availability, model interpretability, computational infrastructure requirements, and ethical and regulatory concerns remain critical issues that require careful attention. Addressing these challenges through standardized datasets, explainable and hybrid AI models, and stronger integration between computational predictions and experimental validation will be essential for sustainable progress. Looking ahead, the future of AI in chemistry lies in effective human–AI collaboration, where intelligent systems complement chemical intuition and expertise rather than replace them. Overall, artificial intelligence is poised to remain a central driver of innovation, shaping chemistry into a more predictive, efficient, and responsible scientific discipline.

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