

Artificial Intelligence in Chemistry: Applications, Challenges, and Pathways Toward Reliable and Sustainable Chemical Discovery

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Abstract—Artificial intelligence (AI) is transforming chemistry by enabling data-driven molecular design, reaction prediction, catalyst discovery, and materials optimization. Machine learning, deep learning, and generative models can accelerate chemical research by identifying patterns in complex datasets and reducing unnecessary experimental trials. However, the reliability of AI-driven chemical discovery remains limited by inconsistent datasets, model interpretability, prediction uncertainty, experimental reproducibility, and computational energy requirements. This review critically examines the applications of AI across chemical synthesis, computational chemistry, materials science, environmental chemistry, and sustainable manufacturing. Particular emphasis is placed on the integration of chemical knowledge, explainable AI, uncertainty quantification, experimental validation, and environmental assessment. By connecting predictive performance with chemical reliability and sustainability, this review identifies important research gaps and proposes a framework for more transparent, reproducible, and environmentally responsible AI-assisted chemical research.

Index Terms—Artificial intelligence; machine learning; computational chemistry; molecular design; reaction prediction; catalysis; explainable AI; sustainable chemistry.

I. INTRODUCTION

Chemistry is essential to the development of pharmaceuticals, advanced materials, energy technologies, agricultural products, and industrial chemicals. However, conventional chemical research often involves time-consuming experiments, extensive material consumption, and complex optimization procedures. The increasing availability of chemical databases, computational resources, and

advanced algorithms has created opportunities to accelerate chemical discovery through artificial intelligence (AI).

AI refers to computational methods that perform tasks such as pattern recognition, prediction, classification, and decision support. Within chemistry, machine learning (ML), deep learning, natural language processing, and generative models are being used to predict molecular properties, identify promising reaction pathways, optimize experimental conditions, and design new materials.

Recent advances demonstrate the potential of AI to improve reaction prediction and synthesis planning, although reliable experimental validation remains essential [1–3]. AI-assisted approaches are also being investigated for catalyst discovery, molecular property prediction, and sustainable chemical production.

Despite this progress, important challenges remain. Chemical datasets may contain incomplete or inconsistent information, and models trained on limited chemical spaces may perform poorly on unfamiliar molecules or reaction conditions. Furthermore, accurate prediction does not necessarily guarantee experimental success, chemical safety, or environmental sustainability.

The central focus of this review is to examine how chemical knowledge, explainable AI, uncertainty assessment, experimental validation, and sustainability metrics can be integrated to improve the reliability of AI-assisted chemical discovery. This perspective moves beyond a general description of AI applications by emphasizing the conditions required for their trustworthy and sustainable implementation.

II. FUNDAMENTALS OF ARTIFICIAL INTELLIGENCE IN CHEMISTRY

2.1 Machine learning

Machine learning enables computational systems to learn relationships from data and use those relationships to make predictions.

In chemistry, ML can be applied to predict solubility, molecular stability, reaction yield, toxicity, catalytic activity, and material properties. Its performance depends on the quality and diversity of the training data, the suitability of the selected model, and the validity of the evaluation procedure.

2.2 Deep learning

Deep learning uses multilayer neural networks to learn complex relationships in large datasets. Graph neural networks can represent molecules as networks of atoms and chemical bonds, making them useful for molecular-property prediction and molecular design. Deep-learning methods can also process reaction representations and spectroscopic data. However, computational complexity, limited interpretability, and dependence on representative training data remain significant challenges.

2.3 Natural language processing and large language models

Natural language processing (NLP) enables computers to extract information from scientific text. It can assist in identifying reported reactions, experimental conditions, chemical compounds, and relationships between chemical structures and properties.

Large language models (LLMs) can support literature analysis, code generation, chemical information retrieval, and research planning. Nevertheless, generated information may contain factual errors or chemically invalid suggestions. All important outputs require verification against reliable scientific sources and experimental evidence [4].

2.4 Generative artificial intelligence

Generative models aim to propose new molecular structures, materials, or reaction pathways that satisfy specified objectives. These methods may help explore chemical spaces that are difficult to investigate experimentally.

However, a generated molecule is not automatically synthesizable, stable, safe, or useful. Candidate structures must be evaluated for chemical validity, synthetic feasibility, predicted properties, toxicity, and practical performance.

III. MAJOR APPLICATIONS OF AI IN CHEMISTRY

3.1 Molecular design and property prediction

AI models can estimate molecular properties such as solubility, acidity, stability, electronic characteristics, and toxicity. These predictions can help researchers prioritize compounds for experimental testing.

The effectiveness of molecular prediction depends on the relationship between the training and test chemical spaces. Models may be unreliable when applied to structures that differ substantially from the compounds represented in their training datasets.

3.2 Reaction prediction and synthesis planning

Reaction-prediction models estimate likely products from reactants and reaction conditions. Retrosynthesis models work in the opposite direction by suggesting possible starting materials and reaction sequences for a desired target molecule.

These techniques can assist organic synthesis, pharmaceutical research, and route optimization. However, proposed pathways require assessment of selectivity, reaction conditions, reagent availability, safety, and experimental feasibility.

3.3 AI-assisted catalysis

Catalyst discovery often involves exploring numerous compositions, structures, and reaction conditions. Machine learning can help identify relationships between catalyst properties and catalytic performance.

AI can prioritize candidate catalysts, predict adsorption properties, and guide the selection of experimental conditions. Integration with computational chemistry and laboratory measurements can improve the efficiency of catalyst development.

A particularly important research direction is the identification of catalysts that reduce dependence on scarce or hazardous materials while maintaining activity, selectivity, and durability.

3.4 Materials and energy chemistry

AI is increasingly applied to the discovery and optimization of materials for batteries, solar cells, hydrogen production, carbon capture, and electronic devices.

Models can predict properties and screen candidate materials before costly synthesis and testing. Nevertheless, predictions must be verified experimentally, and promising materials must also be assessed for stability, resource availability, toxicity, and recyclability.

3.5 Pharmaceutical and medicinal chemistry

AI can support drug discovery by predicting molecular properties, prioritizing potential drug candidates, and assisting in synthesis planning. It may also help identify relationships between molecular structure and biological activity.

However, predicted biological activity does not establish clinical effectiveness or safety. Experimental testing, toxicological evaluation, and appropriate regulatory assessment remain necessary.

3.6 Environmental and green chemistry

AI can contribute to sustainable chemistry by helping optimize reaction conditions, identify less hazardous compounds, predict environmental fate, and improve resource efficiency.

When combined with green chemistry principles, AI may help reduce unnecessary experiments, solvent consumption, and waste generation. However, sustainability must be evaluated using appropriate environmental and life-cycle indicators rather than reaction yield or computational predictions alone.

IV. INTEGRATION OF AI WITH SUSTAINABLE CHEMISTRY

The integration of AI and green chemistry offers opportunities to improve chemical efficiency while reducing environmental impacts.

AI-assisted reaction optimization can identify conditions that balance product yield, selectivity, solvent use, temperature, and energy demand. Predictive models may also support the screening of alternative solvents, renewable feedstocks, and less hazardous reagents.

A major opportunity is **multi-objective optimization**, in which several outcomes are

considered simultaneously rather than optimizing a single parameter. For example, a chemical reaction can be evaluated according to:

- Product yield and selectivity.
- Material consumption and waste generation.
- Energy demand and greenhouse-gas emissions.
- Chemical hazards and environmental persistence.
- Economic feasibility and scalability.

This approach is more informative than selecting a process solely because it produces the highest yield. Nevertheless, the reliability of such optimization depends on the availability of accurate data and appropriate definitions of environmental performance.

V. CHALLENGES AND LIMITATIONS

5.1 Data quality and availability

AI models depend on reliable and representative datasets. Missing experimental conditions, inconsistent reporting, measurement errors, and limited coverage of chemical space can reduce predictive accuracy.

Standardized data formats, transparent reporting, and accessible datasets are therefore important for reproducible chemical AI research.

5.2 Interpretability and chemical reasoning

Complex models may generate accurate predictions without providing a clear explanation of the underlying relationships. Explainable AI methods can help identify influential molecular features and improve scientific interpretation.

However, an explanation generated by a model should not automatically be treated as proof of a chemical mechanism.

5.3 Prediction uncertainty and experimental validation

AI predictions contain uncertainty arising from data limitations, model assumptions, and unfamiliar chemical structures. Uncertainty estimation can help researchers identify predictions that require additional investigation.

Experimental validation remains essential because computational predictions cannot fully capture every feature of real chemical systems.

5.4 Computational cost and environmental impact

Training and operating AI systems require computational resources and electricity. Large-scale calculations can also require substantial data storage and hardware infrastructure.

The environmental benefits of AI should therefore be compared with its computational footprint and the resources consumed by subsequent experiments. Efficient algorithms, targeted experimentation, and renewable electricity may improve overall sustainability.

5.5 Safety, reproducibility, and responsible use

AI-generated chemical suggestions may be incorrect, infeasible, or insufficiently assessed for hazards. Reliable implementation requires expert oversight, independent verification, appropriate safety procedures, and reproducible documentation.

These requirements are particularly important when AI is used to guide laboratory experiments or industrial chemical processes.

VI. A PROPOSED FRAMEWORK FOR RELIABLE AND SUSTAINABLE AI IN CHEMISTRY

A key direction for future research is to integrate predictive performance, chemical reasoning, and sustainability into a single decision-making framework.

The proposed framework consists of five stages:

Stage 1: Data preparation. Collect reliable experimental and computational data, document conditions, and evaluate data quality.

Stage 2: AI-based prediction. Apply suitable machine-learning or generative models to identify promising molecules, reactions, catalysts, or materials.

Stage 3: Uncertainty and safety assessment. Evaluate prediction confidence, chemical feasibility, toxicity, and relevant hazards.

Stage 4: Experimental validation. Test promising predictions under controlled conditions and compare experimental observations with model outputs.

Stage 5: Sustainability assessment. Evaluate material efficiency, waste, energy consumption, environmental impacts, and economic feasibility.

This framework is a proposed synthesis of established research practices rather than a validated

new algorithm. Its practical value should be evaluated through case studies comparing AI-assisted workflows with suitable conventional baselines.

VII. RESEARCH GAPS AND FUTURE PERSPECTIVES

Future advances in AI-assisted chemistry require more than increasingly complex algorithms. Research should prioritize the following areas:

1. Explainable and chemically informed AI: Develop models that provide interpretable predictions consistent with established chemical principles.
2. Reliable uncertainty estimation: Improve the identification of predictions that fall outside the model's reliable domain.
3. Standardized chemical datasets: Encourage consistent experimental reporting, data sharing, and reproducible benchmarking.
4. AI-guided experimentation: Integrate computational predictions with automated or carefully controlled laboratory experiments.
5. Sustainable AI workflows: Evaluate both the environmental benefits of AI-assisted chemistry and the energy requirements of computational methods.
6. Multi-objective chemical design: Combine chemical performance, safety, cost, and environmental impact in the selection of candidate processes.
7. Industrial translation: Validate promising methods at relevant scales and assess their robustness under practical operating conditions.

A particularly promising direction is the development of closed-loop systems in which AI proposes an experiment, laboratory measurements generate new data, and updated models guide the next experiment. Such systems may improve experimental efficiency, provided that uncertainty, safety, data quality, and reproducibility are addressed.

VIII. CONCLUSION

Artificial intelligence is creating new opportunities in molecular design, reaction prediction, catalysis, materials discovery, and sustainable chemical manufacturing. However, its scientific value depends on reliable datasets, interpretable predictions,

uncertainty assessment, and experimental verification. Integrating these requirements with green chemistry principles and quantitative sustainability assessment can help distinguish genuinely useful innovations from predictions that are accurate only within limited computational settings.

The central research opportunity is to develop AI-assisted chemical workflows that optimize not only chemical performance but also safety, reproducibility, resource efficiency, and environmental impact. Achieving this goal will require collaboration among chemists, computer scientists, engineers, and environmental researchers.

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