Macromolecular Symposia
www.ms-journal.de

Advancements in Machine Learning and Artificial Intelligence in Polymer Science: A Comprehensive Review

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Technology, health care, and transport are merely some of the industries that historically rely on polymer-based materials. In past centuries, the creation of innovative polymer materials has been dependent upon extensive experiments and error procedures that require an extensive number of resources as well as time. With the objective to explore the transformative potential of machine learning (ML) and artificial intelligence (AI) in material discovery, design, and optimization, this paper explores the integration of ML and AI in polymer-based materials research. Researchers are able to speed the development of new polymer-based materials with improved properties and functionalities by utilizing sophisticated algorithms and computational models. The use of ML and AI in polymer research is examined, with a focus on how these technologies may stimulate innovation and expand material science research.

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DOI: 10.1002/masy.202400185

1. Introduction

1.1. Polymer

Polymers take up the category of necessary and investigative substances in materials science. From commonplace items like plastic packaging to advanced technologies like lithium-ion batteries, solar power cells, and 3D printing materials, they are used in a large number of applications.[1] The huge quantity of broad monomer atomic structures, intricate chain structures, and diverse synthetic processes of polymers, however, presents major difficulties to human researchers due to the inherent cognitive limitations of humans faced with an enormous amount of articles and high-dimensional data.[2] As the field of polymer output, polymer informatics is a multifaceted field of research that converges polymer science with computer science, information science, and machine learning (ML). Data-driven techniques are being used in polymer informatics to improve and streamline the creation, design, and discovery of polymers in light of the enormous rise of data in research. Artificial Intelligence (AI) applications are used in a variety of sectors such as the food business, cosmetics, polymer design, healthcare, and sustainable agriculture production.

1.2. Machine Learning

ML is an important subset of AI.[3] A portion of the basics of intelligence is overlooked in the initial years of AI research, when the computer's elementary job was to carry out a hard-coded algorithm created by subject matter experts.[4] ML opposes traditional AI, by analyzing the data, ML permits the computer to get rules. Data representation is used in ML by sets of input and related output values. To make it possible for a model to learn, its internal parameters must be modified in a function that describes possible output values given a particular set of input values. After making data-driven variable modifications, the model may determine and predict the ultimate values of newly created data sets.[5] Three components make up ML, as seen in **Figure 1**: supervised learning, unsupervised learning, and reinforcement learning. Supervised learning, support vector algorithms, and artificial neural networks are two examples of technologies used to perform data regression or classification with the output labels of the training set. Unsupervised learning, which performs data clustering or dimensionality reduction by algorithms such as

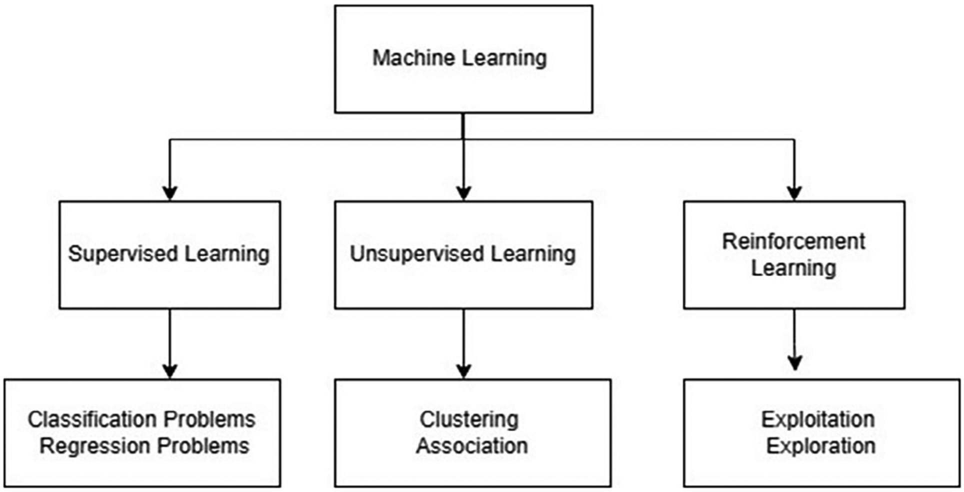

Figure 1. Understanding machine learning types: Classification.

principal component analysis and K-means clustering, is the type of ML that occurs whenever there is no output label present in the data. Reinforcement learning uses a technique of repetition in which an agent moves to modify its state and reacts with the environment in order to maximize the reward value it truly needs. It's the same as a Markov decision process and active learning. ML needs only the right algorithms and enough data for making a successful application. AI is reshaping research and aiding in realizing new and innovative sustainable materials.

The creation of polymers has extended largely more than in the past, and the new artificially intelligent ML systems are the only cause of this. AI is improving in the different fields for improving lifestyle and reaching sustainable development goals (SDGs), AI has contributed to progress. Applications ranging from novel materials to customized treatments and accurate sensor advancements might be changing as a result. The symbiotic relationship between ML and polymetric data insights drives progress in polymer science and materials research, as shown in **Figure 2**. ML techniques, including classification, regression, clustering, and reinforcement learning, are utilized with polymetric data to advance material design, property prediction, process optimization, polymer characterization, and data-driven insights. The insights derived from polymetric data, such as accelerated development of polymeric materials, automated experimentation platforms, actionable designs and predictions, experimental validation of ML models, and pivotal roles in research activities, reciprocally enhance ML, improving its potential and performance.

1.3. Transfer Learning

For solving the problem, the process of transfer learning involves applying or transferring the information. This makes use of an idea that models can utilize pretrained tasks to initialize or change their parameters and weights. **Figure 3** illustrates the subsequent steps in this process. Also, it is beneficial when the dataset for your current task or training is smaller than the dataset for your previously trained task, allowing the acquired dataset to transfer as well. Such as in the image recognition field, you can use a larger dataset involving ImageNet to fine-tune a pretrained model on a smaller data set specific to a particular issue.[5]

1.4. Artificial Intelligence in Polymer Science

The context will ultimately determine whether data fusion is successful or not. If desired quantities are connected, data fusion is able to connect the feature image of one task to that

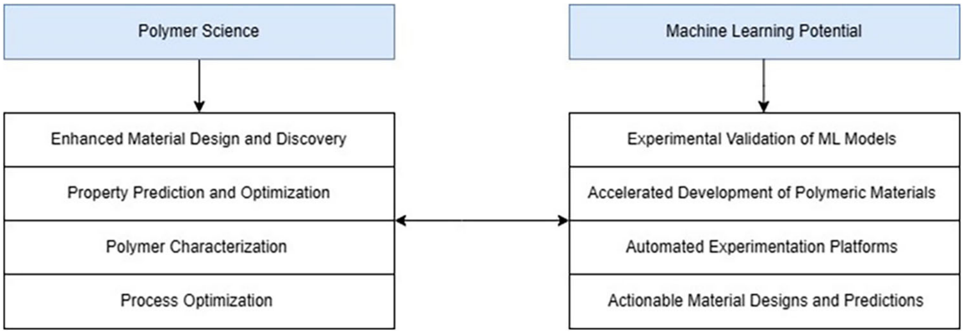

Figure 2. Machine learning potential with polymer science insights.

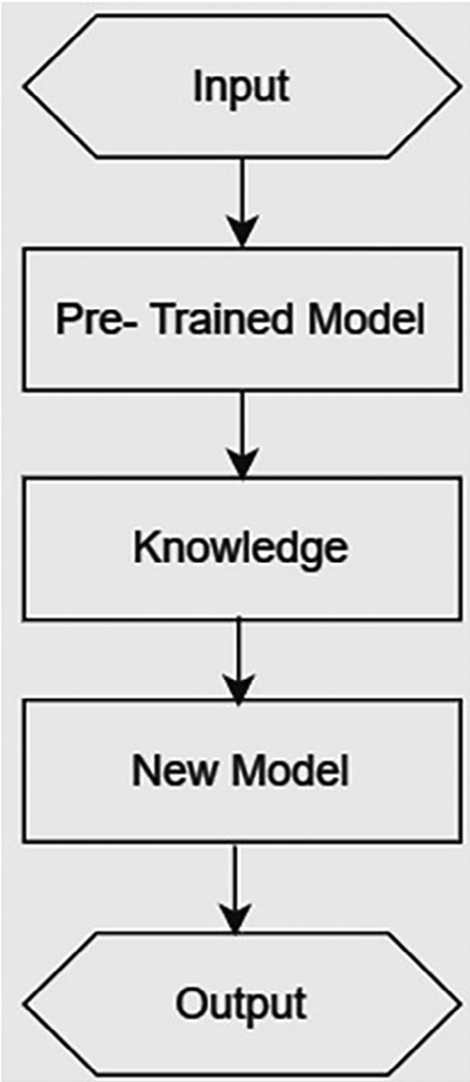

Figure 3. Illustrating transfer learning: Steps to knowledge adaptation.

of another task with a strong chance of success. Correlations between desirable quantities can be explicitly examined in order to partially determine this in advance. Finally, some predictions could derive benefit from multitask learning techniques, while others do not derive the same advantage. However, data fusion shows promise as an efficient method for extrapolating values that are unknown in irregular data sets, used in polymer physics.

The benefits of using ML in polymer-based materials research include:

Quick discovery of new materials and the data: ML technologies hold huge possibilities for predicting and designing innovative material with customized properties by identifying patterns, like increased biocompatibility, strength, or versatility.

Property prediction and optimization: The technique of AI can predict the chemical, mechanical, and physical properties of polymers by directing empirical efforts and permitting researchers to concentrate on the most attractive polymer candidates. AI algorithms may potentially enhance polymer frameworks by placing in place a range of factors and limitations, providing polymers with optimal properties for particular applications.

Process optimization: AI can optimize polymer production for higher productivity, lower costs, and minimize waste. By evaluating sensor information as well as real-time process factors, AI systems may identify the process elements that influence the final properties of polymers, improving product quality and requiring less energy.

Description of Polymer: AI will help with this procedure by automatically interpreting images from microscopes, spectroscopic data, and other analysis outputs. This could lead to a more thorough explanation of puzzling polymer structures and enhance accuracy while streamlining the analytical procedure.

Data-driven insights: Polymer researchers can benefit greatly from AI by using it to find hidden linkages and important patterns in their data. By evaluating vast volumes of experimental data, research papers, and patents, AI algorithms are able to identify patterns, establish theories, and provide fresh insights.

Development of sustainable polymers: AI can help in the creation of sustainable polymers by streamlining manufacturing and material formulation procedures. AI can assist researchers in the design and development of polymers with improved sustainability features by incorporating a number of variables, such as ecologically friendly synthesis procedures, biodegradability, and recycling potential. These advantages, which were taken into account in the study,[20] demonstrate how ML has the ability to significantly alter a variety of polymer research domains, including material creation and research, equitable growth, and process optimization (Table 1).

2. Literature Review

The goal of enhancing polymer science and engineering through the incorporation of ML and huge data resources in polymer informatics is to accelerate forecasting of performance along with process optimization through dependable data-driven methods, with the ultimate goal of improving efficiency and gaining widespread acceptance in materials and AI research.[8] The literature analysis highlights how Chemical Markdown Language (CMDL) has the potential to revolutionize polymer science by facilitating flexible visualization of data and ML incorporation for improved research workflows. Regression transformer models may be optimized with the help of previously collected empirical information through CMDL, demonstrating the technology's adaptability in producing and verifying catalysts and polymers—especially in ring-opening polymerization—and its capacity to work with a variety of polymer classes.[9] The paper highlights how traditional techniques are being challenged by AI and ML, which is transforming the manufacturing and research of polymeric materials. Deep learning algorithms like DNNs, CNNs, GANs, RNNs, and GNNs are increasingly utilized in materials science for property prediction and molecular generation, offering solutions for complex data analysis. These advancements accelerate material innovation by enabling polymer structure identification, material synthesis, property prediction, and molecule generation. However, data scarcity remains a significant obstacle, with online databases facing limitations in data availability and properties, hindering progress in developing polymeric biomaterials, especially in medical applications.[9] The literature review

Table 1. Summary of literature review.

Ref/Year	Title of paper	Findings
[7]/2021	Machine learning in polymer informatics	Enhanced performance prediction through machine learning-driven polymer informatics
[8]/2023	Artificial intelligence driven design of catalysts and materials for ring opening polymerization using a domain-specific language	Shown some applications of machine learning on polymer design process
[9]/2023	Accelerating the design and development of polymeric materials via deep learning: Current status and future challenges	Limited online data makes it hard to develop medical polymer materials.
[10]/2023	Advances in computational intelligence of polymer composite materials: Machine learning assisted modeling, analysis, and design	ML improves polymer composites and suggests using ML to solve problems and guide future research
[11]/2023	Data-driven design of polymer-based biomaterials: High-throughput simulation, experimentation, and machine learning	Machine learning helps design materials by understanding how structure affects properties, especially in polymer biomaterials
[12]/2023	Data and machine learning in polymer science	Using data to solve problems in polymer science is powerful for understanding relationships, patterns, and behaviors.
[13]/2022	New opportunity: Machine learning for polymer materials design and discovery	Discuss future opportunities and challenges for ML in polymer material development.
[14]/2020	Recent advances in polymer-based electronic packaging materials	The research paper reviews polymer materials for electronic packaging, covering EMI shielding, dielectric, flip-chip underfill, and thermal interface.
[15]/2021	Automation and data-driven design of polymer therapeutics	Drug delivery and discovery for small molecules are revolutionized by ML and AI. Data-driven advancements in drug design and synthesis are highlighted in the review, along with research on antimicrobials, bioactive polymers, and drug and gene delivery.
[14]/2020	Application of machine learning in polymer additive manufacturing: A review	The paper explores ML in polymer AM, aiming to improve quality and reduce waste, suggesting future research directions.

underscores the importance of ML in predicting and optimizing the behavior of polymer composites, enabling unprecedented insights beyond traditional computational and experimental analyses. The review discusses ML applications such as prediction, optimization, feature identification, uncertainty quantification, reliability, and sensitivity analysis, along with challenges like the curse of dimensionality, overfitting, noise, and mixed variable problems. The review also highlights the latest ML advancements applicable to polymer composites and offers recommendations for exploiting ML algorithms to address critical problems, while providing insights into future research directions.[10]The rise of data-driven design of polymers for biomaterials, focusing on complex copolymer systems, streamlined modeling of structure-property relationships using ML, high-throughput data generation, surrogate modeling, and property optimization strategies, providing insights for future polymer-based biomaterial design.[11]

In this research paper, Data-driven innovation, integrating data and ML into traditional approaches, has demonstrated significant potential in addressing multifactor correlations, optimization, pattern identification, and phase transitions in polymer science. This literature review of[12] highlights key advances in polymer conformation description, structure identification, and structure-property correlation prediction using data and ML, offering insights and prospects in this emerging direction. In the research and design of polymer materials, ML, research paper reviews, and other data-driven techniques are employed. An overview of the process of ML in polymer materials, as well as the methods that are frequently employed and polymer descriptors and development trends of published papers on the subject, are given in this review. When ML aided in the design and discovery of polymer materials, the authors of this study present two scenarios. The research additionally indicates opportunities and challenges for ML's future progress in the area of polymer materials.[13] This literature review focuses primarily on high-density integration and packaging techniques for electronic devices. Dielectric, flip-chip underfill, thermal interface, and EMI shielding materials are examples of polymer-based electronic packaging materials that are essential to these advancements. The review highlights the obstacles and prospects for future research in the development of advanced polymer-based electronic packaging materials and talks about the variables like filler surface modification, polymer chain orientation, and material microstructures that affect these materials' performance.[14] The literature review highlights the significance of polymers in drug delivery systems, emphasizing the importance of rational design and tunable structural parameters for specific cargo and targeted release, particularly for anticancer drugs. Additionally, the review emphasizes the role of ML and AI in maximizing experimental efficiency in high-throughput synthesis and screening of polymers for drug delivery applications, revealing important lessons for the polymer therapeutics community.[15] In this research paper, the authors explore the integration of ML techniques into polymer additive manufacturing to address technical challenges and enhance efficiency. It provides a detailed analysis of existing research, proposes solutions for challenges, and outlines future research directions in this domain.[16] In conclusion, the literature review reveals a growing trend in polymer science where the application of ML algorithms has been steadily increasing over the past 5 years. This upward trajectory is expected to continue,

Table 2. Applications of AI and machine learning in Polymer Science and Materials Design.

Application	Description	Impact	Benefits
Materials Design and Discovery	AI enhances polymer design, improving properties.	Tailored polymers with better performance.	Innovation, improved material quality.
Property Prediction and Optimization	AI predicts properties, optimizes formulations.	Efficient research, tailored materials.	Research efficiency, optimized properties.
Process Optimization	AI improves manufacturing efficiency, reduces costs.	Cost savings, sustainable production.	Efficiency, cost reduction, sustainability.
Polymer Characterization	AI automates analysis, enhances precision.	Faster analysis, deeper insights.	Speed, understanding, product improvement.
Data-driven Understandings	AI uncovers patterns, guides research.	Novel theories, expanded science.	Enhanced outcomes, innovative discoveries.
Sustainable Polymer Development	AI optimizes for sustainability.	Eco-friendly materials, sustainable practices.	Environmental benefits, sustainability.

AI, artificial intelligence.

indicating a promising future for the integration of AI technologies in this field.

3. Advancements in Polymer Science Through Artificial Intelligence (AI) and Machine Learning (ML)

Polymer research is a specialized field of materials science that focuses on the study of polymers, which are substances composed of lengthy, recurring molecular chains. Polymers can be natural or synthetic and, based on the kind of molecules being bonded and the manner in which they are bonded, hold unique characteristics. From ordinary items like toys, clothes, and packaging to more advanced technologies like pharmaceutical delivery systems, desalination of water membranes, and biomedical implants, polymers have applications in an enormous variety of products. AI is going to have a profound effect on polymer research and transform several of various fields in the industry. Here is **Table 2** which shows applications of AI and ML in Polymer Science and Materials Design.

4. Applications and Future Perspectives

Polymer research shows AI and ML applications in diverse fields like materials, energy, security, catalyst design, and polymer informatics. Here are some examples:

1) *Prediction of Polymer Properties:* The prediction of polymer properties, such as elasticity, tensile strength, and thermal conductivity, can be derived by AI and ML models, specifically those that have been trained on huge datasets. The invention of new materials, optimization of processes, quality control in manufacturing, perception of environmental impacts, and polymer-related pharmaceutical and medical applications are all facilitated by these predictions.[17]
2) *Catalyst and Materials Design:* By predicting the characteristics of polymers and determining the best material combinations, AI systems and ML models facilitate the development of polymeric materials. This can result in the creation of novel polymers with specific properties for specific applications.[18]
3) *Polymer Informatics:* In this, AI systems can understand the complicated grammar and syntax that atoms follow as they merge to form polymers, hence speeding up polymer research. This has the possibility to completely transform how researchers and producers virtually examine the chemical space to find and manufacture these essential polymers (Table 3).
4) *Data Curation and Representation:* AI and ML can be implemented in data curation, feature the next, and material encoding for making ML usage easier. By ensuring transparency, repeatability, and the potential of data mining and the use for more data science-focused research, this can save time down the road. **Table 4** provides the key applications, techniques, and future perspective of ML in polymer science.

5. Machine Learning and AI in Polymer Synthesis and Design

AI and ML techniques have shown significant potential in polymer synthesis and design, paving the way for the synthesis of novel materials with desired features. The two primary tasks in polymer design that these methods can be used for are structure formation (also known as inverse problem design) and property prediction (also known as forward problem design).

The technique of predicting attributes of interest based on a polymer structure is referred to as property prediction. Because it allows for an assessment of the most prospective candidate instead of a complete library, this approach is highly helpful for the initial assessment of prospective materials. Elasticity, tensile strength, and thermal conductivity are among the features of polymers that can be predicted with the use of ML models such as random forests, deep learning, and Gaussian process models. One of the challenges facing this research is the limited and inconsistent research datasets caused by the inconsistent polymer naming standards.

ML challenges linked to property prediction usually call for a multi-phase strategy. Initially, the gathered data is subjected to preparing procedures like feature engineering, standardization, and cleaning. Following that, sets are generated from this data for evaluation, approval, and training. The next phase is to select an

Table 3. Machine learning in Polymer Science: Applications, techniques, and future prospects.

Application	Description	Techniques used	Future perspectives
Polymer modeling	Developing mathematical models to describe polymer behavior	1) Gaussian process regression (GPR) 2) Neural networks (NNs)	1) Improving model interpretability 2) Incorporating quantum-mechanical effects
Property prediction	Predicting polymer properties based on chemical structure	1) Supervised learning (e.g., regression, classification) 2) Transfer learning	1) Expanding to diverse polymer classes 2) Integrating with high-throughput experiments
Polymer Synthesis	Designing new polymers with desired properties	• Generative models (e.g., generative adversarial networks) • Reinforcement learning	• Automating polymer synthesis workflows • Enabling closed-loop optimization
Process Optimization	Optimizing polymer processing conditions	- Bayesian optimization - Reinforcement learning	- Real-time process monitoring and control - Scaling up to industrial production
Polymer Blending	Predicting properties of polymer blends and composites	1) Multiscale modeling 2) Graph neural networks	1) Accounting for complex morphologies 2) Extending to multi-component systems
High-Throughput Screening	Rapid analysis of large polymer datasets	1) Active learning 2) Transfer learning	I) Integrating with robotic experimentation II) Handling diverse data modalities
Sustainability	Assisting in polymer recycling, sorting, and environmental impact prediction	1) Computer vision 2) Life cycle assessment models	1) Enabling closed-loop polymer lifecycles 2) Predicting long-term environmental fate
Quality Control	Real-time monitoring of polymer production	1) Time series analysis 2) Anomaly detection	1) Deploying at industrial scale 2) Coupling with process control systems

Table 4. Polymer modeling, prediction, synthesis, and characterization with ML and AI.

Step	Description	Examples
Polymer modeling	Developing mathematical models to describe polymer behavior	Gaussian process regression (GPR), neural network (NN)
Property prediction	Predicting polymer properties based on ML models	TransPolymer for predicting polymer properties
Synthesis	Designing new polymers using ML models	Chemical-aware polymer tokenization method for modeling polymers
Characterization	Characterizing polymers using ML models	Graph convolutional network for predicting thermal and mechanical properties of polymers

AI, artificial intelligence; ML, machine learning.

algorithm for ML that can be trained on the training data, such as Gaussian algorithm models, random forests, or deep learning.

Then, in order to minimize overfitting, the hyperparameters are adjusted by verifying the model with the validation set. Once the model has been optimized, its performance is evaluated on the testing set. Lastly, the model is used for real-world uses, like polymer property forecasting, process optimization, manufacturing quality control, impact on the environment testing, and improving polymer-related pharmaceutical and medical applications. But the main obstacle facing this investigation is data availability; experimental datasets are frequently small and incompatible with each other because polymer naming rules are not recognized (Figure 4).

6. Examples of Machine Learning Applications

The field of material informatics, which combines ML algorithms with material datasets, has rapidly expanded in its ability to guide the use of polymers because of ML's strong linear and nonlinear fitting capabilities. This section will investigate, using a figure, the ways in which polymer modeling, synthesis, characterization, and property prediction can benefit from data-driven ML.

Here is Table 4 summarizing the key aspects of polymer modeling, property prediction, synthesis, and characterization using ML and AI:

6.1. AI and ML can be Implemented in Medical Science through Polymer Science

With the use of computer-aided material design with a ML algorithm and deep learning method, polymer design with AI and ML can help create high-performance implantable biomaterials with all desired properties. As a result, a highly adaptable and effective zwitterionic polymeric platform with excellent antibiofilm capabilities and adjustable parameters may be created. Property prediction, also known as forward problem design, and structure generation, also known as inverse problem design, are the two main categories into which ML is applied in polymer design. Property prediction entails predicting specific properties of interest given a polymer structure, whereas

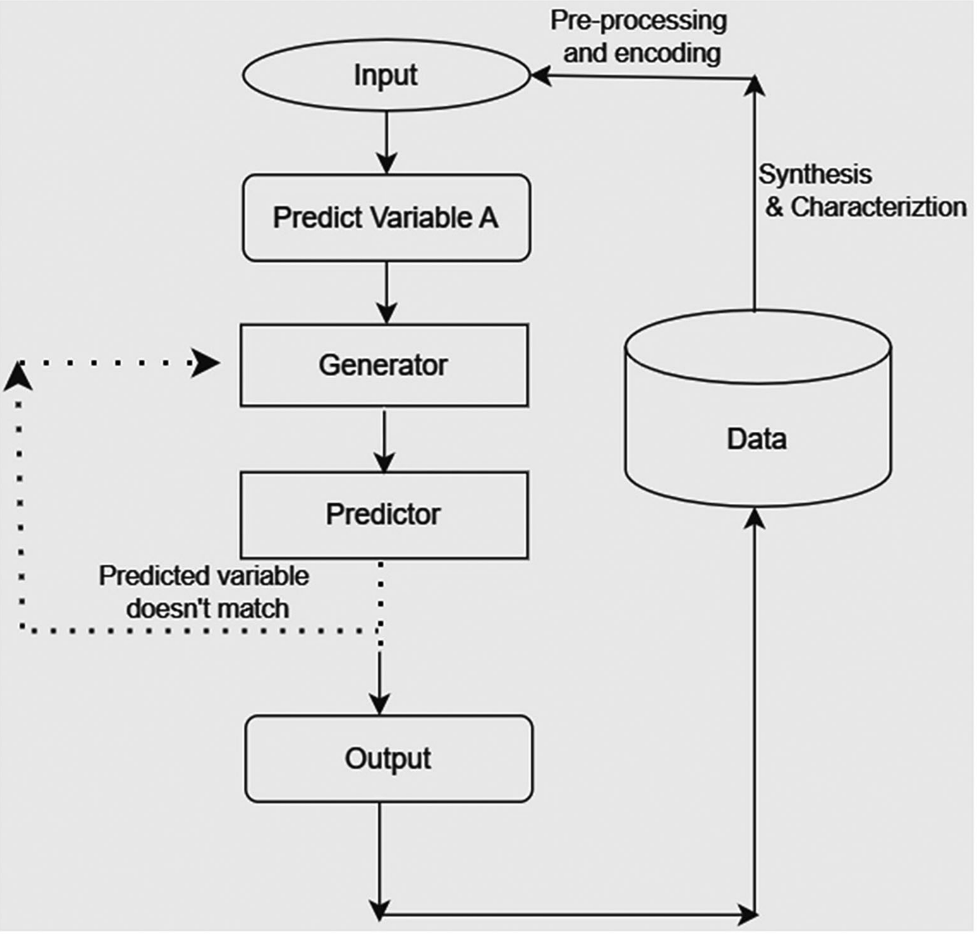

Figure 4. Machine learning and artificial intelligence (AI) in Polymer Synthesis and Design.

structure generation entails predicting polymeric structures that may exhibit the desired properties given properties of interest. By using these methods, the materials design process can be accelerated and user intuition-based constraints can be eliminated.

The main challenge facing this field, though, is data availability. This is the case since polymer naming conventions are not standardized, and experimental datasets are frequently small and incompatible with one another. Online databases include structural photos, various identification techniques, and information on hundreds of polymers and some of their related properties. Yet, their content is limited, and they have a significant data sparsity issue. The traits that supervised learning can predict are limited by these factors. In polymeric biomaterials design, ML offers a hitherto untapped potential to avoid trial-and-error synthesis, saving time and money on breakthrough discoveries that are essential to improving medical therapies. Combinatorial and high-throughput experimental designs have been used in the current efforts to pioneer applied ML in polymer design. The procedure for utilizing the IBM Materials Notebook and CMDL to enable the consumption of automated and historical experimentation data in generative models.[17]

6.2. Challenges

One nearly insurmountable barrier to ML-aided biomaterial design is the lack of available and standardized characterization of parameters relevant to medicine, such as degradation time and biocompatibility.[19] Based on the search results provided, here are the key challenges and conclusions from the research paper on advancements in ML and AI applications in polymer science:

Challenges:

1) **Representation of Polymers in ML Models**: The inherent stochastic nature of polymer structure makes it challenging to represent polymers in ML models, which typically work better with single, well-defined structures.
2) **Lack of Large, High-Quality Polymer Datasets**: The polymer community currently lacks publicly available databases with enough well-annotated polymer data to support “big data” ML approaches that are common in other fields.
3) **Closed Data and Interfaces from Instrumentation Manufacturers**: Many key polymer characterization instruments have closed data models and interfaces, impeding the creation of large, integrated polymer datasets and the integration of these instruments into high-throughput automation platforms.

4) **Need for Interpretable ML Models**: There is a need to develop more transparent, explainable ML models that can provide insights into polymer behavior at the molecular level, beyond just making accurate predictions.

7. Conclusion

The search results highlight that ML and AI are transforming polymer science, enabling new capabilities in areas like polymer modeling, property prediction, synthesis, and process optimization. However, the polymer community still faces unique challenges that need to be addressed to fully unlock the potential of these technologies.

Key future perspectives include:

- Improving model interpretability to gain deeper scientific insights.
- Expanding datasets and promoting open data sharing.
- Integrating ML with high-throughput experimentation and autonomous workflows.
- Developing benchmarks and best practices to drive wider adoption.

Addressing these challenges through collaborative efforts will be crucial to accelerating materials discovery and innovation in polymer science using ML and AI.

Acknowledgements

The authors have nothing to report.

Conflict of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

artificial intelligence, data fusion, machine learning, polymer, transfer learning

Received: April 30, 2024
Revised: May 19, 2024

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