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Predicting Polymer Properties in the Digital Age: AI and Uncertainty Quantification

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ABSTRACT
The digital transformation is rapidly influencing the field of polymer science. While the exact effects on research methods are still unfolding, early signs indicate that digitalization may dramatically enhance how new materials are discovered and developed. For instance, in polymer science, artificial intelligence (AI) has become a potent predictive tool. Compared to traditional methods, AI offers much greater speed and accuracy in forecasting polymer properties. Yet, AI's reliability is under scrutiny—especially for complex structure property relationships in polymers. To boost confidence in predictions, researchers are integrating Uncertainty Quantification (UQ) into their AI models. UQ is a set of methods that provides a measure of "how sure" we can be about an AI prediction. Bayesian neural networks and ensemble learning are among the UQ methods used to make AI more trustworthy for virtual screening and high throughput experiments in polymer informatics. The current state of digital supported materials research is under review, along with the challenges it faces. Our focus is on making AI driven models more scalable, interpretable, and generalizable. This review was written with researchers in mind who are developing new AI tools for use in polymer design and property prediction; we hope it serves as a useful resource for that community.

Keywords: Polymer Property Prediction

INTRODUCTION
The media is currently abuzz with terms like artificial intelligence (AI), automation, deep learning, big data, and machine learning. Their influence and advancements have spread to almost every sector, including science, thanks to cross-functional collaboration. In fact, their application in scientific research is already yielding some exciting results (Nosengo., 2016). For instance, deep learning can help identify genetic disorders (Gurovich et al., 2019); AI can interpret medical images or assist in drug development (Hosny et a;., 2018); and big data can tackle complex life sciences problems (Chen et al., 2016). These are not just trendy tools being applied for the sake of it—each example demonstrates real potential for making science more powerful and effective. There is no reason to think polymer science will be any different. In this context, we should take a closer look at what automation and digitalization might do for polymers research.
The discovery and development of new polymers are crucial for innovation in various sectors. For a long time, polymer research relied on slow and labor-intensive experimental approaches, using trial and error methods to explore the vast chemical space of possible polymer structures. In recent years, however, the advent of big data, automation, artificial intelligence (AI) and machine learning
(ML) has opened new avenues for accelerating the polymer discovery process by predicting material properties quickly and efficiently, thus reducing the need for extensive experimentation (Butler et al.; Jha et al., 2018). AI driven techniques have shown great success in predicting key polymer properties—for example, mechanical strength, thermal stability, and electrical conductivity—which positions AI as a potentially transformative tool in materials science (Chen et al., 2021; Chandrasekaran et al., 2020).
The complex behavior of materials can now be modeled by AI, and this has allowed us to integrate it into high throughput screening and virtual testing pipelines. These developments have meant that we can now explore the vast chemical spaces we are interested in much more quickly than would otherwise be possible. Moreover, these models have shown a potential that could be particularly useful in some of the fields we are interested in—such as sustainable polymers and next generation electronics—in assisting with what is known as

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"inverted design." This is when you generate new structures, such as polymer structures, with optimized properties (Xie & Grossman, 2018).

Yet despite these advances, a critical challenge remains: ensuring that AI predictions are reliable enough to trust when making decisions about which polymers to synthesize and test. In complex materials like polymers, even slight changes in molecular structure can dramatically alter properties. This sensitivity highlights the need for dependable AI models that can predict these property changes and also report how confident we should be in those predictions. Most current AI models are deterministic: they give a single point prediction without addressing the unavoidable uncertainties present in both data and models (Jain et al., 2016). This shortcoming has led to growing interest in methods for quantifying uncertainty (UQ), which aim to make AI driven predictions more trustworthy by assessing both kinds of uncertainty—epistemic (model) and aleatoric (data), and then accounting for them (Gawlikowski et al., 2021).

Uncertainty quantification is becoming recognized as essential not just because it allows us to understand how reliable an AI prediction is but also because it enables us to identify when an AI system is failing. Uncertainty quantification (UQ) serves two primary functions in the evaluation of AI models: it assesses the reliability of model predictions and supports risk-based decision making. These functions are particularly crucial for high stakes applications like biomedical materials and polymers used in extreme conditions, where incorrect AI predictions could have disastrous outcomes (Scalia et al., 2020). In these contexts, UQ allows researchers to trustfully integrate AI into virtual polymer screening and materials informatics pipelines.

This review offers a comprehensive overview of UQ methods as applied to AI driven predictions of polymer properties. We begin by examining the nature and sources of uncertainty in machine learning models, focusing on both model related and data related uncertainties. We will now examine the main uncertainty quantification (UQ) methods—Bayesian neural networks, ensemble techniques, and dropout based approximations—and how well they work for polymer science applications (Kendall & Gal, 2017). We will then explain UQ's place in high throughput screening and virtual polymer design. In these contexts, we will emphasize UQ's importance in improving decision making and speeding up materials discovery. After that, we will discuss some of thechallenges facing the polymer science community as it works to develop AI driven models that are more reliable and robust. Our focus here will be on scalability, interpretability, and generalization.

Finally, we will provide a critical assessment of the current state of uncertainty quantification in AI driven predictions of polymer properties. This review should help guide researchers in developing "trustworthy" AI tools for realizing the next generation of polymer materials.

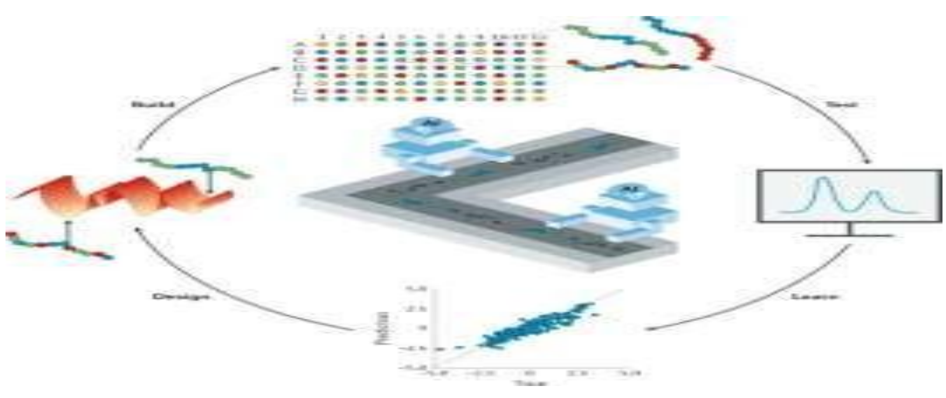

Figure 1 Using machine learning in polymer design (Gormley, A.J et al., 2021)

Review Methodology

The review employs a structured and systematic approach to ensure that relevant, high-quality research is included in the study of uncertainty quantification (UQ) for AI driven predictions of polymer properties.

Literature Search Strategy

The process began with a detailed search across several academic databases: Google Scholar, Web of Science, Scopus, IEEE Xplore, PubMed. Given the interdisciplinary nature of the topic, insights from chemistry, materials science, and other relevant fields were integrated into the search strategy. Additionally, preprints from arXiv

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were consulted to ensure that very recent advancements, particularly in AI and machine learning were captured.

The main body of literature identified consists of peer reviewed journal articles and conference proceedings published between 2010 and 2024. This period covers both foundational techniques in AI as well as more recent innovations pertinent to UQ and polymer property prediction (Jha et al., 2018; Chen et al., 2021).

The search terms and phrases used were centered around the intersection of artificial intelligence, machine learning, and polymer science. They included "uncertainty quantification in machine learning," "AI driven polymer property prediction," "materials science and machine learning," and several others that focused on specific aspects of AI/ML research relevant to materials or polymer science. Given the nascent state of this research area, only a limited number of studies could be

identified. To ensure that key works were located, we employed citation chaining to find seminal papers frequently cited in this domain.

2.1 Inclusion and Exclusion Criteria

We applied inclusion and exclusion criteria during the literature screening process to ensure relevance and rigor. Our focus was on studies directly discussing the application of AI or machine learning to predict properties of polymers or discover new polymers. Uncertainty quantification is a critical aspect of artificial intelligence, especially for high stakes applications like materials science. For this reason, the literature review prioritized papers that address uncertainty quantification in AI models, with a particular focus on their relevance to polymeric materials. Only peer reviewed articles, conference papers, and select high impact preprints were considered to ensure the quality of the sources.

Furthermore, only articles published in English were included. To capture both foundational and cutting-edge work in the field, studies published between 2010 and 2024 were considered. The review excluded any non-AI based studies (e.g., those focused solely on experimental or purely theoretical polymer research) to maintain a sharp focus on the application of AI and machine learning to problems relevant to polymeric materials. We did not include studies on uncertainty quantification that were applied to unrelated fields (e.g., finance, medicine) because we deemed them too far afield. However, some of these studies could have been included if they offered insights directly translatable to polymer science. We excluded non peer reviewed papers and studies with insufficient methodological rigor to ensure the quality of our literature review.

2.2 Selection and Review Process

Our initial literature search resulted in over 300 studies. After applying our inclusion and exclusion criteria, we selected 120 articles for detailed review. The selected papers were organized into thematic categories based on their content. Their focus was either on AI methods for predicting polymer properties, techniques for uncertainty quantification (UQ), or practical applications of UQ in polymer science (Gawlikowski et al., 2021).The first category includes papers that cover a variety of models used for polymer property predictions, such as supervised learning, deep learning, and generative approaches (Chen et al., 2021). The second category includes methods of uncertainty quantification, an important aspect of UQ that involves different techniques such as Bayesian neural networks, ensemble learning, and dropout-based methods (Kendall & Gal, 2017). Finally, the third category includes papers that detail applications of these methods in polymer science, specifically in virtual screening, high throughput experimentation, and materials informatics (Scalia et al., 2020).

2.3 Critical Evaluation and Synthesis

The selected studies underwent a critical evaluation to determine their methodological soundness, originality, and influence on polymer science. The assessment criteria included: 1. Methodological soundness: The robustness of the UQ methods used in the studies and their effectiveness when applied to AI models were examined (Gawlikowski et al., 2021). Priority was given to papers that presented novel approaches to UQ and AI, significantly furthering the field of polymer property

prediction (Jha et al., 2018). The practical applicability of the studies to real world polymer design problems—like high throughput screening and virtual material discovery was evaluated.The synthesis of results is organized into three thematic sections: AI techniques, UQ methodologies, and applications in polymer science. The review highlights new trends, research gaps, and future opportunities to enhance the reliability and scalability of AI driven models used in discovering new materials.

2.4 Limitations

Despite its comprehensive nature, some limitations are inherent to the review's methodology. For instance, it

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may have missed relevant non-English studies due to a reliance on English language literature. Furthermore, while preprints from repositories like arXiv were included, some of these studies might not yet have undergone peer review, which could impact their perceived reliability.

1. Critical Examination

3.1 Overview of AI in polymer prediction

The field of polymer science has been revolutionized by AI and machine learning, which now offer the capability to forecast polymer properties with greater speed and accuracy than the conventional experimental methods of the past. By employing computational models, researchers can delve into vast chemical spaces and unearth new materials that exhibit desired characteristics—all while significantly reducing the number of labor-intensive experiments needed to verify their findings (Chen et al., 2021).Of particular note is the increasing use of certain predictive tools from machine learning. These include supervised learning models such as support vector machines, random forests, and neural networks. When applied to property prediction problems for polymers—especially key properties like glass transition temperature, mechanical strength, and thermal stability—their performance has been impressive (Jha et al., 2018). Deep learning, especially using convolutional neural networks (CNNs) and recurrent neural networks (RNNs), has improved the automatic learning of feature representations from polymer molecular structures. This has enhanced prediction accuracy in polymer science (Chen et al., 2021).An even more significant recent advancement is the use of generative models for polymer design. Generative adversarial networks (GANs) and variational autoencoders (VAEs) are among the most prominent tools for this task. These deep learning-based methods have been particularly effective in virtual screening workflows, wherein new candidate polymers are computationally evaluated before being synthesized.Despite their potential, AI models face several challenges that need to be overcome if they are to achieve widespread reliability and adoption within the field. A key issue relates to the reliability of predictions made by these models when dealing with complex high dimensional data— especially when such data describe polymers with novel structures or compositions. Uncertainty quantification (UQ) has become an essential means for tackling these problems and enhancing the reliability of AI driven forecasts.

3.2 Uncertainty in Data Quality and Machine Learning Models

The key challenge in digitalizing materials research is the collection, management, and interpretation of data, which has not received as much attention as the use of artificial intelligence and machine learning. Data plays a vital role in training these models, but problems persist, such as inconsistent storage formats, limited sharing of experimental outcomes (especially failed experiments), and questionable data quality. Most research data remain confined to local labs, inaccessible to the broader community, which complicates the discovery of structure-property relationships and prevents comprehensive meta-analyses.

One approach to address this is adopting the FAIR principles (Findable, Accessible, Interoperable, and Reusable) for data management, which would enhance the ability to reuse past experiments and prevent unnecessary duplication of efforts (Inau et al., 2021). Centralized repositories like Material Cloud (Materials Cloud, https://www.materialscloud.org/) and Aflowlib (Automatic- Flow for Materials Discovery, http://aflowlib.org/) offer promising examples of open data sharing. However, challenges still exist, such as creating standardized data formats and building a global infrastructure for accessible, high-quality data storage. Success will mainly depend on training researchers and promoting widespread adoption of these data-sharing practices.

Additionally, machine learning models are inherently uncertain, especially when tasked with predicting the properties of polymers. In polymer science driven by artificial intelligence, multiple factors contribute to these uncertainties, including the training data's limitations and the model's generalization capacity for novel materials. Because they affect AI predictions' reliability and accuracy, understanding and addressing these uncertainties is vital.

Two main types of uncertainty afflict machine learning models: epistemic (model) uncertainty and aleatoric (data) uncertainty.

- Epistemic uncertainty stems from the model itself—insufficient training data or an inadequate model structure, for instance, and can often be reduced by improving the model through more data collection or a better-defined model architecture.
- Aleatoric uncertainty stems from the natural variability in the data, such as noise in measurements or a lack of complete information about a polymer's environment. Unlike epistemic uncertainty, which can be reduced by improving our models and understanding, aleatoric uncertainty reflects true randomness and cannot be reduced.

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In polymer science, both types of uncertainty are crucial to consider. Epistemic uncertainty is especially relevant when AI models are applied to predict the properties of new polymers because it highlights situations where those models may not perform well. Aleatoric uncertainty is more prevalent in experimental datasets and reflects the kind of imprecision that often accompanies measurements of material properties.

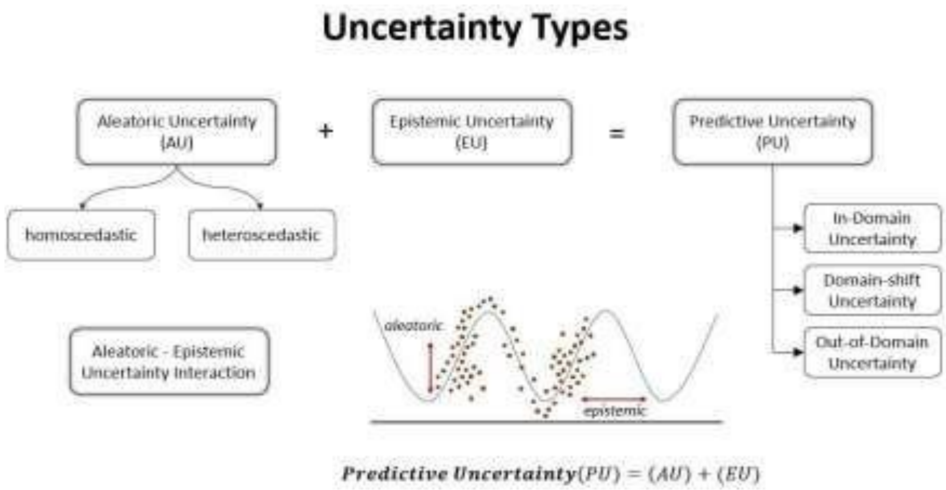

Figure 2 Uncertainty Types (KDnuggets. (2022, April 21). Uncertainty quantification in artificial intelligence-based system)

3.3 Methods for Uncertainty Quantification

To improve the reliability of AI models for predicting polymer properties, researchers have developed several methods for uncertainty quantification (UQ). These methods make it possible to assess both epistemic and aleatoric uncertainties, providing a clearer picture of what the models are actually predicting.

- **Bayesian Neural Networks (BNNs):** One promising approach is to use Bayesian neural networks (BNNs), which offer a way to incorporate probabilistic reasoning into neural networks by placing distributions over parameters instead of single point estimates. BNNs make it straightforward to quantify the uncertainty in predictions because you can sample from the posterior distribution of the model's "weights" to generate predictive distributions. They are particularly useful for capturing epistemic uncertainty—what we do not know about the model itself—which is especially relevant when one has limited training data (Gal & Ghahramani, 2016).
- **Ensemble Learning:** Methods like random forests and deep ensembles enhance accuracy and robustness by combining the predictions of multiple models. These methods provide a way to quantify uncertainty in predictions, as they require training several models with different initial conditions or subsets of data. The variance in predictions across the models is an indicator of epistemic uncertainty. Consistent predictions across models suggest that the system being modeled is not too far from one for which we have low uncertainty (Lakshminarayanan et al., 2017).
- **Dropout as UQ:** Dropout is a regularization technique used to prevent overfitting in neural networks. It can also be repurposed for quantifying uncertainty. By randomly dropping out units during both training and inference, dropout introduces some amount of "controlled" randomness into the model. This randomness allows for an estimation of model uncertainty. The "Monte Carlo dropout" method offers a computationally efficient means to approximate Bayesian inference for deep learning models. This technique provides a way

  to handle model uncertainty, which is especially important when making predictions with limited data (Gal & Ghahramani, 2016).
- **Gaussian Processes (GPs):** In contrast, Gaussian Processes (GPs) are a class of non- parametric models that offer a natural way to quantify prediction uncertainty. For smaller datasets, GPs are particularly effective and provide an excellent fit. In the context of polymer discovery, where only a few data points may be available, GPs are well suited for modeling the kinds of structures that polymers can

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take (Rasmussen & Williams, 2006).

3.4 Applications of UQ in Polymer Science

Uncertainty quantification is crucial in polymer science, especially when reliable forecasts are needed to speed up the discovery process and cut down on experimental expenses.

- **Property Prediction:** When it comes to predicting polymer properties, UQ methods serve as a kind of safety net, catching predictions that are too uncertain to be trusted. For high stakes applications—like polymers for use inside the body or in materials that will be subjected to extreme conditions—it is wise to have not just a property prediction but also an accompanying measure of how confident we can be in that prediction (Scalia et al., 2020). In these cases, UQ enables more informed decisions during the design phase.
- **Virtual Screening:** Uncertainty quantification is also integrated into virtual screening workflows in which thousands of potential polymer candidates are assessed and flagged before synthesis. UQ methods enhance the reliability of predictions about new polymer candidates, making them more trustworthy. This allows researchers to better identify which polymeric materials are most likely to succeed and thus reduces the risk that they will invest in synthesizing and testing materials that ultimately do not work.
- **High-Throughput Testing:** High throughput experimentation is a necessary component of modern materials discovery, but it is also an expensive and resource intensive process. UQ enables adaptive optimization of experimental design, thereby increasing the efficiency of high throughput testing while maintaining its effectiveness.

3.5 Case Studies and Examples

Several studies have highlighted how important it is to quantify uncertainty when designing polymers in the real world. One such study, "Deep Learning for Polymer Dielectrics" by Jha et al. (2018), used deep learning models to predict dielectric properties of polymer materials. These authors incorporated a method called Monte Carlo dropout into their models to estimate uncertainty and improve reliability.Another study, "Bayesian Optimization for Polymer Synthesis" by Scalia et al., used a different method to do the same thing: they quantified uncertainty so that they could reliably identify which predictions needed further validation. In 2017, a research team applied Bayesian optimization with uncertainty quantification to direct polymer synthesis experiments (Li et al., 2017). They prioritized experiments based on how uncertain their predictions were, which allowed them to reduce the number of failed synthesis attempts. At the same time, they discovered new polymers with enhanced properties.These examples highlight how important it is for AI driven polymer research to have reliable and accurate predictions, something that uncertainty quantification helps achieve.

2. Discussion

The review emphasizes the revolutionary impact of AI techniques, especially machine learning and deep learning models, on predicting polymer properties. These computational approaches have made it possible to discover new polymers without heavily relying on expensive and slow experimental methods. Nevertheless, the reliability of these AI predictions is not yet fully trustworthy because both the models and the data contain uncertainties. Uncertainty quantification (UQ) can help make these predictions more reliable by assigning confidence intervals to them.

Current AI models in polymer science—most notably those employing supervised learning, generative models, and ensemble techniques—offer a wide range of predictive accuracies and "uncertainty management" strategies. Bayesian neural networks (BNNs) and ensemble learning have been shown to be effective for capturing epistemic uncertainties. Monte Carlo dropout is another technique that can address both types of uncertainty, with a particular strength in handling aleatoric uncertainty. However, these methods do not always work equally well; their effectiveness can vary based on the complexity of the task at hand, the quality of the data used to train the model, and the amount of computational power available.

Even though impressive progress has been made in uncertainty quantification (UQ), several important gaps remain. One involves making more comprehensive studies of different UQ methods over a larger range of polymer applications. Bayesian optimization has shown promise as a guide for polymer synthesis, but few case studies exist that allow direct comparison between this method and others. Second, there is limited integration

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of UQ into high throughput screening and virtual testing workflows in polymer science. Bringing UQ into these processes more seamlessly could reduce failed experiments significantly and speed up polymer discovery.
Finally, data quality often constrains the use of UQ in polymer science. Many datasets are incomplete or noisy, making it hard to quantify uncertainties. Methods to deal with data related uncertainties need to be developed further to improve predictions and broaden the applicability of UQ techniques in AI driven polymer research.

3. Challenges and Future Directions

Even with the progress made in uncertainty quantification, several hurdles prevent its broad application in polymer science. A major issue is the scalability of current UQ methods. For example, using Bayesian neural networks to quantify uncertainty is often too computationally expensive for large scale tasks, like screening huge libraries of polymers. Another problem is that the most effective methods for quantifying epistemic uncertainty usually need lots of data— something we do not always have in polymer informatics, where our datasets are often limited.

We also need to figure out how to integrate UQ into our high throughput and automated workflows without slowing everything down. Despite the promise that uncertainty quantification (UQ) holds for enhancing decision making in material discovery, its practical application in high throughput systems is still lacking. The reason for this may be the process used to implement UQ, which is not yet sufficiently scalable or efficient for use in a high throughput context.

Another persistent problem relates to data quality. Many experimental polymer datasets are incomplete, noisy, or inconsistent, leading to predictions of questionable reliability. Improving data quality through better experiments and novel techniques for augmenting real data could make a significant dent in reducing aleatoric uncertainties and thus improve the outcomes of UQ.

Future research should aim to create hybrid models that bring together several uncertainty quantification (UQ) methods. These models can more effectively handle the intricate uncertainties involved in predicting polymer properties. AI and physics-based model integration may also offer a path to improved predictive reliability, especially for polymers represented by high dimensional data. Additionally, recent advances in generative models—such as variational autoencoders (VAEs) and generative adversarial networks (GANs)—should be investigated further. In combination with UQ methods, these models could significantly boost the virtual screening of polymers.

4. Conclusion

The future of materials research is becoming more digital, but this shift requires significant changes across various areas, from material synthesis to data management and machine learning. Although progress is being made, the challenge lies in integrating all the above discussed methods into a unified approach. Key steps include creating a centralized data repository, standardizing data formats globally, and improving AI programs tailored for materials science. Additionally, training researchers in fields like computer science, database management, and robotics is crucial. This transformation will enable faster and more reproducible development, allowing scientists to focus on designing new materials while automated systems handle synthesis and characterization. Ultimately, this will lead to greater productivity, improved data quality, and better understanding of material properties and their relationships.

The review has underscored how AI and machine learning are transforming the prediction of polymer properties, with a special focus on the essential role of uncertainty quantification (UQ). In polymer science, where new material discovery is often slowed by data issues, UQ can significantly boost confidence in AI driven predictions. Researchers employing methods like Bayesian neural networks, ensemble learning, and Gaussian processes now have a clearer picture of the uncertainties that accompany their predictions. This allows for better risk assessment in the virtual screening of novel polymers.

Even though UQ is advancing nicely, it still faces some serious challenges—scalability, data quality, and integration into high throughput workflows. These challenges are not insurmountable. Hybrid models that combine the best aspects of different UQ approaches could help tackle the first issue. The second and third issues might be solved by improved data handling methods and enhanced generative techniques. The potential exists for these advancements to greatly speed up the discovery of new materials and lessen the experimental load in polymer science.

To sum up, uncertainty quantification will remain a vital part of the AI driven revolution in polymer research, with the potential to boost how accurately we can make predictions and help us find new polymers with tailored

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properties. Ongoing work on making UQ techniques more scalable, better data quality, and integrating AI models into real world scenarios will be key for determining what comes next in polymer science.

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