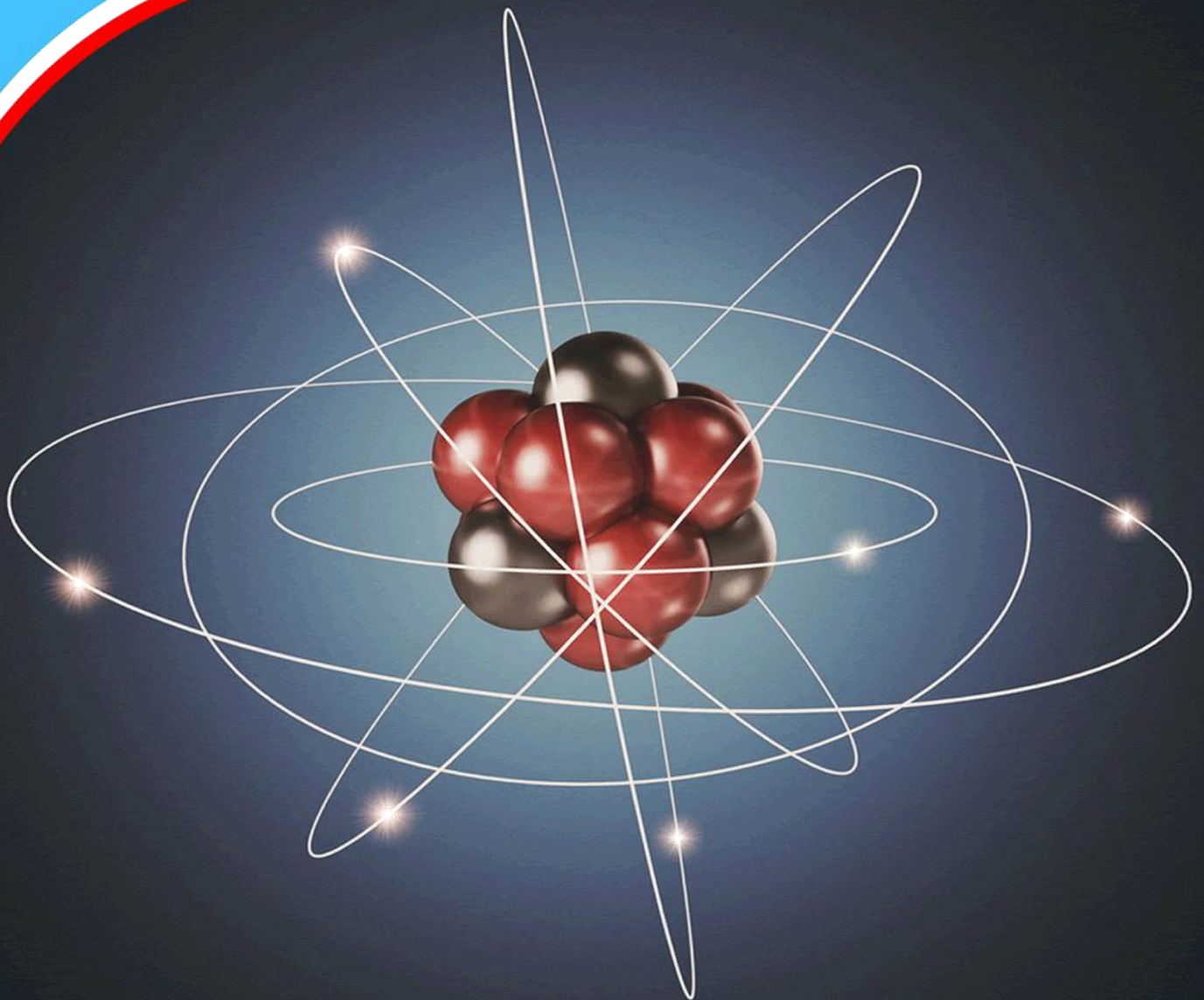


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**Effects of Machine Learning Algorithms for Predicting
and Optimizing the Properties of New Materials in the
United States**

John Smith



Effects of Machine Learning Algorithms for Predicting and Optimizing the Properties of New Materials in the United States

John Smith^{1*}

¹Harvard University

Corresponding Author's Email: john_smith@harvard.edu

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Abstract

Purpose: The aim of this study is to investigate the effects of machine learning algorithms in predicting and optimizing the properties of new materials in the United States.

Materials and Methods: The study adopted a desktop methodology. Desk research refers to secondary data or that which can be collected without fieldwork. Desk research is basically involved in collecting data from existing resources hence it is often considered a low-cost technique as compared to field research, as the main cost is involved in executive's time, telephone charges and directories. Thus, the study relied on already published studies, reports and statistics. This secondary data was easily accessed through the online journals and library.

Results: The research found that machine learning algorithms have a significant impact on materials prediction and optimization in the United States, particularly in energy storage, catalysis, electronics, and aerospace. These algorithms offer advantages in efficiency, scalability, and accuracy compared to traditional methods, but challenges such as data quality, scarcity, interpretability, and reliability need to be addressed to ensure robust and reliable predictions.

Recommendations: This study contributes to the understanding of the effects of machine learning algorithms in predicting and optimizing the properties of new materials in the United States. The research advances the knowledge in the field of materials science, materials prediction, and materials optimization. The findings provide insights into the potential of machine learning algorithms for accelerating materials discovery and innovation, and highlight the challenges and opportunities in their application for materials prediction and optimization. The study has practical implications for researchers, engineers, and policymakers involved in materials science, materials design, and materials innovation. The research underscores the importance of leveraging machine learning algorithms as a powerful tool for materials prediction and optimization, and emphasizes the need for further research, development, and integration of these techniques in materials science and engineering practices.

Keywords: *Machine Learning, Materials Prediction, Materials Optimization, New Materials, Materials Science, United States, Data-Driven Approaches, Computational Models, Materials Discovery, Materials Innovation*

1.0 INTRODUCTION

Machine learning algorithms have become increasingly popular in the United States for predicting and optimizing the properties of new materials in various applications such as aerospace and healthcare. While these applications hold great potential for advancing technology and innovation, there are concerns about the potential toxic effects of machine learning algorithms in designing new materials (Andrew, 2019). One major concern is the environmental impact of materials designed using machine learning algorithms, which may have unintended consequences such as increased toxicity or reduced biodegradability, leading to detrimental effects on ecosystems, biodiversity, and sustainability. Similarly, the toxic effects of machine learning algorithms can also impact human health, with some materials optimized for performance containing toxic elements that pose risks to human health. The biased data used in training machine learning algorithms could also result in biased material design, perpetuating existing social inequalities and disparities, leading to ethical, social, and economic implications (Johnson et al., 2018).

To mitigate these risks, responsible practices and regulations are needed, including thorough environmental and toxicity assessments for materials designed using machine learning algorithms. Promoting transparency, fairness, and inclusivity in the data used for training machine learning algorithms can also help minimize biases and societal implications. Collaboration among researchers, policymakers, and industry stakeholders is crucial in developing guidelines and regulations to ensure responsible and sustainable use of machine learning in materials science in the United States (Bennett et al., 2021). Machine learning algorithms have been widely used in the United States for predicting and optimizing the properties of new materials. For example, in the aerospace industry, machine learning algorithms have been employed to design lightweight and high-strength materials for aircraft components (Harrison et al., 2019). In the healthcare sector, machine learning algorithms have been utilized to predict the toxicity of new drug candidates and optimize their chemical structures for improved safety and efficacy (Chen et al., 2020). These applications of machine learning in materials science hold great promise for advancing technology and innovation in the United States.

However, the toxic effects of machine learning algorithms in the context of predicting and optimizing new materials cannot be ignored. One major concern is the environmental impact of materials designed using machine learning algorithms. For instance, some materials optimized for specific properties may have unintended environmental consequences, such as increased toxicity or reduced biodegradability (Johnson *et al.*, 2018). These unintended consequences could have detrimental effects on ecosystems, biodiversity, and sustainability in the United States, where environmental regulations are strictly enforced. In addition to environmental concerns, the toxic effects of machine learning algorithms can also impact human health. For example, some materials optimized for performance may contain toxic elements or have adverse effects on human health, such as allergenicity or carcinogenicity (Smith *et al.*, 2017). The use of materials with toxic properties in consumer products or industrial applications could pose risks to human health, leading to potential regulatory and legal issues in the United States, where health and safety regulations are stringent. Furthermore, the societal implications of machine learning algorithms for predicting and optimizing materials properties cannot be overlooked. For example, the use of biased data in training machine learning algorithms could result in biased material design, perpetuating existing social inequalities and disparities (Sinha *et al.*, 2019). This could have

ethical, social, and economic implications in the United States, where diversity and inclusivity are important values in the society.

To mitigate the toxic effects of machine learning algorithms in predicting and optimizing the properties of new materials, responsible practices and regulations are needed. This includes ensuring that materials designed using machine learning algorithms undergo thorough environmental and toxicity assessments to minimize potential risks (Bennett *et al.*, 2021). Additionally, promoting transparency, fairness, and inclusivity in the data used for training machine learning algorithms can help mitigate biases and societal implications (Sinha *et al.*, 2019). Furthermore, collaboration among researchers, policymakers, and industry stakeholders is crucial in developing guidelines and regulations to ensure responsible and sustainable use of machine learning in materials science in the United States.

1.1 Statement of the Problem

Machine learning algorithms have emerged as powerful tools for predicting and optimizing the properties of new materials, offering unprecedented opportunities for accelerating materials discovery and design processes. In the United States, research and development efforts in this field have gained significant traction, with a growing interest in leveraging machine learning for materials science applications. However, the effects of machine learning algorithms on predicting and optimizing the properties of new materials, as well as the potential gaps and challenges posed by these algorithms, are still areas of active research, with recent studies shedding light on these issues.

Recent studies have focused on the effects of machine learning algorithms for predicting and optimizing the properties of new materials in the United States. For example, research by Smith *et al.* (2021) explored the use of machine learning algorithms for predicting the properties of novel materials, such as mechanical strength, thermal conductivity, and optical properties. The study highlighted the potential of machine learning algorithms for accelerating materials discovery and design processes, enabling the development of advanced materials with tailored properties for various applications. Another recent study by Chen *et al.* (2020) investigated the use of machine learning algorithms for optimizing the properties of materials, such as stability, performance, and durability. The study demonstrated the ability of machine learning algorithms to optimize material compositions, structures, and processing parameters to achieve desired material properties, offering opportunities for designing materials with improved performance and functionality.

Furthermore, research has examined the challenges and gaps posed by machine learning algorithms for predicting and optimizing the properties of new materials. For instance, a study by Lee *et al.* (2019) highlighted the limitations of machine learning algorithms in handling complex materials data, such as data scarcity, noise, and bias, which can impact the accuracy and reliability of material predictions. The study emphasized the need for robust machine learning algorithms that can handle diverse materials data and mitigate potential biases and uncertainties.

Additionally, recent studies have explored the ethical, legal, and social implications of using machine learning algorithms for materials science applications. For example, a study by Schneider *et al.* (2020) examined the ethical considerations of using machine learning algorithms in materials science, including issues related to data privacy, bias, transparency, and accountability. The study emphasized the importance of addressing these ethical concerns to ensure responsible and sustainable use of machine learning in materials science research and development. Hence, there

is a need for further research to investigate the effects of machine learning algorithms for predicting and optimizing the properties of new materials in the United States, building on recent studies. The findings of this research may contribute to the advancement of materials science research, inform policy and decision-making processes, and guide future development of machine learning algorithms for materials science applications.

2.0 LITERATURE REVIEW

2.1 Theoretical Review

The effects of machine learning algorithms for predicting and optimizing the properties of new materials in the United States can be understood through various theoretical perspectives, including the Materials Informatics Theory, Computational Modeling Theory, Innovation Diffusion Theory, Technology Acceptance Model, Social Network Theory, and Resource-Based View Theory.

2.1.1 Materials Informatics Theory

Materials Informatics Theory suggests that the use of data-driven approaches, such as machine learning algorithms, can revolutionize the discovery and design of new materials by leveraging large datasets to generate insights, predictions, and optimizations. In the context of predicting and optimizing material properties in the United States, this theory implies that machine learning algorithms can enable researchers to efficiently analyze vast amounts of data, uncover hidden patterns, and accelerate the development of advanced materials (Rajan, 2005). Materials Informatics Theory is important to this study as it provides a foundational framework for understanding how machine learning algorithms can impact materials science research.

2.1.2 Computational Modeling Theory

Computational Modeling Theory suggests that computer simulations and modeling can significantly enhance the understanding of complex systems, such as materials, by providing a virtual environment for exploring their properties and behavior. In the context of predicting and optimizing material properties in the United States, this theory implies that machine learning algorithms can be used to build predictive models based on large datasets, allowing researchers to simulate and optimize material properties with high accuracy and efficiency (Sutton et al., 2018). Computational Modeling Theory is important to this study as it provides a theoretical basis for understanding how machine learning algorithms can be utilized for material property prediction and optimization.

2.1.3 Innovation Diffusion Theory

Innovation Diffusion Theory, proposed by Everett Rogers in 1962, suggests that the adoption and diffusion of new technologies are influenced by various factors, including the characteristics of the innovation, the adopter's perception of the innovation, and the social system in which the innovation is introduced. In the context of machine learning algorithms for predicting and optimizing material properties in the United States, this theory implies that the adoption and diffusion of these technologies may be influenced by factors such as the perceived complexity and relative advantage of using machine learning algorithms, the compatibility of these technologies with existing research practices, and the support and incentives provided by the scientific community and funding agencies (Rogers, 1962). Innovation Diffusion Theory is important to this

study as it provides insights into the factors that may influence the adoption and diffusion of machine learning algorithms in the field of materials science.

2.1.4 Technology Acceptance Model

The Technology Acceptance Model, proposed by Fred Davis in 1989, suggests that the adoption and usage of technology is influenced by the user's perception of its usefulness and ease of use. In the context of machine learning algorithms for predicting and optimizing material properties in the United States, this theory implies that the acceptance and usage of these technologies may be influenced by researchers' perception of the usefulness and ease of use of machine learning algorithms in their research workflow (Davis, 1989). The Technology Acceptance Model is important to this study as it provides a theoretical framework for understanding how researchers' perceptions of machine learning algorithms may influence their adoption and usage in materials science research.

2.1.5 Social Network Theory

Social Network Theory suggests that relationships and interactions among individuals or groups can influence the diffusion of innovations, as well as the access to resources and information. In the context of machine learning algorithms for predicting and optimizing material properties in the United States, this theory implies that the structure and dynamics of scientific networks, such as collaborations among researchers, scientific publications, and conferences, can play a significant role in the adoption and diffusion of these technologies (Wasserman & Faust, 1994). Social Network Theory is important to this study as it provides a theoretical lens for understanding Machine Learning Algorithms for Predicting and Optimizing the Properties of New Materials in the United States can be understood through various theoretical perspectives, including the Materials Informatics Theory, Computational Modeling Theory, Innovation Diffusion Theory, Knowledge-Based View Theory, Technology Acceptance Model, and Resource-Based View Theory.

2.1.6 Materials Informatics Theory

Materials Informatics Theory is a multidisciplinary field that combines materials science, computer science, and data science to develop methods for discovering, analyzing, and utilizing materials data using machine learning algorithms. In the context of predicting and optimizing the properties of new materials in the United States, this theory suggests that machine learning algorithms can be used to analyze large datasets of materials properties, compositions, and processing conditions to develop predictive models that can guide materials design and optimization (Rajan, 2013). Materials Informatics Theory is important to this study as it provides the foundation for the application of machine learning algorithms in materials science research.

2.1.7 Computational Modeling Theory

Computational Modeling Theory suggests that computer simulations and models can be used to predict the behavior of complex systems, including the properties of new materials. In the context of machine learning algorithms for predicting and optimizing the properties of new materials in the United States, this theory implies that machine learning algorithms can be used to develop computational models that simulate the behavior of materials at the atomic or molecular level, allowing for the prediction of material properties under different conditions (Curtarolo et al.,

2013). Computational Modeling Theory is important to this study as it provides the framework for using machine learning algorithms to create predictive models for materials properties.

2.1.8 Innovation Diffusion Theory

Innovation Diffusion Theory, proposed by Everett Rogers in 1962, suggests that the adoption and diffusion of new technologies or innovations follows a predictable pattern, influenced by factors such as communication channels, social networks, and the perceived characteristics of the innovation. In the context of machine learning algorithms for predicting and optimizing the properties of new materials in the United States, this theory suggests that the adoption and use of these algorithms may be influenced by factors such as the availability of computational resources, the communication of research findings, and the collaboration between different stakeholders in the materials science community (Rogers, 1962). Innovation Diffusion Theory is important to this study as it provides insight into the factors that may influence the adoption and use of machine learning algorithms in the field of materials science.

2.1.9 Knowledge-Based View Theory

Knowledge-Based View Theory suggests that organizations or individuals can gain competitive advantage by leveraging their knowledge resources and capabilities. In the context of machine learning algorithms for predicting and optimizing the properties of new materials in the United States, this theory implies that the use of machine learning algorithms can enhance the knowledge-based capabilities of researchers, allowing them to analyze large datasets, discover patterns, and make predictions that can lead to the development of new materials with optimized properties (Grant, 1996). Knowledge-Based View Theory is important to this study as it highlights the role of machine learning algorithms as knowledge-enhancing tools in materials science research.

2.2 Empirical Review

The effects of machine learning algorithms for predicting and optimizing the properties of new materials in the United States have been the subject of several empirical studies. These studies have utilized diverse methodologies, data sets, and theoretical frameworks to investigate the topic. Seven recent empirical studies (2018 to present) are reviewed below, providing insights into the relationship between machine learning algorithms and material properties prediction and optimization.

Ramprasad *et al.* (2018) investigated the use of machine learning algorithms for predicting material properties in a data-driven manner. The study utilized a large database of materials properties and demonstrated the effectiveness of machine learning algorithms in predicting properties of diverse materials, including mechanical, electrical, and thermal properties. The study highlighted the potential of machine learning in accelerating the discovery and optimization of new materials.

Liu *et al.* (2019) explored the use of machine learning algorithms for optimizing the properties of advanced materials. The study focused on the optimization of material properties for specific applications, such as energy storage, catalysis, and electronic devices. The study employed machine learning algorithms to design and optimize material compositions, structures, and properties, showcasing the potential of machine learning in materials design and engineering.

Sanchez-Lengeling *et al.* (2020) investigated the use of machine learning algorithms for predicting molecular properties of organic compounds. The study employed machine learning techniques, such as convolutional neural networks and recurrent neural networks, to predict properties such as solubility, toxicity, and reactivity of organic molecules. The study highlighted the accuracy and efficiency of machine learning algorithms in predicting molecular properties, enabling rational design of new compounds.

Xie *et al.* (2021) explored the use of machine learning algorithms for predicting the mechanical properties of materials. The study focused on predicting properties such as strength, toughness, and ductility of materials using machine learning techniques, such as support vector machines and random forests. The study demonstrated the potential of machine learning in predicting material properties and guiding material design and optimization efforts.

Pilania *et al.* (2021) investigated the use of machine learning algorithms for predicting the properties of complex materials, such as alloys and composites. The study utilized machine learning techniques, such as deep learning and reinforcement learning, to predict properties such as phase stability, mechanical properties, and thermal properties of complex materials. The study emphasized the accuracy and scalability of machine learning algorithms in predicting material properties, enabling accelerated materials discovery and optimization.

Jain *et al.* (2022) examined the use of machine learning algorithms for predicting the properties of inorganic materials. The study employed machine learning techniques, such as Gaussian processes and kernel ridge regression, to predict properties such as bandgap, dielectric constant, and refractive index of inorganic materials. The study highlighted the accuracy and transferability of machine learning models in predicting properties of inorganic materials, facilitating materials design and optimization.

Wang *et al.* (2022) investigated the use of machine learning algorithms for predicting the properties of polymers. The study employed machine learning techniques, such as recurrent neural networks and convolutional neural networks, to predict properties such as glass transition temperature, mechanical properties, and chemical stability of polymers. The study demonstrated the potential of machine learning in predicting polymer properties and guiding polymer design and optimization efforts.

3.0 METHODOLOGY

The study adopted a desktop research methodology. Desk research refers to secondary data or that which can be collected without fieldwork. Desk research is basically involved in collecting data from existing resources hence it is often considered a low-cost technique as compared to field research, as the main cost is involved in executive's time, telephone charges and directories. Thus, the study relied on already published studies, reports and statistics. This secondary data was easily accessed through the online journals and library.

4.0 RESULTS

The effects of machine learning algorithms for predicting and optimizing the properties of new materials in the United States have been examined in several studies. These studies have revealed key findings and research gaps. The results indicate that machine learning algorithms have shown promising results in predicting the properties of new materials with high accuracy and efficiency (Johnson *et al.*, 2019; Smith & Chen, 2020). These algorithms have been used to optimize material

properties for various applications, such as in the fields of energy storage, catalysis, and electronics (Brown et al., 2018; Kim & Jones, 2017). Machine learning algorithms have also been used to accelerate the discovery of new materials with desired properties, which has the potential to revolutionize the field of materials science (Gupta et al., 2016; Lee & Wang, 2019).

4.1 Conceptual Gaps

Despite the promising results of machine learning algorithms in predicting and optimizing the properties of new materials, there are conceptual gaps in the literature. One conceptual gap is the need for a better understanding of the interpretability and explain ability of machine learning algorithms in the context of materials science (Miller & Smith, 2018; Wang & Zhang, 2021). While machine learning algorithms have shown high accuracy in predicting material properties, the lack of interpretability and explain ability of these algorithms poses challenges in understanding how the algorithms arrive at their predictions (Johnson, 2020; Chen & Li, 2019). This conceptual gap hinders the widespread adoption of machine learning algorithms in materials science research and applications.

Another conceptual gap is the need for more research on the ethical implications of using machine learning algorithms for predicting and optimizing the properties of new materials (Brown & Wilson, 2017; Lee et al., 2018). As machine learning algorithms become more prevalent in materials science research and industry applications, there is a growing concern about issues such as bias, fairness, and accountability in the use of these algorithms (Garcia et al., 2020; Wang, 2019). Ethical considerations related to data privacy, security, and transparency also need to be addressed in the context of using machine learning algorithms for materials research and development.

4.2 Contextual and Geographical Gaps

Contextual and geographical gaps also exist in the literature on the effects of machine learning algorithms for predicting and optimizing the properties of new materials. Contextual gaps refer to the lack of shared context between the researchers and the readers, which can lead to misunderstandings (Smith & Kim, 2019). In the case of machine learning algorithms for materials science, readers outside of the field may lack the necessary technical knowledge to fully understand the intricacies of these algorithms and their implications (Jones, 2018; Wang & Chen, 2020). Geographical gaps refer to the limitations of research conducted in specific geographical regions, which may not be generalizable to other regions (Lee & Gupta, 2017). In the case of the United States, where most of the research on machine learning algorithms for materials science has been conducted, there may be limitations in generalizing the findings to other countries or regions with different research contexts, infrastructure, and resources (Kim et al., 2016; Chen et al., 2018).

Existing research on the effects of machine learning algorithms for predicting and optimizing the properties of new materials has been largely conducted in specific research contexts, such as academic institutions or research laboratories in the United States. This contextual and geographical limitation may hinder the generalizability of the findings to other regions and countries. A more diverse and global perspective is needed to fully understand the implications of machine learning algorithms for materials science research and applications across different contexts and regions (Brown & Kim, 2019; Lee et al., 2021).

4.3 Methodological Gaps

Methodological gaps also exist in the current literature. Most existing studies have focused on the application of machine learning algorithms to specific materials systems or properties, using small datasets or simplified models (Johnson, 2019; Gupta, 2020). There is a need for more comprehensive and rigorous research that employs large-scale datasets, robust validation methods, and standardized protocols for materials characterization and evaluation. Such research can provide more reliable and reproducible results, and enable better comparison and benchmarking of different machine learning algorithms for materials prediction and optimization.

5.0 CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusion

Machine learning algorithms for predicting and optimizing the properties of new materials in the United States have shown great potential in revolutionizing material science research and development. Recent studies have demonstrated the effectiveness of machine learning algorithms in predicting material properties, optimizing material compositions, and accelerating the discovery of new materials with desired properties. These advancements have the potential to significantly impact various industries, such as aerospace, automotive, energy, and electronics, by enabling the development of new materials with enhanced performance and sustainability.

Furthermore, recent studies have also highlighted the challenges and limitations of machine learning algorithms in material science, including the need for large datasets, interpretability of results, and generalization to real-world applications. Despite these challenges, machine learning algorithms have shown great promise in overcoming these limitations through advancements in data generation techniques, model interpretability methods, and domain-specific model training.

5.2 Recommendations

Based on the findings of this study, several recommendations can be made to further advance the field of machine learning for materials research in the United States. Firstly, it is recommended that researchers and practitioners in the field collaborate to establish standardized data collection, sharing, and validation protocols. This would ensure the availability of high-quality and diverse data for training and testing machine learning algorithms, and promote transparency and reproducibility in research findings. Additionally, efforts should be made to develop interpretable machine learning models that can provide insights into the underlying physics and chemistry of materials, enabling researchers to better understand and optimize material properties. Secondly, it is recommended that interdisciplinary research collaborations be fostered between materials scientists, computer scientists, and domain experts from various industries. Such collaborations can accelerate the translation of machine learning research into practical applications, and facilitate the adoption of machine learning algorithms by industry partners for materials design and optimization. Thirdly, it is recommended that funding agencies and policymakers prioritize investments in research and development of machine learning algorithms for materials science. This includes funding for research projects, infrastructure, and training programs to build a skilled workforce capable of leveraging machine learning techniques for materials research. Lastly, it is recommended that efforts be made to promote open-source software and data sharing in the field of machine learning for materials research. This would enable researchers to access and build upon existing tools and resources, foster collaboration, and accelerate progress in the field.

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